16th International Conference on Liquid and Amorphous Metals
(LAM-16)

Bonn - Bad Godesberg, Germany
September 04-09, 2016

Imprint:
Institute of Materials Physics in Space
German Aerospace Center (DLR)
Priv.-Doz. Dr. Dirk Holland-Moritz, Prof. Dr. Florian Kargl

Linder Höhe
51147 Köln
Germany

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Scope

The 16th International Conference on Liquid and Amorphous Metals (LAM-16) will be held at the town hall of Bonn - Bad Godesberg, Germany, from September 04-09, 2016.
The conference aims to provide a forum for scientists interested in liquid and amorphous metals in order to discuss recent advances and future directions in this intriguing field of condensed matter physics, chemistry and materials sciences. Apart from papers on metallic systems, the LAM conferences traditionally also welcome contributions on liquid and amorphous semi-conductors as well as on molten salts.
The series of LAM conferences has a long standing history dating back to the liquids metal conference LM-1 in Brookhaven (1966). It was followed by the liquid metals conferences in Tokyo (1972) and Bristol (1976). The scope of the conference series was complemented by topics of amorphous metals in the following LAM conferences held in Grenoble (1980), Los Angeles (1983), Garmisch-Partenkirchen (1986), Kyoto (1989), Wien (1992), Chicago (1995), Dortmund (1998), Yokohama (2001), Metz (2004), Ekaterinburg (2007), Rome (2010) and Beijing (2013).
We are planning plenary sessions on hot topics and future advances in the field and there will be thematically focused sessions with invited and selected contributed talks as well as a poster session.
The following topics will be covered by the conference:

- structural and dynamical properties of liquid and amorphous phases
- bulk amorphous glasses (development and properties)
- liquids under extreme and/or highly metastable conditions
- thermophysical properties of metallic melts and amorphous matter
- experimental techniques for investigating liquid and amorphous matter (including state of the art in-situ techniques for studying non-equilibrium states, phase transitions or chemical reactions in liquid and amorphous matter)
- simulation techniques for studying structure, dynamics and properties of liquid and amorphous systems
- investigations on liquid metals under the unique conditions of reduced gravity
- applications of amorphous materials.

Conference Organization

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Travel Information

Conference Venue:

Town Hall Bad Godesberg
Koblenzer Straße 80
53177 Bonn-Bad Godesberg
Germany

Guidelines

Oral Presentations:

1. Prepare Your Presentation:

   Be considerate to the other speakers and audience by staying within your allocated time. The allocated time for your presentation includes a discussion and changeover to the next speaker. This is essential to ensure adequate time for questions and discussion as well as adherence to the schedule. Please discuss the same material as reported in your abstract submission.

   Total duration:

   40 minutes plenary speaker
   30 minutes invited speaker
   20 minutes regular speaker

   You are kindly requested to be at the presentation room at least **15 minutes before the session starts**. In each session, there is one person chairing the session. Session chairs will keep an eye on the time to make sure that all speakers have enough time for their presentations and for questions. Please note that we are unable to provide additional presentation time in case of a delay due to technical issues.

2. Audio-Visual Equipment:
   Each meeting room is equipped with a data projector (with VGA input) and screen, microphone and a laser pointer.
   All presenters should please bring their own laptop from which to present. The conference organisation will not provide laptops for presentations. If you do not have a laptop, please contact the conference organizers by email conference-LAM16@dlr.de. For MAC-laptop users, please bring your own VGA adapter cable and be sure that you have the necessary cords/converters so that your laptop will work with the data projector. Please test the compatibility of your laptop with the data projector before the session starts. An assistant will be assigned to each room to assist with the equipment operation during the session.

3. Backup Copy of Your Presentation:
   We strongly encourage you to have a backup of your presentation on a USB storage device for the case your laptop has a technical problem or is incompatible with the data projector.

4. Microphones:
   The Great Hall is equipped with wireless headsets for the speakers. An assistant will help you to mount the headset. The Small Hall is equipped with a fixed microphone at the speaker desk.

Session Chairs:

Please make sure to arrive at the room where the session takes place **at least 15 minutes in advance**. This will allow you to meet the sessions speakers and to see whether there are any problems with installing their laptops or presentations.

Your main tasks will be:

- To start the session on time
- To very briefly introduce each talk
- To make sure that the speaker will finish her/his talk within the time available. To ensure this, please give the speaker a countdown (e.g., indicating 5 min to end, 2 min to end, finish) and stop her/him if necessary.
- To end the session on time

Poster Presentations

- Poster Session:
  The poster session will be held on Tuesday, September 6 (18:15 - 20:00) in the foyer of the venue Town Hall (Stadthalle) Bad Godesberg.
- Poster Mounting:
  The posters can be mounted on Monday from 08:00 hrs onwards and have to be removed Wednesday until 15:30 hrs
- Poster Size:
  The Poster Boards available at LAM-16 have a maximum usable surface that is 1.80 meters in height x 1.20 m width. Posters can be any size up to this maximum, either landscape or portrait orientation.
- Poster Storage:
  Complimentary poster storage is available at the hospitality desk for posters and poster container. Please make sure that your poster and/or poster container is clearly marked with your name. You may leave it in storage at your own risk.

Posters should be printed and brought to the conference. There will be no possibility of printing posters at the conference site. **Magnets for fixing the posters** on the poster boards will be **available** for all poster presenters at the **LAM-16 Hospitality desk**, located in the entrance hall.

Proceedings LAM-16

Deadline: 01. October 2016

The LAM-16 conference proceedings will be published as **open-access** proceedings in **The European Physical Journal (EPJ) Web of Conferences**.

All the articles should contain new and unpublished results and will be peer reviewed according the Policy on Publishing.

Participants interested in publishing a paper on the work presented on the LAM-16 in the conference proceedings should send a **print-ready** PDF-document of the manuscript together with the signed license agreement to conference-LAM16@dlr.de.

The manuscripts should be formatted in the **EPJ 17 x 25 cm one column format** (please do **not** use the A4 two columns format) and prepared as described in the instructions for authors. There you will also find Word or LaTeX templates as wll guidelines for the preparation of the print-ready PDF documents.

For further information and links to the publishers guidlines please visit the conference home page `https://dlr-mp.meetingmasters.de/LAM16`

Please e-mail your questions regarding LAM-16 proceedings to conference-LAM16@dlr.de.

Program

	Sunday - September 4, 2016
17:00-21:00	**Registration**
19:00-21:00	**Welcome Reception**

Monday - September 5, 2016

			Großer Saal/ Great Hall			Kleiner Saal/ Small Hall
			Opening/Plenary Session			
09:00-09:20			Welcome			
09:20-09:30			Obituary Prof. M. Yao			
09:30-10:10	P	1	**A. L. Greer**			
10:10-10:50	P	2	**T. Egami**			
10:50-11:05			**Conference Photograph (Location tba)**			
11:05-11:30			**Coffee/Tea Break**			
			Glass Transition 1			**Extreme Conditions 1**
11:30-12:00	I	1	**C. Alba-Simionesco**	I	2	**H. Liu**
12:00-12:20	C	1	**M. Sperl**	C	3	**M. Santoro**
12:20-12:40	C	2	**Y. Kajihara**	C	4	**S. Ayrinhac**
12:40-13:50			**Lunch Break**			
			Demixing/Liquid-Liquid Phase Transformations			**Electronic and Magnetic Properties**
13:50-14:20	I	3	**J. Gao**	I	4	**P. Sperling**
14:20-14:40	C	5	**M. Kolbe**	C	9	**H. Shimakura**
14:40-15:00	C	6	**M. Stolpe**	C	10	**S. Ohno**
15:00-15:20	C	7	**S. Hechler**	C	11	**V. Sidorov**
15:20-15:40	C	8	**E. Yahel**	C	12	**B. L. Shen**
15:40-16:10			**Coffee/Tea Break**			
			Applications / Materials Development 1			**Structure and Dynamics 1**
16:10-16:40	I	5	**J. S. Ha**	I	6	**A. P. Seitsonen**
16:40-17:00	C	13	**S. K. Pillai**	C	16	**V. M. Giordano**
17:00-17:20	C	14	**L. Kelhar**	C	17	**C. C. Yuan**
17:20-17:40	C	15	**D. Grell**	C	18	**G. M. Bhuiyan**

P: Plenary Talk I: Invited Talk C: Contributed Talk

Tuesday - September 6, 2016

	Großer Saal/ Great Hall			**Kleiner Saal/ Small Hall**		
	Expanded Liquids / Electronic Properties			**Heat Treatment / Devitrification**		
09:00-09:30	I	7	**K. Matsuda**	I	8	**J. Saida**
09:30-09:50	C	19	**W.-C. Pilgrim**	C	22	**M. Lüttich**
09:50-10:10	C	20	**K. Maruyama**	C	23	**J.-G. Gasser**
10:10-10:30	C	21	**T. Hagiya**	C	24	**S. K. Pillai**
10:30-11:00	**Coffee/Tea Break**					
	Structure and Dynamics 2			**Properties of Metallic Glasses**		
11:00-11:30	I	9	**M. D. Ruiz-Martin**	I	10	**A. Gebert**
11:30-11:50	C	25	**L. E. Gonzalez**	C	28	**M. Eisenbart**
11:50-12:10	C	26	**Z. Wang**	C	29	**P. Ramasamy**
12:10-12:30	C	27	**B. Nowak**	C	30	**B. Bochtler**
12:30-13:40	**Lunch Break**					
	Plenary Session					
13:40-14:20	P	3	**J. Eckert**			
	Dynamics 1			**Structure 1**		
14:25-14:55	I	11	**J.-F. Wax**	I	12	**J.-Z. Jiang**
14:55-15:15	C	31	**H. R. Schober**	C	34	**C. Dong**
15:15-15:35	C	32	**L. W. Wang**	C	35	**P. Popel**
15:35-15:55	C	33	**E. Sondermann**	C	36	**S. Zhang**
15:55-16:25	**Coffee/Tea Break**					
	Dynamics 2			**Solidification**		
16:25-16:55	C	37	**F. Demmel**	I	13	**S. Eckert**
16:55-17:15	C	38	**L. Elizondo Aguilera**	C	42	**C. Karrasch**
17:15-17:35	C	39	**T. Bryk**	C	43	**H.-L. Peng**
17:35-17:55	C	40	**W. Schirmacher**	C	44	**A. Kuball**
17:55-18:15	C	41	**S. V. Divinskiy**	C	45	**R. Kobold**
18:15-20:00	**Poster Session**					

P: Plenary Talk I: Invited Talk C: Contributed Talk

Wednesday - September 7, 2016

	Großer Saal/ Great Hall	**Kleiner Saal/ Small Hall**
	Applications / Materials Development 2	**Structure 2**
09:00-09:30	I 14 **H. Kato**	I 15 **A. Filliponi**
09:30-09:50	C 46 **N. Nollmann**	C 48 **G. Makov**
09:50-10:10	C 47 **F. Gärtner**	C 49 **F. Iesari**
10:10-10:40	**Coffee/Tea Break**	
	Plenary Session	
10:40-11:20	P 4 **C. A. Volkert**	
	Properties	**Excitations in liquids and glasses**
11:25-11:55	I 16 **P. Švec**	I 17 **M. Inui**
11:55-12:15	C 50 **M. Calin**	C 52 **S. Hosokawa**
12:15-12:35	C 51 **O. Gross**	C 53 **S. Hosokawa**
12:35-13:50	**Lunch Break**	
	Glass Transition 2	**Applications / Materials Development 3**
13:50-14:20	I 18 **V. V. Pisarev**	I 19 **Y. Plevachuk**
14:20-14:40	C 54 **E. Pineda**	C 56 **C. M. Fang**
14:40-15:00	C 55 **M. Vasin**	C 57 **V. S. Tsepelev**
15:15-	**Possibility to visit the German Aerospace Center (DLR) or to attend other tours (Bonn, Cologne, or Drachenfels**	

P: Plenary Talk   I: Invited Talk   C: Contributed Talk

Thursday - September 8, 2016

	Großer Saal/ Great Hall	Kleiner Saal/ Small Hall
	Structure and Dynamics 3	**Containerless Processing**
09:00-09:30	I 20 **F. Shimojo**	I 21 **L. Hennet**
09:30-09:50	C 58 **D. J. Gonzalez**	C 61 **J. T. Okada**
09:50-10:10	C 59 **X. D. Wang**	C 62 **G. W. Lee**
10:10-10:30	C 60 **N. Jakse**	C 63 **Y.-H. Lee**
10:30-11:00	**Coffee/Tea Break**	
	Thermophysical Properties	**Modelling / Simulations 1**
11:00-11:30	I 22 **F. Yang**	I 23 **A. Mayer**
11:30-11:50	C 64 **G. Pottlacher**	C 67 **B. Gonzalez del Rio**
11:50-12:10	C 65 **Y. Luo**	C 68 **K. V. Khishchenko**
12:10-12:30	C 66 **T. Ahmed**	C 69 **E. Yahel**
12:30-13:00	**Distribution of Lunch Boxes**	
14:00-22:00	**Excursion and Conference Dinner (Boat tour on the River Rhine)**	

Friday - September 9, 2016

	Großer Saal/ Great Hall	Kleiner Saal/ Small Hall
	Structure and Properties of Glasses	**Modelling / Simulations 2**
09:00-09:30	I 24 **A. Pradel**	I 25 **P. R. Levashov**
09:30-09:50	C 70 **A. Soper**	C 73 **J. Y. Qin**
09:50-10:10	C 71 **A. Tlili**	C 74 **A. Sobolev**
10:10-10:30	C 72 **Y. Dong**	
10:30-11:00	**Coffee/Tea Break**	
	Plenary Session/Closing	
11:00-11:40	P 5 **F. Spaepen**	
11:40-12:30	**Conclusions**	
12:30-14:00	**Lunch**	

P: Plenary Talk   I: Invited Talk   C: Contributed Talk

Abstracts Oral Contributions

P1 - Mon 09:30-10:10 **Plenary** Großer Saal / Great Hall

New perspectives on glasses and glass formation in metallic systems

A. L. Greer

University of Cambridge, Department of Materials Science & Metallurgy, Cambridge, UK.

The properties of liquids are more strongly temperature-dependent than those of the corresponding glasses. It is accepted that the atomistic structure of liquids is dependent on temperature, and glassy states are conventionally taken to be *isoconfigurational*.

Studies of liquid metallic systems reveal interesting complexity: the characteristic haloes in the radial distribution function do not shift equally with temperature change, and nearest-neighbour distances can even appear to shorten on heating. Metallic glasses show an elastic response that is similarly complex, with nearest-neighbour distances appearing stiffer (varying less on loading) than the bulk. Both static and cyclic mechanical loading well within the nominally elastic range can induce significant changes in glass properties, most readily characterized in terms of energy decreases (relaxation/ageing) or increases (rejuvenation) [1,2]. These are considered to be due to local non-reversed configurational changes arising from the non-affine nature of the elastic displacements.

Recent work suggests similar effects from thermal strains [3]. Thermal cycling of metallic glasses (below 0.6 T_g, so relaxation effects are negligible) induces rejuvenation, again interpreted in terms of non-affine strains, raising the question of whether glassy states can, strictly, be regarded as *isoconfigurational* after all. It is striking that, for given composition, temperature and pressure, the range of energy obtainable in the glassy state is very wide, almost as large as the heat of melting [1,2].

We also consider whether pure metals are glass-formers, and the wide range of glass-forming ability of metallic systems [4,5]. Interest in systems of poor glass-forming ability is currently high, because of their potential application in phase-change memory [5]. There are aspects of induced anisotropy in metallic glasses and liquids that are still very far from understood [6], yet anisotropy may be critical in understanding the mechanisms of flow and deformation.

[1] A. L. Greer and Y. H. Sun, *Philos. Mag.* **96** 1643 (2016).
[2] Y. H. Sun, A. Concustell, and A. L. Greer, *Nature Rev. Mater.* **1** 16039 (2016).
[3] S. V. Ketov et al., *Nature* **524** 200 (2015).
[4] J. Orava and A. L. Greer, *J. Chem. Phys.* **140** 214504 (2014).
[5] A. L. Greer, *Nature Mater.* **14** 542 (2015).
[6] Y. H. Sun, A. Concustell, M. A. Carpenter, J. C. Qiao, A. W. Rayment, and A. L. Greer, *Acta Mater.* 112 132 (2016).

P2 - Mon 10:10-10:50 **Plenary** Großer Saal / Great Hall

Cooperative Crossover and the Glass Transition

T. Egami

Shull Wollan Center – Joint Institute for Neutron Sciences, University of Tennessee
and Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

Viscosity of liquid metal at high temperatures shows an Arrhenius behavior, whereas that of supercooled liquid shows a super-Arrhenius behavior with rapid increase with decreasing temperature culminating in the glass transition. Plethora of theories have been proposed in attempt to explain the rapid increase in viscosity. There are two major schools of thought; one attributing it to increased correlation due to some hidden order, such as the icosahedral order, and the other blaming the loss of freedom resulting in jamming. But few have asked the question why the Arrhenius behavior is observed at high temperatures, whereas in my view that is the critical question. Both the hidden order school and the jamming school end up with essentially predicting the gas state at high temperature, not the Arrhenius behavior. Here we propose a different scenario. Through simulation we found that viscosity at high temperature is determined by action of cutting and forming of atomic bond, which is a thermally activated process with the activation energy related to the bond energy [1]. We named this action of cutting and forming the bond “anankeon” [2]. Anankeons are independent from each other above the cooperative crossover temperature, T_{coop}, because phonons are overdamped and atoms cannot communicate, but they become cooperative below. T_{coop} separates “simple liquid” above and “cooperative liquid” below. Because T_{coop} is usually close to the melting temperature T_m, supercooled liquid is cooperative. But this crossover has nothing to do with supercooling. Elastic interaction among anankeons is the mechanism of cooperativity. An effort to create a theory to calculate this cooperativity is in progress. I discuss the effect of increased cooperativity on properties of liquid and glass.

1. T. Iwashita, D. M. Nicholson and T. Egami, *Phys. Rev. Lett.*, **110,** 205504 (2013).
2. T. Egami, *Mod. Phys. Lett. B*, **28,** 1430006 (2014).

I1 - Mon 11:30-12:00 **Glass Transition 1** Großer Saal / Great Hall

The glass formation: a very local structural event

C. Alba-Simionesco, S. Eibl, C. Crauste, A. Raihane, F. Porcher, J. Darpentigny

[1] *Laboratoire Léon Brillouin, UMR CEA-CNRS, Univ. Paris-Saclay, France*

In most reviews on the Glass Transition phenomenon, it is evoked that no remarkable changes happen on the local structure of a liquid or a melt as the glass transition temperature, Tg, is crossed. Above Tg, the static structure factor varies only smoothly with the temperature whereas the dynamical properties evolve dramatically.

While a small increase in dynamical correlation lengths are responsible of the T-dependence of the viscosity, it remains challenging to associate it to a structural length scale or locally preferred structures. We propose to revisit the local organization of some molecular liquids of different complexity and frustration strength: from self-associated mono-alcohols to spherical like van der Waals systems.

Then we intend to answer to Turnbull's statement decades ago, "it not well established whether or not every substance can be put into a glass form", by suggesting the minimal requirements to form a molecular glass in normal conditions.

C1 - Mon 12:00-12:20 **Glass Transition 1** Großer Saal / Great Hall

Theory of Multiple Glass States in Simple Liquids

Matthias Sperl[1]

[1] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, 51170 Köln, Germany*

Multiple glassy states – in addition to being interesting for their experimental relevance – offer a challenge for their theoretical description: The question which theoretical framwork can predict the existence and properties of such amorphous solids allows for highly non-trivial comparisons of different approaches. The existence of some scenarios of multiple distinct glassy states can be inferred from non-standard dynamical features in the liquid or melt such as logarithmic decay laws [1]. Surprisingly, these multiple glass states can already arise from relatively simple interactions among a liquid's constituent particles. And while glass-glass transitions are today well-known in colloidal suspensions when attractive and repulsive length scale compete, recently, glass-glass transition scenarios have been predicted for interactions with distinct repulsive length scales [2].

The presentation shall review the underlying theory, introduce the mathematical origin of the multiple glassy states, discuss the robustness of the predicted phenomena and the consequences for experiments. Results from a recent computer-simulation study are offered as motivation for future experimental studies [3]. The talk will conclude by discussing the relevance of the results for water and certain metallic melts.

[1] W. Götze and M. Sperl, *Logarithmic relaxation in glass-forming systems,* Phys. Rev. **E 66,** 011405 (2002).
[2] Matthias Sperl, Emanuela Zaccarelli, Francesco Sciortino, Pradeep Kumar, and H. Eugene Stanley, *Disconnected Glass-Glass Transitions and Diffusion Anomalies in a Model with Two Repulsive Length Scales,* Phys. Rev. Lett. **104,** 145701 (2010).
[3] Nicoletta Gnan, Gayatri Das, Matthias Sperl, Francesco Sciortino, and Emanuela Zaccarelli, *Multiple Glass Singularities and Isodynamics in a Core-Softened Model for Glass-Forming Systems,* Phys. Rev. Lett. **113,** 258302 (2014).

C2 - Mon 12:20-12:40 **Glass Transition 1** Großer Saal / Great Hall

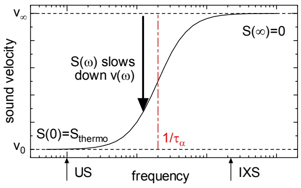
Time concept of entropy: from “fast sound” to glass transition

Y. Kajihara[1], M. Inui[1] and A. Chiba[2]

[1] Graduate School of Integrated Arts and Sciences, Hiroshima University, Higashi-Hiroshima 739-8521, Japan

[2] Department of Physics, Keio University, Yokohama 223-8522, Japan

Recent years, we have studied so-called “fast sound” phenomena by using inelastic x-ray scattering (IXS) technique. “Fast sound” is a historical expression that the sound velocity of liquids measured by microscopic methods (molecular dynamics simulation or inelastic neutron / x-ray scattering) is much (about two times) faster than those by macroscopic methods (ultrasonic=US etc.). It was first observed in an ambient water and now it seems to be concluded that it is a huge frequency- (or momentum transfer-) dependence of the sound velocity in terms of the “relaxation” phenomena [1,2]. But we think we can make much more fruitful discussion about it. We have found “fast sound” state, not only for water but also for liquid Te system (Te [3], Se-Te and Ge-Te mixtures [4]). Already discussed by Tanaka [5] and Tsuchiya et al. [6], the anomalous slowing down of US sound velocities in both systems originates from the mixing entropy due to the continuous liquid-liquid phase transition. In our IXS measurements, there are almost no anomalies in estimated sound velocities. Our conclusion is that, though the system has large thermodynamic entropy (S(0) in figure), there is no entropy in this frequency range ($S(\omega=\text{THz})$). That is, to introduce time concept to entropy: it is zero when the frequency is high enough compared to the inverse of the characteristic time (τ_α) of “relaxation”. We think that it is a natural extension of the Boltzmann’s definition: “entropy is a measure of the number of microstates”. If the given time is shorter, the number of realized microstates, entropy, is smaller.



Our concept is similar to what has been discussed for glass transition phenomena [7]. We believe that the generalization of entropy can give a new viewpoint combining fast sound and glass transition phenomena and it will be a key to understand “broken ergodicity” [8] phenomena.

In the conference, we will present a summary of our IXS study and how simply the concept can explain the anomaly of the heat capacity at the glass transition.

[1] F. Sette et al, *Phys. Rev. Lett.* **77**, 83 (1996), [2] S. C. Santucci et al, *Phys. Rev. Lett.* **97**, 225701 (2006), [3] Y. Kajihara et al, *J.Phys.:Condens. Matter* **20**, 494244 (2008), [4] Y. Kajihara et al, in preparation, [5] H. Tanaka, *J. Chem. Phys.* **112**, 799-809 (2000), [6] Y. Tsuchiya and E.F.W.Seymour, *J. Phys.* **C15**, L687-695 (1982), [7] J.C.Mauro et al, *J.Chem.Phys.***126**, 184511 (2007) and references therein, [8] R.G.Palmer, *Adv. Phys.* **31**, 669 (1982)

I2 - Mon 11:30-12:00 **Extreme Conditions 1** Kleiner Saal / Small Hall

Metallic glasses and melt under compression: Universal behavior patterns on power law for their density and the corresponding fractal dimensionality

Haozhe Liu [1], Luhong Wang [2]
[1] *HPSTAR, Beijing, China*
[2] *Harbin Institute of Technology, Harbin, China*

The usage of the so called First Strong “Diffraction” Peak (FSDP) in scattering patterns of non-crystalline materials to estimate their density change has long history, and the physics meaning and structure origin behind this method is extremely controversial. After this discovery of the power-law and fractal nature using this method in metallic glasses at ambient conditions [1], the high pressure researches revealed “universal” fractional non-cubic power law for density of metallic glasses, and the constant fractal dimensionality under compression is presented, for several typical metallic glass case under high pressure conditions [2-4]. In this report, we will present the updated result on this topic, based on the experimental data for metallic glass sample at broader pressure range using synchrotron x-ray scattering and tomography techniques. Furthermore, gallium met upon compression was investigated, and the physics picture of relative higher fractal dimensionality will be demonstrated.

References:

1. Ma, D., Stoica, A. D. & Wang, X.-L. Power-law scaling and fractal nature of medium-range order in metallic glasses. *Nature Mater.* **8**, 30-34 (2009)
2. Zeng, Q. *et al.* Universal fractional noncubic power law for density of metallic glasses. *Phys. Rev. Lett.* **112**, 185502 (2014)
3. Chen. D. Z. *et al.* Fractal atomic-level percolation in metallic glasses. *Science* **349**, 1306-1310 (2015)
4. Zeng, Q. *et al*, General 2.5 power law of metallic glasses, PNAS, **113**, 1714 (2016).

C3 - Mon 12:00-12:20 **Extreme Conditions 1** Kleiner Saal / Small Hall

Liquid and Solid Rubidium at Extreme Conditions

Mario Santoro[1,2], Simone De Panfilis[3], Federico A. Gorelli[1,2], E. Gregoryanz[4]

[1] *Istituto Nazionale di Ottica, CNR-INO, 51019 Sesto Fiorentino, Italy*

[2] *European Laboratory for non Linear Spectroscopy (LENS), 51019 Sesto Fiorentino, Italy*

[3] *Centre for Life Nano Science IIT@Sapienza, Istituto Italiano di Tecnologia, I-00161 Roma, Italy*

[4] *School of Physics and Astronomy, CSEC, Univ. of Edinburgh, Edinburgh EH9 3JZ, UK*

Transformations of alkali metals at high pressures is one of the hot topics of modern condensed matter physics. Exotic crystalline structures with very large and complex unit cells, unusual melting lines showing maxima and minima, pressure induced metal to non-metal transitions are some examples of this fascinating scenario emerging recently. I will describe recent spectroscopy studies (Raman and X ray absorption experiments) on solid Rubidium at extreme pressures. Furthermore preliminary XRD data show a transformation in the liquid state at high pressures and temperatures. Ab initio simulations have also been performed to help the data analysis and to show the evolution of the electronic, structural and dynamic properties in Rubidium extending to conditions still difficult to reach experimentally.

Thermodynamic properties of liquid metals measured by picoseconds acoustics

S.Ayrinhac[1], M.Gauthier[1], M.Morand[1] , G.Le Marchand[1] ,F.Bergame[1] and F.Decremps[1]

[1] *Institut de minéralogie, de physique des matériaux et de cosmochimie (IMPMC), Université Pierre et Marie Curie, Paris, France*

Currently, the existence of liquid–liquid phase transition (LLPT), i.e. the transition between two liquids with different local structure, is one of the most interesting topics in condensed matter physics. LLPT are rare or controversial because they occur in highly reactive systems or metastable phases and more generally in challenging P-T conditions.

Recent technical achievements in picosecond acoustics associated with a diamond anvil cell permit to measure elastic properties at high pressures in liquid metals [1,2,3]. The acoustic waves are generated by picoseconds optical pulses at one side of the sample from a point source; they are detected on the opposite side and visualized by surface phonon imaging. The analysis of the images gives the sample thickness and the sound velocity. From sound velocities we can extract the equation of state $\rho(P,T)$ by a numerical procedure.

Those achievements have been applied firstly to metals which melt at low temperature, such as liquid mercury [2] and liquid gallium [4]. In the case of l-Ga, our measurements do not show a LLPT expected around 300 K and 2 GPa [5,6]. This technique can be also applied to alkali metals, considered as simple metals at ambient pressure but which get intriguing properties at high pressures. Among alkali metals, liquid rubidium is interesting because it presents a little-known phase diagram and simulations revealed the existence of a LLPT at 573 K and 12.9 GPa [7]. We will present sound velocity measurements in l-Rb which can bring informations on these two issues.

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I3 - Mon 13:50-14:20 **Demixing/LL Phase Transf.** Großer Saal / Great Hall

Liquid-liquid decomposition and rapid solidification of undercooled Co-Cu melts under high magnetic fields

Jianrong Gao

Key Laboratory of Electromagnetic Processing of Materials (Ministry of Education),
Northeastern University, Shenyang 110819, China

A homogeneous liquid will be decomposed into two liquids of different densities and properties if it is cooled to the binodal line of a liquid miscibility gap. This liquid-liquid decomposition is completed by nucleation and growth of a minor phase or by spinodal decomposition depending on bulk composition of the parent liquid phase [1]. The nucleation mechanism in principle allows for production of a finely dispersed structure, which is pursued in many applications of metal-metal composite material. But, the liquid-liquid decomposition can be accelerated by the gravitational field of the Earth leading to serious spatial separation of two product phases. Microgravity experiments were already performed in an attempt to solve this problem [2]. But, solidified samples show a separated structure yet due to Marangoni convection. Thus it seems difficult to produce a finely dispersed structure by solidification processing of immiscible bulk alloys either on the Earth or in Space. Recent work showed that application of high magnetic fields during solidification may provide a solution to this issue [3]. However, the complex dynamics of the liquid-liquid decomposition and the following solidification process of immiscible alloys occurring under the high magnetic fields is not well understood yet. In this talk, advances in our studies of liquid-liquid decomposition and rapid solidification of undercooled immiscible Co-Cu alloys under high magnetic fields are presented. Our studies show that the magnetic fields alter the liquid-liquid decomposition kinetics and the crystallization kinetics of the separated liquid phases as well. Our studies also shed light onto the magnetism of the Co-rich liquid at its highly undercooled state and its correlation with experimentally observed crystallization kinetics.

Acknowledgment: This work is financially supported by National Natural Science Foundation of China (51271033).

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C5 - Mon 14:20-14:40 **Demixing/LL Phase Transf.** Großer Saal / Great Hall

Liquid-liquid demixing of Co-Cu alloys under various convective conditions

M. Kolbe[1]

[1] *Institut für Materialphysik im Weltraum, DLR, 51170 Köln, Germany*

Monotectic metallic systems show phase demixing in the region of the liquid melt. As metallic melts are not transparent for visible light, it is difficult to observe the process of demixing and phase growth directly. Stable monotectic Al-based systems have been investigated by X-ray radiography and show a strong influence on phase growth by convection in the melt and sedimentation. A different approach is to study phase growth in a *metastable* miscibility gap. Co-Cu alloys exhibit a metastable miscibility gap in a wide composition range, approximately 120 K below the liquidus. This degree of undercooling is accessible by various techniques as processing in an electromagnetic levitation facility, melt fluxing and rapid solidification in sprayed droplets [1]. The analysis of microstructure is performed by standard metallographic techniques with the quenched solid samples. Each technique has its advantages and disadvantages, special focus is on experiments carried out in microgravity [2]. In general, sedimentation and fluid flow is reduced in these experiments, but residual convection has an influence on the solidified microstructure. Results from microgravity experiments are presented and compared to results obtained by terrestrial solidification experiments.

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C6 - Mon 14:40-15:00 **Demixing/LL Phase Transf.** Großer Saal / Great Hall

Liquid-liquid transition in the deeply undercooled $Zr_{58.5}Cu_{15.6}Ni_{12.8}Al_{10.3}Nb_{2.8}$ bulk metallic glass forming melt

Moritz Stolpe[1], Isabell Jonas[2], Shuai Wei[3], Zach Evenson[4], Fan Yang[2], Will Hembree[1], Andreas Meyer[2], and Ralf Busch[3]

[1] *Chair of Metallic Materials, Department of Material Science and Engineering, Saarland University, 66123 Saarbrücken, Germany*

[2] *Institute for Materials Physics in Space, German Aerospace Center (DLR), 51147 Cologne, Germany*

[3] *School of Molecular Science, Arizona State University, Tempe, Arizona 85287, USA*

[4]*Heinz Maier-Leibnitz Zentrum (MLZ) and Physik Department, Technische Universität München, 85748 Garching, Germany*

Apart from the question whether a highly dynamic system such as a liquid can exist in different modifications that are equal in composition but differ in local structure and thermodynamic properties [1], liquid-liquid phase transitions (LLTs) are of particular interest due to their implications on the dynamics [1,2,3]. LLTs are proposed as a possible source to explain anomalous changes in the viscous behavior, a phenomenon known as fragile-strong transition [1,2]. More precisely, it has been postulated that strong liquids differ from fragile liquids by occupying opposite flanks of an underlying order-disorder transition [1].

Using synchrotron X-ray scattering combined with electrostatic levitation we investigated the structural evolution of Zr-based metallic glass forming alloy from above the liquidus temperature down to the glass transition temperature T_g [4]. Our study reveals strong evidence for a LLT in the deeply undercooled liquid state at T ~ $1.2T_g$, in which a less ordered high temperature phase transforms into a more ordered low temperature phase [4]. This manifests as a smeared-out peak in the heat capacity over emissivity data as well as discontinuities in the evolution of the total structure factor *S(Q)* and its corresponding Fourier Transforms. Although no notable density change is observed, marked structural changes involving short- (SRO) and medium range order (MRO) occur during the LLT. These findings indicate that the experimentally observed difference between the high temperature viscous behavior of the melt close to the liquidus and the low temperature behavior close to T_g [5] indeed results from an underlying order-disorder transition in the deeply undercooled liquid state [4].

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C7 - Mon 15:00-15:20 **Demixing/LL Phase Transf.** Großer Saal / Great Hall

Signature of a Liquid-Liquid Transition in a Gold-Based Metallic Glass revealed by X-ray Photon Correlation Spectroscopy (XPCS)

S. Hechler[1], B. Ruta[2], Z. Evenson[3], M. Stolpe[1], W. Hembree[1], I. Gallino[1], and R. Busch[1]

[1] *Saarland University, Chair of Metallic Materials, Saarbruecken, Germany*

[2] *European Synchrotron Radiation Facility, Grenoble, France*

[3] *Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany*

Although structural relaxation is a universal feature of glasses, the atomic-level processes involved still remain a puzzling mystery. X-ray photon correlation spectroscopy (XPCS) has emerged as a novel technique for studying the microscopic dynamics of non-equilibrium condensed matter [1] among which also metallic glass systems [2]. Understanding the fundamental mechanism of structural relaxation is particularly important, since structural relaxation produces changes in the physical properties of glasses that can have profound impact on their performance stability over time.

Here, we report on XPCS experiments, which follow the equilibration process from the glass into the supercooled liquid of a $Au_{49}Cu_{26.9}Si_{16.3}Ag_{5.5}Pd_{2.3}$ metallic glass. The as-cast alloy shows different dynamical regimes as it approaches the glass transition. At low temperature, the relaxation time is almost temperature independent. Upon heating, closer to the glass transition, the glass shows dynamics that are highly temperature dependent. In the supercooled liquid region, the material changes the equilibrium dynamics upon cooling, without freezing and transforms into a liquid with significantly stronger fragility. Such crossovers in the dynamics of the supercooled liquid have not been observed in XPCS studies before [2,3] and suggest the existence of a liquid-liquid transition at temperatures just above the glass transition.

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Liquid-liquid phase transformations and the shape of the melting curve

Eyal Yahel[1] and Guy Makov[2]

[1] *NRCN, Department of Physics, Beer-Sheva, Israel*

[2] *Ben Gurion University, Department of Material Engineering, Beer-Sheva, Israel*

The phase diagram of elemental liquids has been found to be surprisingly rich, including variations in the melting curve and transitions in the liquid phase. The effect of these transitions in the liquid state on the shape of the melting curve is analyzed. First-order phase transitions intersecting the melting curve imply piecewise continuous melting curves, with solid-solid transitions generating upward kinks or minima and liquid-liquid transitions generating downward kinks or maxima. For liquid-liquid phase transitions proposed for carbon, phosphorous, selenium, and possibly nitrogen, we find that the melting curve exhibits a kink. Continuous transitions imply smooth extrema in the melting curve, the curvature of which is described by an exact thermodynamic relation. This expression indicates that a minimum in the melting curve requires the solid compressibility to be greater than that of the liquid, a very unusual situation. This relation is employed to predict the loci of smooth maxima at negative pressures for liquids with anomalous melting curves. The relation between the location of the melting curve maximum and the two-state model of continuous liquid-liquid transitions is discussed and illustrated by the case of tellurium.

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I4 - Mon 13:50-14:20 **Electronic and Magnetic Prop.** Kleiner Saal / Small Hall

Free-electron x-ray laser measurements of collisional-damped plasmons in isochorically heated warm dense matter

P. Sperling[1,2], L. B. Fletcher[1], E. Galtier[1], E. J. Gamboa[1], H. J. Lee[1], R. Redmer[3], H. Reinholz[3], G. Röpke[3], B. B. L. Witte[1,3], U. Zastrau[2], S. H. Glenzer[1]

[1] *SLAC National Accelerator Laboratory, HED Science Devision, Menlo Park, USA*

[2] *European XFEL GmbH, HED Group, Hamburg, Germany*

[3] *Universität Rostock, Institut für Physik, Rostock, Germany*

We present highly-resolved measurements of inelastic x-ray scattering spectra in ultrafast heated aluminum [1]. X-ray pulses from the seeded Linac Coherent Light Source delivering an average of 0.3 mJ of 8 keV x-ray photons in a 0.005 % bandwidth pulse, have been focused to micrometer diameter focal spots isochorically heating solid materials to temperatures up to several eV. The inelastic forward scattering spectra resolve electronic plasma oscillations that directly allow an accurate determination of the electron temperature and density indicating a strongly coupled, warm dense matter state. This accuracy enables us to extract plasma properties, which show a reduced electrical conductivity as well as a non-quadratic electron plasma oscillation dispersion relation in disagreement with the Born approximation. These properties are best described by taking into account electron-electron collisions as well as strong electron-ion collisions and dynamical screening effects that are beyond the Born approximation. First results from one-temperature density-functional theory simulations confirm these findings but simulations using two-temperatures [2] have to be applied.

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C9 - Mon 14:20-14:40 **Electronic and Magnetic Prop.** Kleiner Saal / Small Hall

Magnetic susceptibility of liquid Gd-M (M =Cu, Zn, Ga, Ge)

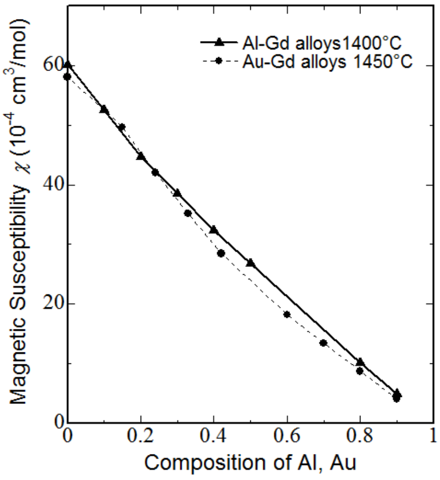
Hironori Shimakura[1], Shuta Tahara[2], Tatsuya Okada[3] , and Satoru Ohno[1]

[1] *Niigata University of Pharmacy and Applied Life Sciences, Faculty of Pharmacy, Niigata, Japan*

[2] *University of the Ryukyus, Faculty of Science, Okinawa, Japan*

[3] *Niigata Colledge of Technology, Niigata, Japan*

Al-Gd alloys have a lot of intermetallic compounds and high melting temperature at Al_2Gd composition. Au-Gd alloys also have a lot of intermetallic compounds and high melting temperature at AuGd composition. To analyze the electronic state of f-electron of REM, we had performed the magnetic susceptibility measurements for Al-Gd and Au-Gd. Figure shows the composition dependence of magnetic susceptibility of Al-Gd and Au-Gd alloys. The magnetic susceptibility of Al-Gd alloys shows linearly decreasing with increasing Al compositions. In the case of Au-Gd alloys, however, the value decreases parabolic with increasing Au compositions. It can be interpreted that the differences relates to the RKKY interaction. The intensity of RKKY interaction is represented as, $H_{RKKY} = -9\pi(J^2/\varepsilon_F)(N_e/N)^2\ f(2k_F R)\ \vec{S}_1\ \vec{S}_2$ and the intensity decreases parabolic with decreasing conduction electrons. The magnetic susceptibility of Au-Gd decreases parabolic since the number of conduction electrons of Au-Gd alloys decreases with increasing Au composition.



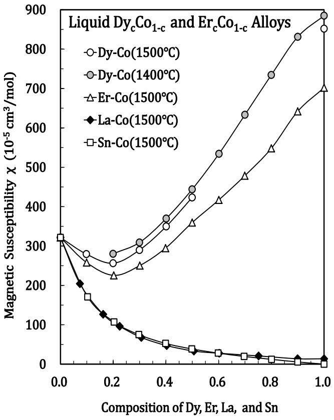
To reveal the effects of the number of conduction electrons for magnetic susceptibility, we performed the magnetic susceptibility measurements for liquid Gd-M (M = Cu, Zn, Ga, Ge). These metals belong to fourth period in periodic table and the valence shows 1, 2, 3 and 4, respectively. By systematic measurements, the detailed relationship between the valence and magnetic susceptibility will reveal. We will present the effect of 4f electrons and conduction electrons for magnetic susceptibility.

C10 - Mon 14:40-15:00 **Electronic and Magnetic Prop.** Kleiner Saal / Small Hall

MAGNETIC PROPERTIES OF LIQUID RE-Co (RE = Dy, Er) ALLOYS

Satoru Ohno[1], Hironori Shimakura[1] Shuta Tahara[2], and Tatsuya Okada[3]

[1] Niigata University of Pharmacy and Applied Life Sciences, Niigata 956-8603, Japan
[2] Faculty of Science, University of the Ryukyus, Nishihara, Okinawa 903-0213, Japan
[3] Niigata College of Technology, Niigata 950-2076, Japan



Magnetic susceptibility measurements were carried out by Faraday method with a torsion balance. The force applied to the specimen in the capsule was quantified by an automatic method of feedback current control. A RE-Co alloy specimen was placed in a magnesia capsule and was melted and homogenized under purified argon gas using a silicon carbide furnace. The magnetic susceptibility χ of liquid Dy-Co and Er-Co alloys is given by

$$\chi = \chi_{dia} + \chi_{el} + \chi_{3d} + \chi_{5d} + \chi_{4f} , \qquad (1)$$

where χ_{dia} is the diamagnetic susceptibility due to the RE and Co ions and χ_{el} is the paramagnetic susceptibility due to the conduction electrons. The paramagnetic susceptibility χ_{3d} of Co-rich alloys obeys the Curie-Weiss law as $\chi_{3d} = C/ (T - \theta)$, where C and θ are the Curie constant and the Curie temperature, respectively. Similarly, the paramagnetic susceptibility, χ_{4f}, of alloys on the RE-rich side is given by; $\chi_{4f} = (C/T) + \alpha$, where α is the residual magnetic susceptibility. χ_{5d} is the paramagnetic susceptibility due to the 5d electrons of RE ions. On the La-rich side, this value can be estimated from the data of liquid La-Co and Sn-Co alloys obtained in the early works.[1,2] As shown in Fig.1, the composition dependence of χ of liquid Dy-Co and Er-Co alloys reaches a minimum at the composition c=0.2 and rapidly increases with increasing RE component, respectively. Roughly speaking, the composition dependence of χ_{4f} for liquid RE-Co alloys corresponds to the difference between the experimental values of χ for liquid RE-Co and La-Co alloys. We compare the composition dependence of χ_{4f} of liquid Dy-Co, Er-Co and Gd-Co, and study the effective number of Bohr magnetons obtained. Liquid Co has a large θ of 1415 K. For the Co-rich alloys, the rapid decrease in θ was found to occur with decreasing Co component. It indicates that the magnitude of exchange interaction between Co ions similarly decreases by the addition of Dy, Er, La and Sn.

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C11 - Mon 15:00-15:20 **Electronic and Magnetic Prop.** Kleiner Saal / Small Hall

Electrical and magnetic properties of CoFeBSiNb alloys at high temperatures

Valeriy Sidorov[1,2], Vitaliy Mikhailov[1], Alexander Sushkevich[2]

[1] Ural State Pedagogical University, Institute of Physics, Technology and Economics, Ekaterinburg, Russia
[2] Ural Institute of State Fire Service of EMERCOM of Russia, Ekaterinburg, Russia

Co-based bulk metallic glasses have a unique combination of physical properties: high strength and plasticity, excellent corrosion resistance and good soft magnetic properties. However, their industrial application is limited due to low glass forming ability (GFA) and their physical properties at high temperatures are practically unknown. In this work we investigated the influence of gallium, tin, antimony and zirconium small additions on electrical resistivity and magnetic susceptibility of CoFeBSiNb alloys with different combination of the main elements. The temperature dependences of properties were investigated in a wide range including liquid state, and some parameters of electronic structure were obtained. In particular, the liquidus temperatures determined from resistivity and susceptibility temperature curves coincide within ± 3 K.

Electrical resistivity was studied by a contact-less method in rotating magnetic field. The temperature dependences $\rho(T)$ were found to be linear both in crystalline and liquid states. The used additions increase resistivity of investigated samples in both solid and liquid states. From the results it comes that Ga (Sn, Sb, Zr) atoms exist in the melt not in a form of individual pseudoatoms, but create some clusters around them. At high temperature the “influence” of doped atom on its neighbors weakens due to the increase in atoms heat motion.

Magnetic susceptibility measurements were performed on an equipment using a relative variant of Faraday’s method. The property was found to decrease with temperature growth and all the doped elements diminish susceptibility values. To obtain some information on electronic structure of the alloys in liquid phase, the experimental $\chi(T)$ curves were fitted by the generalized Curie-Weiss law. It was found that Ga and Zr additions increase interatomic interaction in the melt, whereas Sb and Sn additions decrease it. The paramagnetic Curie temperature θ can be used as indicator for impurity’s influence on GFA of the alloy: GFA improves when θ rises and falls down when θ decreases.

The work is partially supported by the Ministry of Education and Science of the Russian Federation (Project no. 4.1177.2014/K).

Structure, Magnetic and Mechanical Properties of Fe-based Bulk Metallic Glasses

B. Shen[1]

[1] *School of Materials Sciences and Engineering, Southeast University, Nanjing, China*

Fe-based bulk metallic glasses (BMGs) have attracted great attention ever since their first synthesis in 1995 due to their unique magnetic and mechanical properties. In this talk, I will report a series of novel Fe-based BMGs, such as FeREBNb (RE=Dy, Gd, Tb, Ho, Er, Tm) and FeNiPC alloys. These Fe-based BMGs exhibit good soft magnetic properties, large magnetostriction, large magnetic entropy change, high strength and unprecedented compressive plasticity at room temperature, which have not been obtained in conventional Fe-based crystalline alloys. This uniqueness has led to practical uses of these bulk glassy alloys as soft magnetic and structural materials. Meanwhile, the mechanism of ductile-to-brittle transition for Fe-based BMGs were also investigated. It was discovered that the ductile Fe-based BMG is composed of unique clusters mainly linked by less directional metal-metal bonds which are inclined to accommodate shear strain and absorbed energy in the front of crack tip. This conclusion was further verified by the X-ray photoelectron spectroscopy and ultraviolet photoelectron spectroscopy experiments of brittle to ductile Fe-based glassy systems. The results also indicate a strong correlation between the p-d hybridization and plasticity, verifying that the transition from brittle to ductile is due to the change of bonding characteristics in atomic configurations.

I5 - Mon 16:10-16:40 **Applications/Mater. Devel. 1** Großer Saal / Great Hall

Liquid Metal for Stretchable Devices

Jeong Sook Ha[1,2]
[1] *Korea University, Department of Chemical and Biological Engineering, Seoul, Korea*
[2] *Korea University, KU-KIST Graduate School of Converging Science and Technology, Seoul, Korea*

Recently, there has been extensive research on body-attachable/implantable devices. In order to achieve stable performance of such devices under mechanical deformation accompanied with body-movements, their stretchability as well as flexibility is required. For satisfying the desired stretchability of the devices attached and/or implanted onto body, many different kinds of strain-relieving approaches adopted novel design and materials where various stretchable conductors such as serpentine-shaped or pre-wrinkled interconnections, liquid metals, polymer-conductor (carbon nanotubes, Ag nanowires) composites, and ionic conductors were used. In this work, we report on the use of Galinstan, an eutectic alloy liquid metal consisting of gallium (68.5%), indium (21.5%), and tin (10%), which has excellent electrical conductivity (3.46×10^6 S m^{-1} at 20 ºC), a low melting point (-19 ºC), low vapor pressure, and low toxicity when compared with mercury,[1] in the fabrication of stretchable devices including a stretchable loudspeaker and stretchable interconnections among integrated active devices.

A simple fabrication of a stretchable acoustic device (SAD) is demonstrated by replacing the conventional rigid metal coil with a deformable liquid metal coil of Galinstan in a flexible polymer microchannel where the fabricated stretchable loudspeaker is driven by the dynamic interaction between the Galinstan coil and a permanent Neodymium magnet. The fabricated SAD exhibited very stable acoustic performance in the audible frequency range from 20 Hz to 20 kHz, upon repeated cycles of mechanical deformation of uniaxial stretching up-to 50% and biaxial stretching up-to 30%. The results intuitively show the high applicability of the Galinstan-based SAD to various stretchable acoustic devices. In addition, Galinstan-filled elastomeric polymer microchennels were successfully applied to the body-attachable integrated system of energy storage devices and bio-environmental sensors, as stretchable interconnections. These works clearly suggest the high potential of liquid metal in fabricating high performance body-attachable/implantable devices.

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C13 - Mon 16:40-17:00 **Applications/Mater. Devel. 1** Großer Saal / Great Hall

Synthesis and Characterization of a Novel High Entropy Glass

Suresh Kumar Pillai and Julien Zollinger

Research group: Solidification, Institut Jean Lamour - UMR 7198, Université de Lorraine -
Parc de Saurupt, CS 50840, 54011 Nancy cedex, France
Email : suresh-kumar.pillai@univ-lorraine.fr

High entropy glass-forming alloys have compositions that depend on the ‘confusion principle’ during liquid-solid transformation for their enhanced glass forming ability. A new empirical criterion for designing glass forming alloys based on calculations of thermodynamic, kinetic and topological parameters is introduced. A novel Zr-based high entropy glass forming alloy was synthesized. The processed samples of the aforementioned alloy were characterized by X-ray diffraction, electron microscopy and differential thermal analysis.

C14 - Mon 17:00-17:20 **Applications/Mater. Devel. 1** Großer Saal / Great Hall

Stability of amorphous alloys in the system Ce-Cu-Fe with additions of Al

Luka Kelhar[1,2,4], Spomenka Kobe[1,2,4] and Jean-Marie Dubois[1,2,3,4]

[1]Jožef Stefan Institute, Jamova cesta 39, Ljubljana 1000, Slovenia

[2]International Postgraduate School "Jožef Stefan", Jamova 39, Ljubljana 1000, Slovenia

[3]Institut Jean Lamour (UMR 7198 CNRS-Université de Lorraine), Parc de Saurupt, CS 50840, 54011 Nancy Cedex, France

[4]International Associated Laboratory PACS2, CNRS-Nancy, France and JSI-Ljubljana, Slovenia

Our study is dedicated to the quaternary system $(Al_{1-x}Ce_x)_{62}Cu_{25}Fe_{13}$, where x stands for the relative Ce concentration in the Al+Ce mixture, x=Ce/(Al+Ce). We used a processing route that features arc-melting of ingots from pure raw elements under Ar atmosphere followed by rapid quenching on a copper wheel to yield around 30 micrometers thick ribbons. Variation of x greatly influences the glass forming ability. The best glasses are found at compositions where $0.67 \leq x \leq 0.83$. Alloys with more or less Ce exhibit nanocrystallites embedded in an amorphous matrix. A stable icosahedral quasicrystal forms only at very low Ce content: $x \leq 0.03$. The temperature of the onset of crystallization (T_x) is sensitive to the amount of Ce. It extends from 590K for x=0.5 down to 390K for x=1. The variation in glass transition temperature (T_g) is consistent with that of T_x, featuring a shift to lower temperatures with higher concentration of Ce. Alloys within the range $0.67 \leq x \leq 0.83$ exhibit good glass forming ability (GFA), indicated by a pronounced supercooled liquid region, reaching extension in temperature range up to 60K.

The investigated series of Ce-rich amorphous alloys exhibit a composition range with significant GFA. Two eutectic compositions in the Al-Ce binary system [1] fall in the range $0.67 \leq x \leq 0.83$, which describes the most pronounced GFA. Thus, the mechanism responsible for superior GFA could be bound to the existence of a high amount of undercooled liquid in the vicinity of deep eutectic points. Additionally, we show that a powder prepared by crushing melt-spun ribbons with extended supercooled liquid region has a good potential to be consolidated into bulk amorphous specimens via thermoplastic forming. Such centimeter-size specimens open an avenue to in-depth measurements of properties like hardness, yield stress, etc. Application to mechanical devices is found realistic.

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C15 - Mon 17:20-17:40 **Applications/Mater. Devel. 1** Großer Saal / Great Hall

Mechanically induced surface modifications affecting the quasi-static and cyclic properties of bulk metallic glasses

Daniel Grell[1] and Eberhard Kerscher[1]

[1] University of Kaiserslautern, Materials Testing, Kaiserslautern, Germany

Beside their outstanding mechanical properties, such as high compressive strengths combined with large elastic strains, good wear resistance, and high hardness, bulk metallic glasses (BMGs) show only poor plasticity and mostly low fatigue limits. Therefore, their application as structural materials has been strictly restricted so far, but various approaches have already been taken to improve their plastic deformation behavior. By mechanical pre-treatments, e.g. surface imprinting[1] or shot-peening[2], plasticity can be significantly enhanced due to surface near residual stresses, which directly affect shear banding mechanisms in bulk metallic glasses.

While the influence of mechanically induced surface modifications on the compressive[3] and tensile[4] behavior of Zr-based BMGs has already been properly investigated, our recent investigations deal with the effect of these surface modifications on the three-point bending properties of fully amorphous $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ (Vitreloy 105) produced by suction casting. Therefore, bar-shaped samples were cut from the casted plates and one side was modified by micro-milling, micro-eroding and laser ablation. Thereby, the process parameters were varied for each manufacturing method to generate two different surface morphologies. We have tested the samples under quasi-static and cyclic three-point bending as well as with load increase tests. In this framework, our recent work focusses on the comparison of the different loading conditions concerning the achieved maximum strengths of Vitreloy 105 BMG. Furthermore, the mechanical properties of the different surface states were compared to each other and to a reference state of untreated bulk amorphous Vit-105. The fracture surfaces were additionally analyzed in SEM to gain further information about the fracture mechanisms. All tests were carried out in order to find a material's surface state with improved mechanical properties under given loading conditions.

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I6 - Mon 16:10-16:40 **Structure and Dynamics 1** Kleiner Saal / Small Hall

Investigation of dynamics and structure in liquid (alkali) metals via density functional theory-based molecular dynamics

Taras Bryk[1,2], Ivan Klevets[1], Giancarlo Ruocco[3,4], Tullio Scopigno[3,5] and Ari P Seitsonen[6,7]

[1] *Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, UA-79011 Lviv, Ukraine*
[2] *Institute of Applied Mathematics and Fundamental Sciences, Lviv Polytechnic National University, UA-79013 Lviv, Ukraine*
[3] *Dipartimento di Fisica, Universita di Roma La Sapienza, I-00185 Roma, Italy*
[4] *Center for Life Nano Science @Sapienza, Istituto Italiano di Tecnologia, I-00161 Roma, Italy*
[5] *IPCF-CNR, Universita di Roma, I-00185 Roma, Italy*
[6] *Institut für Chemie, Universität Zürich, CH-8057 Zürich, Switzerland*
[7] *École Normale Supérieure, Departement de Chimie, F-75005 Paris, France*

Alkali metal solids and fluids were for long time regarded as simple nearly-free electron metals also under applied pressure, until evindence emerged on the contrary, and subsequently the electron wave functions of the highly compressed Li were found [1] to be mostly of *p* type and localised in the interstitial regions.

We have performed molecular dynamics simulations, based on density functional theory to yield the forces on the atoms *on the fly*, on liquid alkali metals. In particular we have investigated the properties of *l*-Rb [2] and *l*-Li [3] at elevated temperatures and varying pressures. We concentrate our analysis on the collective dynamics and electronic structure in these fluids. In *l*-Rb the results from our simulations agree well with inelastic X-ray scattering experiments, and we find evidence of a liquid-liquid phase transition. In *l*-Li we evaluated the charge-density correlation functions. In both cases we find non-sphericality in the electronic structure around the ions.

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C16 - Mon 16:40-17:00 **Structure and Dynamics 1** Kleiner Saal / Small Hall

Unveiling the structural arrangements responsible for the atomic dynamics in metallic glasses during physical aging

V. M. Giordano[1] and B. Ruta[2]

[1] *Institute of Light and Matter, UMR5306 Université Lyon 1-CNRS, Université de Lyon, 69622 Villeurbanne Cedex, France.*
[2] *ESRF-The European Synchrotron, CS 40220, 38043 Grenoble Cedex 9, France*

The unique structural features and outstanding mechanical and physical properties of glasses have put them at the focus of an intense research activity for both fundamental understanding and technological applications. Notwithstanding, their intrinsic non equilibrium nature still poses formidable problems to broad applications, and one of the main challenges is to avoid aging during processing and annealing. This requires an understanding of the microscopic mechanisms behind aging and of the relation between the structure and the atomic motion, which is still missing due to
the lack of information on the dynamics with both experiments and simulations.
Recent studies have revealed the existence of a complex atomic motion in metallic glasses, with different aging regimes in contrast with the typical continuous aging observed in macroscopic quantities. By combining dynamical and structural synchrotron techniques, for the first time we directly connect previously identified microscopic structural mechanisms with the peculiar atomic motion, providing a broader unique view of their complexity. We show that the atomic scale is dominated by the interplay between two processes: rearrangements releasing residual stresses related to a cascade mechanism of relaxation, and medium range ordering processes, which do not affect the local density, likely due to localized relaxations of liquid-like regions. As temperature increases, a surprising additional secondary relaxation process sets in, together with a faster medium range ordering, likely precursors of crystallization. [1].

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C17 - Mon 17:00-17:20 **Structure and Dynamics 1** Kleiner Saal / Small Hall

Effects of alloying elements on the viscosity of ternary glass-forming Zr-(Co,Ni)-M melts

C. C. Yuan[1,2], F. Yang[2], F. Kargl[2], D. Holland-Moritz[2], G. G. Simeoni[3], and A. Meyer[2]

[1] *Southeast University, School of Material Science & Engineering, Nanjing 211189, P. R. China*
[2] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany*
[3] *Heinz Maier-Leibnitz Zentrum (MLZ) and Physics Department, Technische Universität München, 85748 Garching, Germany*

Addition of a third component to a binary metallic glass forming melt can significantly improves its glass forming ability. In some cases only a very small amount of such elements is necessarily. The underlying mechanism is so far not very well understood. Particularly, very little attention has been paid to the change of melt properties in this respect. We thus studied the microscopic mass transport and the macroscopic flow behavior of the Zr-(Co,Ni)-(Al,Pd,Ti) melt with a systematic variation of the third component. Utilizing the containerless processing technique of electrostatic levitation allows us to obtain precise data on diffusion coefficient and melt viscosity over a wide temperature range, without artifacts caused by container-melt reactions. We shows that the addition of the of Al to the binary Zr-(Co,Ni) melt leads to an increase of the melt viscosity of system accompanied by a remarkable decrease of the Co, Ni self-diffusion coefficient [1]. In contrast, upon alloying of Ti and Pd the effect of slowing-down of the liquid dynamics is much weaker. However, the average packing fraction of the Al contained melt derived from the measured macroscopic density is smaller than that of the corresponding binary alloys. This indicates that apparently such slowing down of the liquid dynamics cannot be explained a hard-sphere like model of packing, although metallic glass-forming melts in which is absent are often considered to be most closed to a hard-sphere like system [2]. Instead, the chemical interactions of Al with transition metal atoms should play an important role here, which also contribute to their improved glass-forming ability.

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C18 - Mon 17:20-17:40 **Structure and Dynamics 1** Kleiner Saal / Small Hall

OF-AIMD Study of Static and Dynamic Properties of some Liquid transition Metals

G. M. Bhuiyan[1], Md. Riazuddin Molla[1], A. Z. Ziauddin Ahmed[1], L. E. González[2], and D. J. González[2]

[1] *Department of Theoretical Physics, University of Dhaka, Bangladesh*
[2] *Department of Physics, University of Valladolid, Spain*

Some static and dynamic properties of liquid transition metals namely l-Cr, l-Mn and l-Co are studied for the first time using the orbital free *ab-initio* molecular dynamics simulation (OF-AIMD) method near their respective melting temperatures. The OF-AIMD method is based on the density functional theory (DFT) which provides the electronic energy of the system; the necessary interionic interaction is then derived from the electronic energy via the Hellman-Feynman theorem. The exchange and correlation energy in the DFT are described by the local density approximation. The external energy term is treated with a local pseudopotential. Results for static structure factors, isothermal; compressibility, diffusion coefficients, sound velocity and viscosity for the above systems are found to be good in agreement with available experimental data and with other theoretical values.

*Corresponding author: gbhuiyan@du.ac.bd

I7 - Tue 09:00-09:30 **Expanded Liqu./Electronic Prop.** Großer Saal / Great Hall

Inelastic x-ray scattering study on the electronic state in fluid alkali metals

Kazuhiro Matsuda

Kyoto University, Graduate School of Science, Kyoto, Japan

Fluid metals have been regarded as a system whose physical properties are strongly dependent on the thermodynamic state [1]. Liquid metals near the melting point exhibit a typical metallic character, whereas the vapor phase of metals is an insulator which consists of atoms or molecules. Vaporization of the fluids across the liquid-vapor coexistence curve accompanies a substantial and abrupt decrease in the electrical conductivity, thus a metal-insulator transition occurs in a discontinuous manner. On the other hand, a continuous volume expansion along the coexistence curve causes a gradual loss of metallic nature with a continuous reduction in the conductivity. A dilute metallic system is realized where the valence electrons and ions are in highly correlated state.

Among the metallic elements, alkali metals are a simple metal since their valence electrons originate from *s*-state, this " simple metal" picture is basically preserved in the liquid state near the melting point. However, the situation drastically changes when they are expanded. The breakdown of the nearly free electron picture was indicated through the measurement for the electrical conductivity of Rb and Cs [1]. It is remarkable that such breakdown appears in the density region still far apart the critical point (around 3 times critical density, $3\rho_c$) where the fluids are still metallic. X-ray diffraction and small-angle x-ray scattering measurements for fluid Rb observed that structural changes occur also in the early stage of expansion ($\approx 3.5\ \rho_c$). The nearest neighbor distance decreases and the density fluctuation increases with decreasing density [2]. It was indicated that charge fluctuation of the low-density electron gas makes a significant contribution to such structural features, making the interatomic force more attractive [3].

In order to gain further insights into the electronic states in fluid alkali metals, a direct experimental observation for the electronic states is of crucial importance. Inelastic X-ray scattering technique has been a powerful tool for investigating the electronic states in materials [4]. We have thus far carried out X-ray Compton experiments to measure the momentum distributions of electrons in fluid alkali metals, and X-ray Raman scattering experiments to measure plasmon excitations of valence electrons in the fluids. Recent experimental results will be reported.

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C19 - Tue 09:30-09:50 **Expanded Liqu./Electronic Prop.** Großer Saal / Great Hall

Metal to Nonmetal Phase Separation in Expanded liquid Rubidium

Wolf - C. Pilgrim[1], Daniel Szubrin[1], Franz Demmel[2], Andrea Orecchini[3], Alessio De Francesco[3] and Stephane Rols[3]

[1.] Physical Chemistry, University of Marburg, Hans-Meerwein-Str., D-35032 Marburg, Germany

[2] Molecular Science Group, ISIS Facility RAL, OX11 0QX Chilton Oxfordshire, United Kingdom

[3] Institute Laue-Langevin, ILL, 71 Avenue des Martyrs, F-38042 Grenoble, France

Quantum mechanical calculations of the ground state energy in pure electron gases reveal a mechanical instability, i.e. a negative compressibility, if they are sufficiently expanded [1]. Appropriate scaling [1,2] allows relating these gas densities to mass densities in real liquid alkali metals which are regarded as perfect model systems for free electron gases. It is found that the region of instability corresponds to about 3-4 times the critical density. This however contradicts the common view of the density induced metal to non-metal transition in liquid alkali metals which is believed to set in at about 2-3 times the critical density, i.e. at considerably lower density (see e.g. [3]). We have investigated the density dependence of the collective modes in liquid Rubidium to understand this discrepancy. Collective modes were chosen as suitable probes for this investigation because their properties are highly sensitive to variations in the interatomic interactions, which are expected to occur if the electron gas ceases to exist.

Experiments were carried out on the time of flight instruments IN4 and BRISP, located at the ILL in Grenoble. As a result, we find that all $S(Q,\omega)$-properties show distinctive variations when the density range is approached where the electron gas instability is predicted. Variation of mode- and $S(Q,\omega)$-maximum properties will be discussed. It is demonstrated that the observed behavior can be understood within a scenario recently suggested for the metal to non-metal transition in liquid mercury [4]. There, the localization of the conduction electrons forces the formation of a micro emulsion consisting of a dense metallic and less dense non-metallic phase. The densities of these phases remain constant with further expansion but the volume fraction of the non-metallic phase increases causing the observed overall density reduction. This scenario fully explains the observed $S(Q,\omega)$ density dependence along the explored density range and throws new light on the mechanism of the density-induced metal to non-metal transition in liquid metals.

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C20 - Tue 09:50-10:10 **Expanded Liqu./Electronic Prop.** Großer Saal / Great Hall

The packing of helical and zigzag chains and distribution of interstitial voids in expanded liquid Se near the semiconductor to metal transition

K. Maruyama[1], S. Hiroi(Sato) [2], H. Endo[3], H. Hoshino[4], T. Odagaki[5], and F. Hensel[6],

[1] *Department of Chemistry, Faculty of Science, Niigata University, Niigata, JAPAN*

[2] *Toyota Technological Institute, Nagoya, JAPAN*

[3] *Department of Physics, Faculty of Science, Kyoto University, Kyoto, JAPAN*

[4] *Faculty of Education, Hirosaki University, Hirosaki, Aomori, JAPAN*

[5] *School of Science and Engineering, Tokyo Denki University, Hatoyama, Saitama, Japan*

[6] *Physikalische Chemie, Philipps-Universität Marburg, Marburg, Germany*

The RMC and Voronoi-Delaunay void analyses were applied to study the modification of chain geometries in expanded liquid Se up to 1600 ºC and ~ 1500 bar. The shortening of chains, fluctuations of dihedral angles and branched chains with increasing temperature and pressure cause modification of the helical chain to the planar zigzag chain conformations.

The structural data for the distribution of voids and distances to the 4th or 6th neighbor atoms on the chain segments provide information for stacking of planar zigzag chains which leads to the formation of metallic domains involving voids with radius ~2.3 Å. Near the semiconductor to metal (SC-M) transition region the number fraction N_Z / N_H for zigzag(Z) and helical(H) chain segments is to be ~ 1.

The description of structures built with corner-sharing triangle blocks for contiguous atoms along the chains is used to characterize the spatial correlation between chain segments and voids near the SC-M transition.

C21 - Tue 10:10-10:30 **Expanded Liqu./Electronic Prop.** Großer Saal / Great Hall

Inelastic X-ray Scattering Measurements of Plasmons in Expanded Liquid Alkali Metals

T. Hagiya[1], K. Matsuda[1], N. Hiraoka[2], K. Kimura[3], H. Hayashi[1], M. Inui[4], Y. Kajihara[4], and M. Yao[1]

[1] *Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan*

[2] *National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan*

[3] *Graduate School of Engineering, Nagoya Institute of Technology, Nagoya 466-8555, Japan*

[4] *Graduate School of Integrated Arts and Sciences, Hiroshima University, Higashi Hiroshima 739-8521, Japan*

It has been regarded that the conduction electrons in liquid alkali metals can be described with the nearly free electron approximation. However, as the density of the liquid is reduced, they depart from such a description and are gradually transformed into a highly correlated state [1]. This indicates the effect of the electron-electron interaction (the exchange and correlation interaction) becomes increasingly important with the volume expansion in liquid alkali metals.

In order to understand the electronic state in liquid alkali metals, we have so far carried out inelastic X-ray scattering (IXS) experiments focusing on the behaviors of plasmon, a collective excitation of conduction electrons. The results of the plasmon dispersions of liquid Rb near the melting point [2] show that the effect of electron-ion interaction is reduced upon melting. This indicates the conduction electrons are more suitably described with the electron gas model in the liquid state than in the solid state. It is a matter of concern how the electron-electron interaction is reflected in the plasmon dispersion in expanded liquid alkali metals.

In this study, we have investigated the plasmon behaviors in liquid alkali metals (Rb and K) at lower densities by IXS experiments. The experiments were performed on the IXS beamline BL12XU at SPring-8 in Japan. High-temperature and high-pressure conditions were achieved by using an internally heated high-pressure vessel. The IXS spectra exhibit a distinct excitation of plasmon, and we could determine the plasmon excitation energy from them. The present results of liquid Rb show that the plasmon energy increases with the momentum transfer (positive dispersion) at high densities (1.37~1.28 g/cm^3, 573~773 K). This dependence is qualitatively consistent with the prediction of the electron gas model. However, at a low density (1.15 g/cm^3, 1073 K), the dispersion tends to be flat in a low momentum transfer region and deviates from the electron gas model. We calculated the plasmon energy by taking account of the electron-electron and electron-ion interaction, and the calculated results qualitatively reproduce the experimental results.

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I8 - Tue 09:00-09:30 **Heat Treatment/Devitrification** Kleiner Saal / Small Hall

Structural rejuvenation with the change of local structure and mechanical properties in recovery annealed Zr-based metallic glasses

Junji Saida[1], Rui Yamada[1], Wei Guo[1], Masato Wakeda[2] and Shigenobu Ogata[2]

[1] Frontier Research Institute for Interdisciplinary Sciences (FRIS), Tohoku University, Sendai, Japan

[2] Graduate School of Engineering Science, Osaka University, Osaka, Japan

Recently, structural rejuvenation, *i.e.*, recovery of the less relaxed state, in metallic glasses has been attracted attention from the viewpoints of improving mechanical properties as well as understanding a relaxation phenomenon originating from the intrinsic random atomic configuration. Relaxation state is generally regarded as one of the important parameters on various properties of metallic glass. Especially, since the good mechanical properties are usually lost by relaxation, we have to control it carefully for industrial use. The authors have investigated that the relaxation state is fixed by the cooling rate in the lower temperature region of the supercooled liquid state [1]. Based on the results, we have reported the recovery of less relaxed state (rejuvenation) of metallic glass through a simple thermal processing by annealing just above glass transition temperature followed by an appropriate cooling using the experimental [2] and simulation studies [3]. Here, it is found that the history of the relaxation is reset in the temperature around 1.1-1.2T_g, and the new relaxation state is introduced depending on the following (final) cooling rate by molecular dynamics (MD) simulation. Actually, the relaxation enthalpy can be got back (*that is*, the glassy alloy can be rejuvenated) for the almost fully relaxed glassy alloy by post annealing at 1.07T_g followed by the appropriate cooling at approximately 4 K/s in the $Zr_{55}Al_{10}Ni_5Cu_{30}$ metallic glass. In this presentation, we intend to evaluate the condition for rejuvenation in metallic glass and discuss on the change of local structure and mechanical properties by rejuvenation. The present study proposes a novel method on controlling relaxation state and provides useful information on the application of metallic glasses.

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C22 - Tue 09:30-09:50 **Heat Treatment/Devitrification** Kleiner Saal / Small Hall

Tuning the memory dependence of vapour deposited metallic glasses

M. Lüttich[1,2], B. Ruta[1], Y. Luo[2], K. Samwer[2], V.M. Giordano[3], E. Pineda[4]

[1] ESRF-The European Synchrotron, 38043 Grenoble Cedex 9, France

[2] I. Institute of Physics, University of Göttingen, Germany

[3] Institute of Light and Matter, Université de Lyon 1-CNRS, France

[3] Polytechnic University of Catalonia Barcelona, Catalunya, Spain

Metallic glasses (MGs) show outstanding mechanical, physical and chemical properties and so provide a whole class of materials at the cutting-edge research in metallic and glassy systems [1]. By exposing them to thermal treatments, their properties get affected in a subtle and complex way. We present here a study of memory effects due to different thermal treatments in the atomic motion of rapidly quenched and vapour deposited CuZr MGs by means of x-ray photon correlation spectroscopy (XPCS). Vapour deposition is supposed to give rise to ultra-stable MGs, that is MGs with improved stability [2]. However information on their dynamics at the atomic level is still missing.

While cycling through a temperature protocol and measuring the dynamics of density fluctuations at different isothermal temperature steps, we find that vapour deposited MGs show a vanishing history dependence with rising annealing temperatures $T_\mathrm{a} < T_\mathrm{g} \lesssim T'_\mathrm{a}$; although the absolute value of the relaxation time τ behaves inversely proportional with T_a. Moreover the dynamics in vapour deposited MGs is stationary while, in contrast, the fast quenched MG show the occurrence of aging during isotherm measurements.

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C23 - Tue 09:50-10:10 **Heat Treatment/Devitrification** Kleiner Saal / Small Hall

Structural changes of amorphous $Fe_{86}Cr_6P_6C_2$ alloy according to temperature and time determined by resistivity, thermopower, and DSC

L. Abadlia[1,2], F. Gasser[3], K. Khalouk[3], M. Mayoufi[1], and J. G. Gasser[3,*]

[1] *Laboratoire de Chimie des Matériaux Inorganiques (LCMI), Université Badji-Mokhtar Annaba, BP12, 23000 Annaba, Algeria*

[2] *Laboratoire de Physique de la Matière et du Rayonnement (LPMR), Université Mohamed Chérif Messaadia B.P. 1553, 41000, Souk-Ahras, Algeria*

[3] *Laboratoire de Chimie et Physique - Approche Multi-échelle des Milieux Complexes (LCP- A2MC) Institut de Chimie, Physique et Matériaux, Université de Lorraine, 1 Boulevard Arago - 57078 Metz cedex 3, France*

In this work, we characterize structural changes of $Fe_{86}Cr_6P_6C_2$ alloys, particularly the recrystallization of amorphous alloys but also transformations between different crystalline phases, by resistivity, Absolute Thermoelectric Power and by Differential Scanning Calorimetry measurements. We deduce the activation energy by three independent “resistivity versus time” measurements where the sample can be kept at constant temperature during a very long time (several minutes to several days) when phase changes are occurring.

Keywords: Metallic glasses, amorphous alloy, recrystallization, resistivity, thermopower, DSC, scientific instrumentation

[*]Corresponding author: jean-gorges.gasser@univ-loraine.fr, Tel: + 33 (0)3 87 31 58 59, Fax+ 33 (0)3 87 31 58 84

C24 - Tue 10:10-10:30 **Heat Treatment/Devitrification** Kleiner Saal / Small Hall

Estimation of crystal growth velocity in a chalcogenide glass by fast scanning calorimetry

S. K. Pillai[1], Ch. Schick[2], J. Málek[3], and J. Zollinger[1]

[1] *Research group: Solidification, Institut Jean Lamour - UMR 7198, Université de Lorraine - Parc de Saurupt, CS 50840, 54011 Nancy cedex, France*

[2] *Faculty of Chemical Technology, University of Pardubice, Studentská 573, Pardubice 532 10, Czech Republic*

[3] *University of Rostock, Institute of Physics, Wismarsche Str. 43-45, 18051 Rostock, Germany*

A novel approach for measurement of crystal growth velocities by fast differential scanning calorimetry is discussed. A theoretical model using the Johnson–Mehl–Avrami–Yerofeeyev–Kolmogorov (JMAYK) is presented to deduce the growth information from the calorimetric melt peak data. A well-documented and commercially important Se 0.9 Te 0.1 alloy that readily forms a stable chalcogenide glass was used in this study. The fast-DSC results compared well with micrographic data from the literature.

I9 - Tue 11:00-11:30 **Structure and Dynamics 2** Großer Saal / Great Hall

Microscopic and macroscopic properties of Zr_2Co melts

M.D. Ruiz-Martín[1,2], D. Holland-Moritz[2], F. Yang[2], C. C. Yuan[2], G.G. Simeoni[3],
T. Hansen[4], U. Rütt[5], O. Gutowski[5], J. Bednarčik[5], and A. Meyer[2]

[1] *Universitat Politècnica de Catalunya, Departament de Física I Enginyeria Nuclear, Grup de Caracterització, Barcelona, Spain*

[2] *Deutsches Zentrum für Luft- und Raumfahrt, Institut für Materialphysik im Weltraum, Köln, Germany*

[3] *Technische Universität München, Forschungsquelle Heinz Maier-Leibnitz (FRM-II), Garching, Germany*

[4] *Institut Laue-Langevin, Grenoble, France*

[5] *DESY Photon Science, Hamburg, Germany*

Zr-based alloys have attracted broad interest because of their ability to form metallic glasses even when cooling down the melts at moderate cooling rates. In order to understand the microscopic processes that determine the macroscopic physical properties of the melt (such as density, viscosity, surface tension and electrical resistivity) or the solidification behaviour, we have conducted an extensive study combining X-ray and neutron diffraction as well as quasielastic neutron scattering.

In order to undercool the melts deeply below the melting temperature and to avoid reactions with crucible materials, the liquids are containerlessly processed in an electrostatic levitation furnace [1]. Using this technique in combination with neutron and X-ray diffraction yielded the static structure factors of binary Zr_2Co alloy melts. Furthermore, the Co self-diffusion coefficient of liquid Zr_2Co as a function of temperature was investigated using quasielastic neutron scattering.

The results of the studies reveal that the short-range order, the number density and the Co self-diffusion coefficient of the Zr_2Co melts closely resemble those observed for $Zr_{64}Ni_{36}$ melts of similar composition [2]. An explanation based on similar atomic radii is obviously not sufficient, as different structural and dynamical properties have been observed in liquid Zr-Cu and Zr-Pd.

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C25 - Tue 11:30-11:50 **Structure and Dynamics 2** Großer Saal / Great Hall

Structure and dynamics of liquid Zn. An ab-initio molecular dynamics study.

Luis E. González[1] and Beatriz G. del Rio[1]

[1] *Universidad de Valladolid, Dept. Fisica Teórica, Valladolid, Spain*

The static and dynamic properties of liquid Zn have been studied using an ab initio molecular dynamics method. Results are reported for the thermodynamic states at 723K for which inelastic neutron scattering data are available [1]. The calculated static structure shows very good agreement with experimental measurements, including an asymmetric second peak. The dynamic structure reveals the existence of propagating density fluctuations and the associated dispersion relation has also been calculated. The possible coupling between longitudinal and transverse excitation modes has been investigated by looking at specific signatures in two wavevector regions: the first one is located around the position of the main peak of the structure factor, Qp, as suggested by the recently reported appearance of high frequency transverse waves in several liquid metals under high pressures [2]; the second region is around Qp/2, as suggested by inelastic scattering experiments for liquid Zn [1] and other metals.

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C26 - Tue 11:50-12:10 **Structure and Dynamics 2** Großer Saal / Great Hall

Structural and dynamical evolution in binary and ternary La-based glass-forming melts

Zheng WANG[1], Fan YANG[1] and Andreas MEYER[1]

[1] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany*

The substitution of similar sized transition metals (TM= Ni, Co or Cu) in La-TM-Al metallic glasses (MGs) alters the local relaxation behavior in glassy state [1], which cannot be simply interpreted under hard sphere packing assumption. The copper containing alloy exhibits distinct characteristic for this MG system, compared to nickel or cobalt. The absence of separately local relaxation peak on mechanical spectrum implies some additional effect, like chemical interaction, should play an important role in the relaxation behavior. The local relaxation behavior is also considered to be related with weakly bonded and rich free volume region here. Whether this behavior roots in properties of corresponding glass-forming melts is worthy to find out. Furthermore, addition of Al is found to dramatically improve the GFA for many MG systems, and recent experiment suggests that the chemical interaction leads to a sluggish transport behavior in Zr-Co-Al melts [2]. However, whether other glass-forming alloy systems exhibit similar behaviors is still unclear.

Here, in this study, an elaborate selection of binary La-TM/Al and ternary La-TM-Al glass-forming melts are systematically studied. Combing the newly developed containerless electrostatic levitator (ESL) method and *in-situ* synchrotron X-ray scattering experiment [3], density and total structure factor are obtained over a wide temperature range. Macroscopic and microscopic properties can be analyzed simultaneously at same temperature. La-Cu melts are found to present a positive excess volume, compared to the negative excess volume for La-Ni/Co melts. Total structure factor $S(Q)$ is also differ between Cu and Ni/Co containing melts. Such difference is likely also has its origin in the chemical interaction between La and TM, which may persist in glass and cause different local relaxation behavior. The Al addition slows down the liquid dynamics and changes the property of glass-forming melts, which come along with an improved GFA. Moreover, similar to that in Zr-Co-Al melts, the slower liquid dynamics by adding Al is associated with an increase of molar volume V_m.

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C27 - Tue 12:10-12:30 **Structure and Dynamics 2** Großer Saal / Great Hall

Structural and dynamical investigations on $Hf_{35}Ni_{65}$ metallic melts by Neutron- and X-ray-scattering

B. Nowak[1], D. Holland-Moritz[1], F. Yang[1], E. Ritter[1], D. Brüggemann[1], A. Meyer[1], T. Hansen[2], W. Lohstroh[3], A. Bernasconi[4]

[1] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany*
[2] *Institut Laue-Langevin (ILL), 38042 Grenoble, France*
[3] *TU München, Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching, Germany*
[4] *European Synchrotron Radiation Facility (ESRF), 38000 Grenoble, France*

The glass formation in metallic melts is controlled by dynamical and structural properties on the atomic scale. We studied these properties for the binary eutectic system $Hf_{35}Ni_{65}$ and compared results with the more common glass-forming $Zr_{36}Ni_{64}$ system. Hf and Zr are chemically similar, as they are in the same main group in the periodic table and have approximately the same atomic size. The great advantage of investigating Hf containing alloys is the significant incoherent neutron scattering cross section of Hf in contrast to Zr, which allows for the measurment of the Hf self-diffusion coefficient by quasielastic neutron scattering (QNS).
We investigated the structure factors of liquid $Hf_{35}Ni_{65}$ by X-ray and Neutron diffraction and the self-diffusion coefficients by QNS. The melts have been processed by use of the containerless electrostatic levitation technique [1]. By applying this technique, it is possible to avoid chemical reactions of the melt with crucible materials and to undercool the sample below the melting temperature. Additionally we measured density and viscosity of $Hf_{35}Ni_{65}$ by the oscillating drop technique. Comparing the results with $Zr_{36}Ni_{64}$ led to the conclusion, that the structure of both systems is similar [2], but diffusion coefficients exhibit deviations, particularly the activation energy E_A differs by almost a factor of two [3]. This results in a different temperature dependency of the diffusion coefficients. Furthermore, QNS measurements of liquid $Hf_{35}Ni_{65}$ prepared with ^{60}Ni, which has an incoherent scattering cross section of zero, have demonstrated, that self-diffusion of Hf does not differ from the combined concentration weighted self-diffusion of Hf and Ni. This implies the same self-diffusion coefficients for Ni and Hf within the accuracy limit of the measurement.

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I10 - Tue 11:00-11:30 **Properties of Metallic Glasses** Kleiner Saal / Small Hall

Electrochemical properties of metallic glasses and related composites

Annett Gebert[1], Petre Flaviu Gostin[1], Daniel Grell[2], Eberhard Kerscher[2]

[1] Leibniz-Institute for Solid State and Materials Research (IFW) Dresden, Institute for Complex Materials, Dresden, Germany

[2] University of Kaiserslautern, Materials Testing, Kaiserslautern, Germany

The corrosion behaviour of glassy alloys is principally determined by various material-dependent factors, i.e. metastability of the amorphous state, alloy composition and ideally, lack of microstructural defects and chemically homogeneous nature. However, under real casting and rapid quenching conditions the preparation of absolutely defect-free amorphous alloys is nearly impossible. In particular in case of Zr-based glasses, though exhibiting excellent passivity in many environments, those defects cause a strong susceptibility to local corrosion. Moreover, recent studies on most prominent Zr-based BMGs revealed that their Cu content decisively determines the corrosion performance in chloride-containing solutions[1]. Developments towards in situ formed composite microstructures with dendrite phase and glassy matrix yield compositional variations that can be critical for the corrosion stability.

For metallic glasses the resistance against crack propagation is a critical aspect. Superposition of environmentally induced reactions gives rise to significant stress corrosion cracking and corrosion fatigue phenomena, which are poorly understood at present. Since cracks initiate and grow along shear bands, present work is focused on studying the interplay of shear bands with corrosive media as well as on clarifying the crack growth behaviour under various mechanical loading and corrosion conditions. Firstly it is shown how ex situ formed shear bands act as preferential sites for local corrosion initiation, while pre-formed corrosion pits are favorable surface sites to which shear bands are linked. It is further demonstrated that the in situ electrochemical response analysis of a Zr-based glass during quasistatic loading is a sensitive tool for detection of early shear banding[2]. Besides the corrosion fatigue behaviour under anodic polarization, stress corrosion cracking processes of bulk glassy $Zr_{52.5}Cu_{17.9}Al_{10}Ni_{14.6}Ti_5$ (Vit 105) under three-point bending in chloride electrolyte were studied by in situ stress and current measurements and subsequent fractography analysis. A mechanism is proposed in which cracks initiate from pits, crack tip blunting is attributed to shear banding and re-sharpening is due to preferential dissolution at shear bands[3].

Funding from the DFG in the framework of SPP-1594 under grant numbers GE 1106/11 and KE 1426/4 is acknowledged.

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C28 - Tue 11:30-11:50 **Properties of Metallic Glasses** Kleiner Saal / Small Hall

Improved Tarnishing Behavior of New Gold-based Bulk Metallic Glasses

Miriam Eisenbart[1], Oliver Gross[2], Ulrich E. Klotz[1], Isabella Gallino[2], Ralf Busch[2]

[1] fem Research Institute Precious Metals, Physical Metallurgy, 73525 Schwäbisch Gmünd, Germany

[2] Saarland University, Chair of Metallic Materials, 66123 Saarbrücken, Germany

The amorphous 18 karat gold alloy of composition Au49Ag5.5Pd2.3Cu26.9Si16.3 at% possesses a premium white-gold color and a Vickers hardness value of 360 HV1 in as-cast condition. These properties, together with the low melting temperature (range 340-380°C) and good processability are highly desired for jewelry applications.

However, the alloy shows an unusually fast tarnishing behavior as reported in [1, 2]. This is the main obstacle for the application of gold-based bulk metallic glasses (BMG) in decorative products like jewelry or watch making. The extraordinarily fast tarnishing even at room temperature could be attributed to a detrimental interaction of the alloying elements silicon and copper. Based on these findings, an extensive alloy development study was carried out with the aim to suppress the tarnishing effect.

We present new BMG alloys designed for decorative applications with largely improved tarnishing behavior. The tarnishing behavior was observed in various environmental conditions (gaseous and liquid) and quantified by the measurement of the Yellowness Index (YI1925) and metal release into the test solution. The characterization of the corroded surface was performed with SEM, STEM, TEM and XPS measurements.

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C29 - Tue 11:50-12:10 **Properties of Metallic Glasses** Kleiner Saal / Small Hall

Influence of Copper and Gallium addition on properties of $[Fe_{74}Mo_4P_{10}C_{7.5}B_{2.5}Si_2]_{100-x,\,y}$ (Cu_x, Ga_y) bulk metallic glasses

Parthiban Ramasamy[1,*], Supriya Bera[1], Mariana Calin[1], Jürgen Eckert[2, 3] and Mihai Stoica[1, 4]

[1] *IFW Dresden, Institute for Complex Materials, Helmholtzstr. 20, D-01069 Dresden, Germany*

[2] *Erich Schmid Institute of Materials Science, Austrian Academy of Sciences (ÖAW), Leoben, Austria*

[3] *Department Materials Physics, Montanuniversität Leoben, Jahnstraße 12, A-8700 Leoben, Austria*

[4] *Politehnica University Timisoara, P-ta Victoriei 2, RO-300006 Timisoara, Romania*

Fe based bulk metallic glasses are gaining more importance in recent decades due to their high strength and excellent soft magnetic properties, combined with low materials cost [1, 2]. Fe-based bulk metallic glasses usually suffer from very poor ductility, which limits their industrial applications. Recently, the improvement of the room temperature plasticity of bulk metallic glasses (BMGs) has become a hot topic in the development of advanced structural materials [3,4].The synthesis of ductile Fe-based BMGs with enhanced glass-forming ability (GFA) has also been performed in recent years, which is important for the further extension of the application fields as Structural and functional materials. Fe-Mo-P-C-B-Si glasses are more promising because of their of their good glass forming ability, which can be cast as amorphous rods with a diameter up to 5mm [5]. This BMG can reach a compressive strength of 3200 MPa and a DC magnetization of 1.3T [5]. It was proven that the minor addition of Ga will improve the glass forming ability and also the soft magnetic properties of the Fe-P-C-B-Si glass [6].

In this present work we will discuss about the changes in the GFA, mechanical and magnetic properties brought by the addition of (x = 0.5, 1, 2...) Ga and Cu. The Ga added glass shows good GFA and improved plastic deformability, with 1 at. % Ga the plastic strain of 4 % was obtained for 1.5 mm diameter rod. With increase in the Ga% the coercivity of the glass increases. The addition of small amount of copper does not really affect the GFA but with increase in the Cu% the GFA decreases and also the magnetic saturation also started to decrease. With 0.5 at. % Cu the plastic strain of 3 % was obtained for 1.5 mm diameter rod.

The financial support provided by the European Commission (FP7 Marie Curie ITN “VitriMetTech”-607080) is fully acknowledged.

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C30 - Tue 12:10-12:30 **Properties of Metallic Glasses** Kleiner Saal / Small Hall

Characterization of the $Fe_{67}Mo_6Ni_{3.5}Cr_{3.5}P_{12}C_{5.5}B_{2.5}$ bulk metallic glass forming alloy

B. Bochtler *, O. Gross, I. Gallino and R. Busch

Saarland University, Chair of Metallic Materials, Campus C6.3, 66123 Saarbrücken, Germany
* *corresponding author: benedikt.bochtler@uni-saarland.de*

Fe-based metallic glasses gained considerable interest as they show extraordinary material properties, like high strength and high hardness even compared to other metallic glasses [1]. A further crucial advantage is the low price and good availability of iron, thus making Fe-based glasses interesting for industrial applications. Of special interest is the production of small and/or complicated structures, like precision gears or micro actuators, where the high hardness and wear resistance of Fe-based BMGs come into effect.

In the present work, the bulk metallic glass steel $Fe_{67}Mo_6Ni_{3.5}Cr_{3.5}P_{12}C_{5.5}B_{2.5}$ (0.52 wt% C) is characterized in detail in order to evaluate its general applicability. This alloy was designed by Johnson and co-workers [2] and provides a high critical casting thickness of 13 mm, thus allowing for the casting of amorphous parts with a considerable size and a high yield strength of 3.1 GPa. For the casting of amorphous parts, as well as the processing via thermoplastic forming, thermodynamics and viscosity of an alloy are crucial.

The thermophysical properties including the specific heat capacity were measured using calorimetric methods. The crystallization behavior of amorphous samples upon heating was characterized by differential scanning calorimetry and X-ray diffraction and a time-temperature-transformation diagram was constructed. The equilibrium viscosity below the glass transition as well as volume relaxation behavior were measured by three-point beam bending and dilatometry, respectively, in order to assess the kinetic fragility [3]. Viscosity in the liquid state was determined, using electromagnetic levitation in microgravity on a reduced gravity aircraft during the TEMPUS campaign of the German Aerospace Center (DLR). The alloy displays a strong liquid behavior at low temperatures (three-point beam bending) and a fragile behavior at high temperatures (electromagnetic levitation). These results are analog to the ones observed in several Zr-based bulk metallic glass forming liquids [4], indicating a strong to fragile liquid-liquid transition.

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P3 - Tue 13:40-14:20 **Plenary** Großer Saal / Great Hall

Tailoring structure formation and properties of glass-forming systems

J. Eckert[1,2]

[1] Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, A-8700 Leoben, Austria

[2] TU Department Materials Physics, Montanuniversität Leoben, Jahnstraße 12, A-8700 Leoben, Austria

Metallic glasses and composites with unique combinations of strength, toughness, ductility and other properties are of increasing interest for a variety of applications as structural and functional materials. However, room temperature plasticity in metallic glasses is localized on shear bands often resulting in limited deformability. Hence, finding ways to induce more homogeneous deformation characteristics is not only highly interesting with respect to basic scientific questions but also urgent to further promote the use of these materials for engineering applications.

A lot of attempts have been made to tune the atomic short- and medium-range order so that to obtain sufficient ductility through promoting local shear events and to distribute them as homogeneously as possible throughout the material. An alternative approach is to create unique heterogeneous materials with different type and length-scale of *in-situ* formed heterogeneities / phases / structure modulations. Moreover, subsequent heat treatment and/or mechanical treatment can be used to further improve the properties of the material.

The recent developments along this line will be summarized and results for different types of metallic alloys will be presented to illustrate how the structural and functional properties can be tuned by appropriate phase and microstructure control. The phase and structure formation will be described under consideration of the solidification parameters and the conditions governing the development of atomic short- and medium-range order or composite formation. The deformation behaviour and possible phase transitions during deformation will be related to the structure of the glass including heterogeneities and the microstructure of the material in order to derive guidelines for the design of macroscopically ductile high strength materials.

I11 - Tue 14:25-14:55 **Dynamics 1** Großer Saal / Great Hall

Analyzing the dynamic structure of liquid metals and alloys

WAX Jean-François[1], BRYK Taras[2,3]

[1] *Laboratoire de Chimie et de Physique—A2MC, Université de Lorraine—Metz, 1, boulevard Arago 57078 Metz Cedex 3, France*

[2] *Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, 1 Svientsitskii Street, UA-79011 Lviv, Ukraine*

[3] *Institute of Applied Mathematics and Fundamental Sciences, Lviv Polytechnic National University, UA-79013 Lviv, Ukraine*

Experimental improvements in the inelastic x-ray and neutrons scattering techniques have stimulated a great interest in the dynamic structure of liquids during the last decades. Many unexpected or anomalous phenomena have been unfolded among which fast sound, positive dispersion and possible coupling between transverse and longitudinal excitations can be mentioned. Numerical simulations have been really helpful in interpreting the experimental observations. But, whatever the origin of the data, their analysis is usually based on fitted analytic expressions. Of course, such approaches depend on the hypotheses made in building the model and care must be taken in its elaboration.

In this presentation, a recently developed analysis scheme [1,2] inspired from the Generalized Collective Modes approach is presented and applied to simulation results of liquid metals and alloys. We will focus on several aspects and discuss which information can be accurately obtained from these data and which is more questionable.

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C31 - Tue 14:55-15:15 **Dynamics 1** Großer Saal / Great Hall

Heterogeneous diffusion, viscosity and the Stokes Einstein relation in binary liquids

H. R. Schober[1] and H. L. Peng[2]

[1] *Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany*

[2] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany*

We investigate the origin of the breakdown of the Stokes-Einstein relation (SER) between diffusivity and viscosity in undercooled melts. A binary Lennard-Jones system, as a model for a metallic melt, is studied by molecular dynamics. A weak breakdown at high temperatures can be understood from the collectivization of motion, seen in the isotope effect. The strong breakdown at lower temperatures is connected to an increase in dynamic heterogeneity. On relevant timescales some particles diffuse much faster than the average or than predicted by the SER. The van-Hove self correlation function allows to unambiguously identify slow particles. Their diffusivity is even less than predicted by the SER. The time-span of these particles being slow particles, before their first conversion to be a fast one, is larger than the decay time of the stress correlation. The contribution of the slow particles to the viscosity rises rapidly upon cooling. Not only the diffusion but also the viscosity shows a dynamically heterogeneous scenario. We can define a "slow" viscosity. The SER is recovered as relation between slow diffusivity and slow viscosity.

H. R. Schober and H. L. Peng, arXiv:1604.02045 [cond-mat.dis-nn]

C32 - Tue 15:15-15:35 **Dynamics 1** Großer Saal / Great Hall

Possible crossover in self-diffusion of liquid metals above the melting point?

Lianwen Wang

School of Physical Science and Technology, Lanzhou University, Lanzhou, P. R. China

A possible high temperature kinetic crossover was noticed long ago in liquid Ga (Fig.1) but is neither explained nor confirmed in other metallic elements [1]. Difficulties are from both measurements and understanding of liquid metals. Here, with the microgravity self-diffusion data reported on Sn, In, and Pb (see Fig. 2 for liquid In as an example) [2], we found that a crossover in self-diffusion may do exist at temperatures above the melting point. Interestingly, this scenario seems incorporative with a microscopic liquid model that we developed in recent years [4], see Fig. 3.

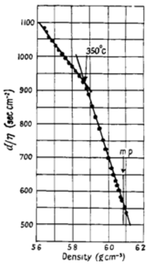

Fig. 1 Density *d* over viscosity η of liquid Ga. [1] m.p. is the melting point

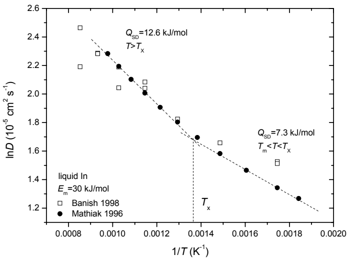

Fig. 2 Self-diffusion coefficient *D* of liquid In plotted against inverse temperature *T*. [2,3]

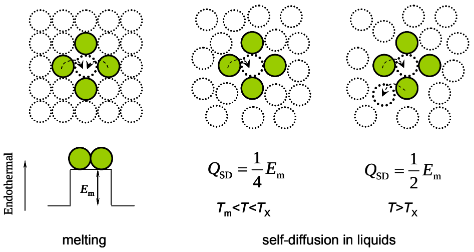

Fig. 3 (left) A liquid nucleus is formed at melting when a vacancy is squashed by two migration atoms, with the migration energy $2E_m$ stored. [4]
(middle) Diffusion in liquids may be superdiffusion of four atoms and the activation energy of self-diffusion Q_{SD} equals to a quarter of E_m.
(right) When two vacancies are available in the liquid nucleus, diffusion in liquids may turn to superdiffusion of two atoms, leading Q_{SD} to half E_m.

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C33 - Tue 15:35-15:55 **Dynamics 1** Großer Saal / Great Hall

Diffusion in liquid Al-rich alloys and the influence of cross-correlations

Elke Sondermann[1], Florian Kargl[1] and Andreas Meyer[1]

[1] *German Aerospace Center (DLR), Institute of Materials Physics in Space, Cologne, Germany*

Diffusion in the melt impacts on the formation and evolution of microstructure during solidification. This makes diffusion coefficients in the liquid an important parameter in the simulation of cast alloys. Al-based alloys are used widely in construction and aeronautic industry due to their high strength and light weight. Moreover there are numerous studies on e.g. the structure of the melts and different thermophysical properties. To reveal fundamental relations, binary mixtures are often studied in place of multicomponent mixtures. Thus Al-based alloys are of both scientific and industrial interest.

Here we present interdiffusion measurements in Al-rich Al-Cu and Al-Ni melts. To obtain accurate data, a combination of X-ray radiography and the shear-cell technique is used. This avoids disturbances during melting and solidification of the samples and provides time-resolved information as well as an improved process control. Contrary to earlier publications the interdiffusion coefficient in Al-Cu is found to decrease slightly with decreasing Al-concentration. In liquid Al-Ni the interdiffusion coefficients is almost constant for concentrations up to 14 at.% Ni. Since diffusion measurement can be hampered by buoyancy, selected samples were additionally measured under microgravity. For these experiments the same combination of X-ray radiography and shear cell was implemented aboard the sounding rocket MAPHEUS.

The interdiffusion data are related to experimental self-diffusion coefficients via the extended Darken equation. The required thermodynamic factor is derived from thermodynamic descriptions by Witusiewicz *et al.* [1] in the case of Al-Cu and by Ansara *et al.* [2] for Al-Ni. It is then possible to determine the influence of cross-correlations on interdiffusion. We show that in both Al-rich alloys interdiffusion is slowed down by cross-correlations.

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I12 - Tue 14:25-14:55 **Structure 1** Kleiner Saal / Small Hall

Temperature-induced structural evolution in metallic melts

X.D. Wang[1], Q. Yu[1], Q.P. Cao[1], D.X. Zhang[2] and J.Z. Jiang[1,3]

[1] *International Center for New-Structured Materials (ICNSM) and Laboratory of New-Structured Materials, School of Materials Science and Engineering, Zhejiang University, Hangzhou 310027, People's Republic of China*

[2] *State Key Laboratory of Modern Optical Instrumentation, Zhejiang University, Hangzhou, 310027, People's Republic of China*

[3] *State Key Laboratory of Silicon Materials, Zhejiang University, Hangzhou, 310027, People's Republic of China*

Email: jiangjz@zju.edu.cn

Here we report that the average atomic distance between centre atom and atoms in the first shell contracts for several metallic liquids upon heating. This anomaly could be caused by the redistribution of polyhedral clusters affected by temperature. In metallic liquids the high-coordinated polyhedra are inclined to evolve into low-coordinated ones with increasing temperature. As the coordination number decreases, the average atomic distance between centre atom and atoms in the first shell of polyhedral clusters is reduced. Temperature dependent atomic structure evolution in liquid gallium has been investigated in a temperature range of 300 - 1375 K by *in situ* high temperature X-ray diffraction and *ab initio* molecular dynamics simulation. A reversible liquid-to-liquid crossover, separated by a temperature zone of about 900 - 1250 K, is discovered. Remarkable agreements between experimental and computational structure factors demonstrate two pronounced liquid gallium states: the one below the temperature zone exhibits low activation energy of self-diffusion coefficient, high temperature dependences of heat capacity and the average string length, being composed of relatively high fractions of large coordination-number polyhedral clusters, and the other above the temperature zone displays high activation energy of self-diffusion coefficient, low temperature dependences of heat capacity and the average string length, being composed of relatively high fractions of small coordination-number polyhedral clusters. This work will further trigger more studies for the liquid-to-liquid crossover in liquids.

C34 - Tue 14:55-15:15 **Structure 1** Kleiner Saal / Small Hall

Cluster-based short-range-order structural model of binary eutectics and relevant metallic glasses

Chuang Dong[1]

[1] *Key Laboratory for Materials Modification by Laser, Ion and Electron Beam (Dalian University of Technology), Ministry of Education, Dalian 116024, China*

Previously we have established the composition formulas for ideal metallic glasses (the glasses that exhibit the highest stabilities and the largest glass forming abilities in given alloy systems), by introducing a new structural tool for the description of short-range-order structural unit, the cluster-plus-glue-atom model. In this model, any structure is dissociated into a 1st-neighbor cluster and a few glue atoms between the clusters, expressed by a cluster formula [cluster](glue atoms)$_{1 \text{ or } 3}$. Such a formulism well explains all binary bulk metallic glasses and some typical multi-component ones. This model also applies in interpreting binary eutectic points, by assuming that a eutectic liquid consist of two subunits issued from relevant eutectic phases, each being expressed by the cluster formula for ideal metallic glasses. A structural unit is then composed of two clusters from relevant eutectic phases plus 2, 4, or 6 glue atoms. Such a dual cluster formulism is well validated in all boron-containing (except those located by the extreme phase diagram ends) and in some commonly-encountered binary eutectics, within accuracies below 1 at.%. The dual cluster formulas are generally formed with two distinctly different cluster types, with special cluster matching rules such as cuboctahedron plus capped trigonal prism and rhombidodecahedron plus octahedral antiprism.

C35 - Tue 15:15-12:35 **Structure 1** Kleiner Saal / Small Hall

On the existence of metastable microheterogeneities in metallic melts

P.Popel[1], U.Dahlborg[2], M.Calvo-Dahlborg[2] , X.X. Dong[3]

[1] *Ural State Pedagogical University, 26 Cosmonavtov ave., Ekaterinburg, 620017, Russia*

[2] *GPM-UMR6634-CNRS, University of Rouen Normandie, Campus Madrillet, BP12, 76801 Saint-Etienne-du-Rouvray, France*

[3] *BCAST, Brunel University London, Uxbridge, Middlesex, UB8 3PH, United Kingdom*

Whether a molten alloy after melting is homogeneous or not on the atomic scale has been an issue for many experimental investigations using a manifold of techniques. In most of these investigations anomalies in measured property/temperature curves found at temperatures well above the liquidus temperature have been interpreted as indications for the existence of a dissolution process of alloy microheterogeneities which are inherited from the precursor solid alloy. In other investigations the observed anomalies have been interpreted as evidence for the existence of a liquid/liquid phase transition while in some investigations no anomalies have been found in the measured property/temperature curves. Most of the anomalies have been found in metal-semimetal alloys while in ordinary alloys they have scarcely been observed. The reason for this disparity of results will be discussed in the paper and new results on the structural and transport properties of Al-Si and Al-Cu alloys will be presented. Furthermore, the influence of the thermal history of the melt on the microstructure of rapidly solidified Al-Si alloys will be discussed.

In particular, new accurate measurements of the viscosity and the density of Al-Cu liquid alloys are reported. This alloy system which has a complicated phase diagram with two eutectic points is suitable in order to investigate the structural phenomena occurring after melting and how the melt transforms to a true solution depending on the phase composition of the solid precursors. A large difference between the measured quantities during heating and subsequent cooling was observed in narrow composition ranges corresponding to the stoichiometric compositions AlCu and Al_2Cu.

From a technological point of view, results obtained by ultrasound velocity and viscosity measurements on alloys suggested to be used as heat carriers in nuclear power plants (Pb-Bi, Pb-Sn and Ga-In alloys of near-eutectic concentrations) will be presented. The results show that microheterogeneities exist in the melts at their planned temperatures of use. Melt homogenization temperatures are much higher and thus in order to avoid temperature instabilities of the heat carriers they have to be heat treated at high temperatures before use.

C36 - Tue 15:35-15:55 **Structure 1** Kleiner Saal / Small Hall

Spherical periodicity as structural homology hidden in crystalline and glassy states

Shuang Zhang[1], Dandan Dong[1], Chuang Dong[1], Peter Häussler[2]

[1] *Key Laboratory for Materials Modification by Laser, Ion and Electron Beam (Dalian University of Technology), Ministry of Education, Dalian 116024, China*

[2] *Chemnitz University of Technology, 09107 Chemnitz, Germany*

Recently it has been reported that fcc-typical periodicity exists in some metallic glasses [1], and abundant experimental and simulated data have suggested tight relationships between glassy and crystalline solids. It seems that both phases share a nontrivial structural homology at short-to-medium range and their hidden local atomic-packing modes are similar. Here we show that spherical periodicity can be seen as the structural homology of crystalline and glassy states.

During structure formation at a very early stage as in liquid and amorphous systems, local spherical periodicity occurs optimizing the total energy along a spherical resonance between the electronic system and the self-organizing static structure. Both, the short- and medium-range can be described globally by the so-called spherical periodic order, with unique characteristic distances between the concentric equidistant spherical shells [2].

Due to spherical periodic order and hence isotropy, we propose a 1-dimensional structural view on crystals and analyze the structural features along the radial distribution functions. Furthermore, the hidden spherical periodic order in crystalline solids will be revealed and the stability mechanism will be well understood. Finally, how the crystalline phases relate to glassy states at short- and medium-range will be explained.

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C37 - Tue 16:25-16:55 **Dynamics 2** Großer Saal / Great Hall

Experimental evidence for two different dynamical regimes in liquid metals

F. Demmel[1], C. Morkel[2]
[1] *ISIS Facility, Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK*
[2] *Physikdepartment, TU München, Garching, Germany*

The solidification process is still one of the great mysteries in condensed matter research. Cooling down a liquid and avoiding crystallization the viscosity will increase dramatically and finally the viscous liquid will arrest into a glass. This process is accompanied by slowing down of the structural relaxation process.

We measured the temperature dependence of the dynamics at the structure factor maximum of liquid Rubidium [1], Lead [2] and more recently Aluminium [3]. This correlation function is a sensitive parameter for changes in the local environment and its Fourier transform was obtained through a coherent quasielastic neutron scattering experiment. The derived amplitude demonstrates a changing slope with increasing temperature and the lineshape of the intermediate scattering function becomes non-exponential towards the melting point [4].

Calculated generalized viscosities and collective inelastic dynamics indicate a change in dynamics in the same temperature range [5]. All these findings point to a change in dynamics of the equilibrium liquid metal state and indicate a crossover from a fluid-like dynamics to a viscous liquid dynamics well above the melting point. The similarity of the changes in the studied metals is evidence for a universal character of this change in dynamics.

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C38 - Tue 16:55-17:15 **Dynamics 2** Großer Saal / Great Hall

Glassy dynamics and dynamical arrest in binary mixtures of hard spheres: asymmetric glasses, mixed states and anomalous diffusion.

L.F. Elizondo Aguilera[1], E. Lázaro Lázaro[2], J. A. Perera Burgos[3], R. Castañeda Priego [4], T. Voigtmann[1] and M. Medina Noyola[2]

[1] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft-und Raumfahrt (DLR), 51170 Köln, Germany*

[2] *Instituto de Física Manuel Sandoval Vallarta, Universidad Autónoma de San Luis Potosí, Alvaro Obregón 64, 78000 San Luis Potosí, SLP, México.*

[3] *Facultad de Ciencias Química y Petrolera, Universidad Autónoma del Carmen, C. 56 No.4 Esq. Avenida Concordia, Col. Benito Juárez, C.P. 24180, Cd. del Carmen, Campeche, México.*

[2] *Departamento de Ingeniería Física, División de Ciencias e Ingenierías, Universidad de Guanajuato, Loma del Bosque 103, 37150 León, México.*

A wide range of materials, with which the human beings have a daily interaction, belong to a special category of physical systems whose fundamental description entails one of the first principles of physics: understanding of dynamically arrested states of matter. Such is the case of many amorphous solids, like gels and glasses, with a high technological impact. One of the main features of such systems is their inability to reach thermodynamic equilibrium within experimental accessible times. Among the variety of model systems to study the essential features of the glassy behavior, the asymmetric binary mixture of hard spheres is a suited model that provides a rich dynamical scenario. In particular, we provide a physics oriented overview of the different dynamically arrested states occurring in a highly asymmetric mixture, combining theoretical calculations and numerical simulations, which are also contrasted against recently reported experimental data of colloidal mixtures. The resulting general scenario for dynamical arrest obtained within these independent, but complementary approaches, is in qualitatively agreement, providing mutual support and suggesting that this is, to our best knowledge, one of the most general descriptions of the glassy behavior in amorphous materials.

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C39 - Tue 17:15-17:35 **Dynamics 2** Großer Saal / Great Hall

Thermo-viscoelastic model for collective dynamics of liquid metals and alloys: Theory and ab initio simulations

T. Bryk[1,2]

[1] *Institute for Condensed Matter Physics, NASU, Lviv 79011, Ukraine*
[2] *Lviv Polytechnic National University, Lviv 79013, Ukraine*

A very specific feature of collective dynamics in liquids is the role of thermal fluctuations, because macroscopic propagation of sound which is the adiabatic one causes different temperatures for the compression and decompression regions in the sound wave. The permanently fluctuating temperature field in liquids causes diffusivity of local temperature (thermal diffusivity), that makes thermal relaxation as the leading relaxation process on macroscopic scales in liquids. On molecular spatial scale non-hydrodynamic propagating processes contribute to thermal fluxes too. These features of temperature fluctuations in liquids must be taken into account in analysis of collective dynamics outside the hydrodynamic regime.

Solutions of a thermo-viscoelastic model [1] for collective dynamics of simple and binary liquids are reported for several pure liquid metals (Li, Na, Tl, Rb)[2,3] and liquid alloys (Li_4Tl and Li_4Pb). I will show analytical solutions of the model in macroscopic limit, as well as numerical solutions from ab initio simulations in a wide range of wavenumbers, which allow classification of relaxing and propagating modes contributing to dynamic structure factors. Additionally I will discuss an issue of possible manifestation of transverse excitations in dynamic structure of liquid metals [2].

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C40 - Tue 17:35-17:55 **Dynamics 2** Großer Saal / Great Hall

Theory of heterogeneous viscoelasticity in glass-forming metallic and nonmetallic liquids

Walter Schirmacher[1,3], Giancarlo Ruocco[2,3] and Valerio Mazzone [2]

[1] *Institut für Physik, Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany*
[2] *Dipartimento di Fisica, Universitá di Roma “La Sapienza”, P’le Aldo Moro 2, I-00185, Roma, Italy*
[3] *Center for Life Nano science@Sapienza, Istituto Italiano di Tecnologia, Viale Regina Elena, 291, I-00161 Roma, Italy,*

We present a theory for the viscoelastic properties of glass-forming liquids near and below the glass transition, which is based on the assumption of a spatially varying viscosity (dynamical heterogeneity) [1,2]. Applying the ideas of the shoving model [3,4] we relate the local activation energies of the viscosity to the local high-frequency elastic constants within Maxwell’s viscoelasticity theory. The model is solved in coherent-potential approximation and gives good account of the mechanical alpha relaxation curves of metallic and non-metallic glass-forming liquids, if Gaussian distributions of activation energies are used. Beta relaxation can be included into the theory by assuming a second Gaussian with much smaller energy scale. The theory may also be used for dielectric relaxation using the coupling scheme of Gemant and DiMarzio.

At low temperatures/high frequencies the theory reduces to earlier theories assuming parallel relaxation processes with distributed relaxation times. This is not so at low frequencies, where many important relaxation processes occur in series. In this regime the theory allows for the calculation of the overall viscosity, which gives the linearly increasing low-frequency branch of the alpha relaxation curves, observed in all materials. At very high frequencies (THz range) the theory goes over to heterogeneous relaxation theory [5,6], which explains the vibrational anomalies (boson peak, etc.) in glasses

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Probing the glassy dynamics in deformed bulk metallic glass by radiotracer diffusion

S.V. Divinski[1], I. Binkowski[1], M. Seleznev[1,2], V. Schmidt[1], H. Rösner[1], and G. Wilde[1]

[1] *Institute of Materials Physics, University of Münster, Germany*

[2] *Togliatty State University, Togliatty, Russia*

Diffusion in bulk metallic glasses was considered to represent a comprehensively investigated and in depth understood phenomenon [1]. However, almost nothing was known about atomic motion in deformed glasses. Recently, we measured a significant enhancement, by orders of magnitude, of tracer diffusion in cold-rolled PdNiP glass [2] and this enhancement was unambiguously attributed to diffusion along shear bands which represent zones of plastic deformation localization in amorphous materials. The activation enthalpy of shear band diffusion occurred to be small, about one third of that for bulk diffusion [3]. Moreover, the diffusion enhancement evolves in a strongly non-monotonous manner during annealing, revealing a cross-over type of relaxation behavior [3]. In this report an overview of recent findings is presented where the radiotracer diffusion is used as a sensitive and specific probe of local changes of the glassy states induced by plastic deformation and subsequent annealing. The diffusion behavior is correlated to local density variations in the shear band as revealed by TEM observations [4] and mesoscopic data on the stick-slip character of the shear band propagation [5].

Financial support of DFG via SPP 1594, the research project WI 1899/27-2 is acknowledged.

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C13 - Tue 16:15-16:45 **Solidification** Kleiner Saal / Small Hall

In-situ X-ray observations of dendritic solidification under the influence of natural and forced convection

Sven Eckert[1], Natalia Shevchenko[1],Olga Roshchupkina[1] and Olga Sokolova[2]

[1] *Helmholtz-Zentrum Dresden-Rossendorf, Department of Magnetohydrodynamics, Dresden, Germany*

[2] *Perm National Research Polytechnic University, Perm, Russia*

The directional solidification of Ga–25wt%In alloys within a Hele-Shaw cell was investigated by means of X-ray radioscopy. This diagnostic technique offers a visual access to opaque metal alloys and enables a basic, intuitional understanding of the complex interplay between melt flow and dendritic growth. Natural convection occurs during a bottom up solidification because lighter solute is rejected at the solid-liquid interface leading to an unstable density stratification [1]. Forced convection was produced by a rotating wheel with two parallel disks containing at their inner sides a set of permanent NdFeB magnets with alternating polarization. The direction of forced melt flow is almost horizontal at the solidification front whereas local flow velocities in the range between 0.1 and 1.0 mm/s were achieved by controlling the rotation speed of the magnetic wheel.

Melt flow induces various effects on the grain morphology primarily caused by the convective transport of solute. Our observations show a facilitation of the growth of primary trunks or lateral branches, suppression of side branching, dendrite remelting and fragmentation. The manifestation of all phenomena depends on the dendrite orientation, local direction and intensity of the flow [2]. The forced flow eliminates the solutal plumes and damps the local fluctuations of solute concentration. It provokes a preferential growth of the secondary arms at the upstream side of the primary dendrite arms, whereas the high solute concentration at the downstream side of the dendrites can inhibit the formation of secondary branches completely. Moreover, the flow changes the inclination angle of the dendrites and the angle between primary trunks and secondary arms.

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C42 - Tue 16:45-17:05 **Solidification** Kleiner Saal / Small Hall

Growth Velocity of Undercooled Fe-B under Different Fluid Flow Conditions

C. Karrasch[1,2], T. Volkmann[1], M.Kolbe[1], and D.M. Herlach[1,2]

[1] *Institute of Materials Physics in Space, German Aerospace Center DLR, 51147 Köln, Germany*

[2] *Institute of Experimental Physics IV, Ruhr-Universität Bochum, 44780 Bochum, Germany*

Fe-B as a metallic glass former has the ability to solidify amorphous. The glass temperature for Fe-17 at.% B is about 800 K [1]. However to form an amorphous Fe-B glassy alloy, a high cooling rate of approximately 1000 K/s (e.g. rapid quenching technique) is necessary, which cannot be achieved by the used electromagnetic levitation method.

The Fe-B system offers to study dendritic (Fe-1, 5, 10 at.% B) and eutectic solidification (Fe-17 at.% B) [2]. Electromagnetic levitation technique (EML) is used for containerless in-situ studies on deeply undercooled Fe-B melts. The transformation of the undercooled liquid into the solid leads to a visible contrast due to the release of latent heat during rapid solidification which is recorded by a high-speed video camera. Concerning terrestrial EML under 1g, the electro-magnetic field necessary for levitation induces strong convective fluid flow (0.3 m/s) inside the melt (electromagnetic stirring). In order to verify the influence of convection on the growth morphology (bent dendrite [3]) and growth velocity, melt fluxing and parabolic flight experiments are carried out under reduced gravity conditions with reduced fluid flow velocity (0.05 m/s).

This work is supported by the German Research Foundation DFG within contract HE1601/18 and by the European Space Agency ESA under contracts 4200020277 and 4200014980.

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C43 - Tue 17:05-17:25 **Solidification** Kleiner Saal / Small Hall

Crystal growth under shear flow on Molecular Dynamic Simulation

H. L. Peng[1,2], Th. Voigtmann[2,3] and D. M. Herlach[1,2])

[1] *Experimentalphysik IV, Ruhr-Universität Bochum, Universitätsstrasse 150, 44780 Bochum, Germany*
[2] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany*
[3] *Department of Physics, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany*

Understanding the mechanism of solidification is one of the central points for exploiting the merits of materials' application in industry. In realistic situation, Convective flow is commonly present in many technical solidification processes, usually induced by external field, e. g. gravity and electromagnetic, or possible internal mass or heat gradient. Although effect of the flow field has been investigated in experiment and theoretical modelling, atomic level understandi ng is still lacking.
In this work, by using non-equilibrium molecular dynamic simulation, the first time, we explore the kinetics of crystal-liquid interface under the influence of shear flow. We find that shear flow can both enhance and suppress the interface velocity, depending on the interplay between diffusion-limited growth and destablization effect of shear flow. This interplay also changes the balance point between stationary crystal and sheared liquid, from where we obtain an additional undercooling due to shear flow, which is not reported before. Our results give new perspective on interface kinetic under shear flow from atomic level, and are also of great importance for theoretical modelling of solidification in non-equilibrium state.

C44 - Tue 17:25-17:45 **Solidification** Kleiner Saal / Small Hall

Crystallization behavior upon rapid cooling of Al-based glass forming liquids in the ternary Al-Ni-Y system

Alexander Kuball*, Moritz Stolpe and Ralf Busch

Saarland University, Chair of Metallic Materials, Campus C6.3 66123 Saarbruecken, Germany
**corresponding author: alexander.kuball@uni-saarland.de*

Aluminum-based metallic glasses are of great interest for lightweight technology because of their unique mechanical properties. Their tensile strength exceeds that of common crystalline Al-alloys by up to five times. Especially the ternary Al-Ni-Y system consists of elements that are suitable for industrial application, but exhibits low glass forming ability (GFA). In order to understand the reason for the limited GFA, it is important to identify the competing crystalline phases and to understand the crystallization mechanism during quenching.

In this study the crystallization behavior of $Al_{86}Ni_8Y_6$ upon rapid cooling from the equilibrium melt was investigated and the competing crystalline phases, which reduce glass formation, were identified. $Al_{86}Ni_8Y_6$ is close to the eutectic point of [$L \Leftrightarrow Al_{23}Ni_6Y_4 + \beta\text{-}Al_3Y + \alpha\text{-}Al$] [1] and corresponds to one of the best glass formers in the ternary Al-Ni-Y systems possessing a critical casting thickness of up to 600 µm [2]. Samples of $Al_{86}Ni_8Y_6$ were produced by suction casting the alloy into copper molds and analyzed by scanning electron microscopy (SEM), X-ray diffraction and calorimetric measurements. Our study reveals that glass formation is strongly restricted by the primary precipitating metastable ternary intermetallic compound $Al_{19}Ni_5Y_3$. The nucleation of $Al_{19}Ni_5Y_3$ appears to be favored by yttrium oxides present in the melt which are spread from the slag during casting and act as heterogeneous nucleation sites. Once the primary metastable phase $Al_{19}Ni_5Y_3$ has formed further crystallization of the Ni and Y depleted melt occurs via the eutectic reaction of $L \Leftrightarrow Al_{19}Ni_5Y_3 + \alpha\text{-}Al$.
Based on these findings, attempts to destabilize the formation of the intermetallic phase $Al_{19}Ni_5Y_3$ by substitution and addition of different elements have been performed. The corresponding results are shown and discussed in terms of their effects on the glass forming ability.

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Quasicrystal nucleation in an intermetallic glass-former

R. Kobold[1,2a], W. Hornfeck[1b], M.Kolbe[1c] and D.M. Herlach[1,2d]

[1] *Institute of Materials Physics in Space, German Aerospace Center DLR, 51147 Köln, Germany*

[2] *Institute of Experimental Physics IV, Ruhr-Universität Bochum, 44780 Bochum, Germany*

The solidification of the intermetallic, congruently melting binary alloy NiZr is studied in a temperature regime of the undercooled melt between the melting and the glass transition temperature. The NiZr system is well known as a good glass former in a broad concentration range of 30 to 70 at.% Zr. We use electrostatic levitation technique to melt and undercool samples with a diameter of 3 - 4 mm under ultra-high-vacuum conditions. Containerless processing is an effective tool for undercooling metallic melts far below their equilibrium melting temperatures since heterogeneous nucleation on container walls is completely avoided. During crystallization the release of the heat of fusion leads to a rapid increase of the temperature at the solid-liquid interface. This makes the solidification front visible by optical observation. The rapid propagation of the solidification front is recorded by using a high-speed camera with a frame rate of 10.000 (1024x744 pixels) frames per second. At high undercoolings the solidification front of NiZr shows features, which make the investigation of its solidification behavior particularly interesting. We observed the growth of a solidification front with 10-fold symmetry at large undercoolings of approximately 300 K and a cooling rate of 35 K/s. A detailed picture of the solidification process was gained, correlating the macroscopic decagon-shaped growth front to the microscopic dendrite growth into a tenfold twinned microstructure and eventually to the crystal structure, whose metrical properties explain the mechanism of twinning, at the atomic scale.

An atomistic twin model is proposed which has the potential to represent a missing link connecting quasicrystals and multiple twinned structures shedding light on intermediate states of order between glasses, crystals and their twins, and quasicrystals.

Funding by Deutsche Forschungsgemeinschaft, under grant HE1601/28 is gratefully acknowledged.

I14 - Wed 09:00-09:30 **Applications/Mater. Devel. 2** Großer Saal / Great Hall

High aspect ratio grating by imprinting Gd-based metallic glass with less viscous workability for neutron phase imaging

Maryam Sageghilaridjani[1], Kosuke Kato[1], Takenao Shinohara[3], Wataru Yashiro[3], Atsushi Momose[3], and Hidemi Kato[3]

[1] *Department of Materials Science, Graduate School of Engineering, Tohoku University, Sendai, Japan*

[2] *Japan Atomic Energy Agency, Tokai, Japan*

[3] *JST, ERATO, Momose Quantum Beam Phase Imaging Project, Sendai, Japan*

[4] *Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai, Japan*

[5] *Institute for Materials Research, Tohoku University, Sendai, Japan*

In this study, we report imprinting Gd-based MG gratings with a high aspect ratio, which have, for a long time, been expected to fabricate for a Talbot-Lau interferometer of the neutron phase imaging [1] as Gd can absorb neutrons efficiently compared with the other elements [2, 3]. The difficulties of imprinting Gd-based MGs arise from the higher viscosity (~$10^{8–10}$ Pa s) and the lower thermal stability compared with the low viscosity of Pd- (~$10^{4–7}$ Pa s [4]), Pt- (~10^4 Pa s [4]), Au- (~10^7 Pa s [5]) and Zr- (~$10^{4–5}$ Pa s [6]) based MGs. Having taken into account the aforementioned, the present paper intends to demonstrate alloy selection and optimization of imprinting condition of Gd-based MGs to prepare high aspect ratio gratings, followed by neutron phase imaging with the produced grating.

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C46 - Wed 09:30-09:50 **Applications/Mater. Devel. 2** Großer Saal / Great Hall

The critical fictive temperature of the bulk metallic glass former PdNiP an the influence of micro-alloying

Niklas Nollmann[1], Isabelle Binkowski[1], Harald Rösner[1], Gerhard Wilde[1]

[1] *University of Münster, Institute of Materials Physics, Münster, Germany*

Deformation of bulk metallic glasses (BMGs) at low temperatures and high stresses lead to an inhomogeneous plastic flow. During plastic deformation, bulk metallic glasses show almost no ductility and fail alongside shear bands where the strain is localized. This limited ductility has led to substantial effort in order to improve the plasticity of BMGs. We investigated PdNiP based glasses which feature a rather high ductility in bending, compared to other bulk metallic glasses. By the use of micro alloying, the mechanical properties of metallic glasses can be influenced. Adding Iron or Cobalt to the PdNiP BMG leads to a huge change in ductility. While analyzing the dependence of the ductility of the present glasses on relaxation treatments, we utilize the fictive temperature concept to investigate the impact of minor alloying on the relative amount of free volume [1]. Also the critical fictive temperature was measured to characterize the ductility of the new BMGs [2]. There for the PdNiP based BMGs were annealed at different temperatures in the undercooled liquid region and bended afterwards in a three point bending test. To adjust several fictive temperatures different concrete cooling rates had been used.

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Processing of bulk metallic glass coatings or parts by cold gas spraying

F. Gärtner, A. List, H. Assadi, T. Klassen

Helmut Schmidt University, Institute of Materials Technology, Hamburg, Germany

Well defined temperatures well below the melting point and low expose times to the ambient atmosphere during cold gas spraying enable processing of bulk metallic glass powder to coatings or parts by retained the amorphous structure. The coating formation in cold spraying is attributed to high kinetic energy impacts of respective particles and related phenomena at the surface under high strain rate deformation. For different BMG types, studies of individual splat morphologies indicated shear banding, viscous flow and mixed modes with very localized, viscous-like behavior. The bonding mechanisms of BMG powders in cold spraying are still controversially discussed. On the one hand, bonding is attributed to localized heat creation and flow; on the other hand it is assumed that the particle temperature should be above Tg allowing for viscous deformation of the undercooled liquid state.

The present study summarizes results on single particle impact phenomena and coating formation for Vit 101, AMZ 4 and FeCoCrMoBC metallic glasses. Under well-tuned impact conditions, dense coatings can be obtained. Possible separation of interfaces and crystallization can be avoided by fast heat extraction from the liquefied interfaces. Possible explanations for needed bonding and undesired crystallization are discussed in terms of the ultra-high deformation velocities and associated fast heating and quenching rates.

I15 - Wed 09:00-09:30 **Structure 2** Kleiner Saal / Small Hall

The structure of liquid metals probed by X-ray absorption spectroscopy

Adriano Filipponi[1], Andrea Di Cicco[2], Fabio Iesari[2] and Angela Trapananti[2]

[1] *Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, I-67100 L'Aquila, Italy*

[2] *CNISM, Scuola di Scienze e Tecnologie, Sezione di Fisica, Camerino I-62032, Macerata, Italy*

X-ray absorption spectroscopy (XAS) provides a unique probe to investigate the average structure around selected atomic species in condensed matter, including metallic liquids at ambient and high pressure, as a function of temperature [1]. XAS measures the photo-absorption cross section for processes promoting core electrons to unoccupied states of increasing energy above the Fermi level. The cross-section oscillations are interpreted in terms of interference signals associated with multiple scattering process of the final state wave-function over the surrounding atoms. This signal is dominated by the distance distribution of the neighboring atoms but also contains detectable contributions associated with atomic triplets involving the photoabsorber atom. The problem of implementing an efficient data analysis strategy will be addressed with emphasis on the role of Reverse Monte Carlo and related techniques. Examples of model (pair and triplet) signals will be illustrated and recent applications (including [2]) will be reviewed.
The absorption spectra display a detectable discontinuity at first order phase transition. Melting at T_m can be easily detected since the changes in the absorption cross-section can be of the order of a few % at selected energies in the edge region. This phase sensitivity can be exploited, using temperature scans, to monitor the occurrence of undercooling in micrometric powder samples dispersed in an inert matrix and to prepare the sample in the desired state prior to collecting high quality spectra at a fixed temperature. In is also possible to monitor the crystalline nucleation process, obtaining an *in-situ* measurement of the nucleation rate in a (deep undercooling) temperature range [2] that is often not accessible by repeated recalescence experiments on mm size samples [3].
The possibility to perform a temperature dependent sample structural characterization sensitive to local coordination geometries and simultaneously to obtain information on the nucleation rate, makes this spectroscopy an ideal probe to address the fundamental issue on how these two aspects are related.

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C48 - Wed 09:30-09:50 **Structure 2** Kleiner Saal / Small Hall

Short range order in liquid metals

Guy Makov[1], Martin Mayo[2], Yaron Greenberg and Eyal Yahel[3]

[1] *Dept. of Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel*

[2] *Dept. of Physics, Cavendish Laboratory, Cambridge University, Cambridge, UK*

[3] *Dept. of Physics, NRCN, Beer-Sheva, Israel*

Evolution of short range structure in liquid metals of elements of groups IV and V is analysed within the quasi-crystalline model of liquid structure. Many of these systems exhibit anomalous thermophysical properties such as decreasing melting curves and sound velocity maxima. It has been suggested that these anomalies reflect an underlying liquid-liquid phase transition in the supercooled regime which is not directly accessible and which leads to a change in the liquid structure. The quasi-crystalline model allows quantitative characterization of the short range order in liquids by identifying a reference lattice.

It is found that the liquid pnictides are characterized by a short range order which reflects a Peierls distorted structure. This distortion decreases as the elements progress down the periodic table column V and explains the large change in coordination number from 3 to 8. Surprisingly the distortion is found to increase with temperature and correlates with the appearance of a sound velocity maximum with respect to temperature. Column IV elements exhibit a very different short range order which is found to remain constant with temperature, possibly indicating that the origin of the sound velocity anomaly in these systems is not related to any structural rearrangement of the liquid unlike in the pnictides.

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X-ray absorption spectroscopy: new insights on the three-dimensional liquid structure

F. Iesari[1], A. Trapananti[2], and A. Di Cicco[1]

[1] *School of Science and Technology, Physics Division, University of Camerino, Camerino (MC), Italy*

[2] *CNR-Istituto Officina dei Materiali, c/o Department of Physics, University of Perugia, Perugia, Italy*

The local structure of liquid metals and binary metal alloys may differ significantly from that of the corresponding crystalline systems, possibly containing icosahedral local ordering, forbidden in periodic structures. The application of Reverse Monte Carlo (RMC) for combined refinements of XAS and diffraction data allowed us to obtain in selected liquid metals an ensemble of realistic three-dimensional models of the liquid structure, compared also with the results of molecular dynamics simulations.

In previous works, signatures of short-range fivefold ordering have been investigated by x-ray absorption spectroscopy (XAS) experiments in elemental liquids including for example, liquid and undercooled copper and nickel for which estimates of the fraction of nearly-icosahedral configurations were obtained [1,2].

We have recently improved our RMC-XAS method [3], extending its application to multi-atomic substances, performing also several XAS experiments in liquid metals at high temperatures. In this work, we report RMC refinements of accurate XAS data of several molten elemental metals and binary alloys showing that an accurate reconstruction of the three-dimensional local structure is feasible. The results of our work include estimates of the fraction of atoms having local icosahedral symmetry, in elemental metals like Cu, Ni, Cd. Moreover, a detailed analysis of local coordination and geometry in molten alloys such as Cu-Sn and In-Sn is presented.

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P4 - Wed 10:40-11:20 **Plenary** Großer Saal / Great Hall

Early Plasticity in Metallic Glasses

C.A. Volkert[1,*], D. Tönnies[1], K. Samwer[2] and R. Maass[3]

[1] Georg-August University, Institute of Materials Physics, Göttingen, Germany

[2] Georg-August University, First Physics Institute, Göttingen, Germany

[3] University of Illinois, Department of Materials Science and Engineering, Urbana-Champain, USA

Plastic deformation of metallic glasses at technically relevant temperatures is mediated by the operation of localized shear bands. Understanding the emergence of shear bands from smaller deformation entities, such as shear transformation zones, has become a topic of intense research in the past years, with the goal of ultimately mediating the brittle behavior the shear bands cause. However, since shear transformation zones as well as shear bands may operate at time and length scales that are barely accessible experimentally, systematic studies must often be performed to gain indirect insight.

We present several small-scale mechanical studies on metallic glasses which have been designed to test our understanding of the emergence of shear bands [1-3]. We vary specimen size [1,2], strain rate [2], acquisition rate, and stress state in microcompresson or spherical nanoindentation studies, and by analyzing the mechanical response and the distributions of strain bursts, infer certain limits on the inherent behavior of emerging shear bands and the cooperativity of the shear transformation zones.

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I16 - Wed 11:25-11:55 **Properties** Großer Saal / Great Hall

Structure-property relationship in rapidly quenched alloys correlated with melt precursor processing

P. Svec[1], I. Janotova[1], J. Zigo[1], I. Matko[1], D. Janickovic[1], V. Sidorov[2], I. Skorvanek[3], P Svec Sr. [1]

[1] Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia
[2] Ural State Pedagogical University, Ekaterinburg, Russia
[3] Institute of Experimental Physics, Slovak Academy of Sciences, Kosice, Slovakia

Recently attention in rapidly quenched amorphous and nanocrystalline materials is focused on soft magnetic systems with high saturation magnetization while preserving low coercivity. Diverse systems based on Fe-B with additions of Co, Cu, Si, C, P and other elements were developed and tested. Successful compositional and processing design has lead to a new class of so-called NANOMET alloys [1], [2] which fulfill such requirements. Selected results will be presented on these alloys together with results obtained on a still relatively new and promising system based on Fe-Sn-B, where the effect due to the presence of Nb or Zr in NANOPERM and HITPERM alloys, namely nanograin size control, is obtained by addition of Sn [3]. The effect of compositional tuning and pre-preparation processing will be investigated. In addition, enhanced functionality will be presented in systems of rapidly quenched alloys with enhanced thickness achieved by layering during preparation or by combination of layers with different compositions. The structure of the individual layers and of the interfaces between the layers as well as properties of mono-, bi and trilayered metallic glasses prepared from soft magnetic alloys will be discussed. Added value of such materials will be shown on specific cases of applications.

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C50 - Wed 11:55-12:15 **Properties** Großer Saal / Great Hall

Improved mechanical behavior of Ni-free Ti-based bulk metallic glasses by minor In/Ga additions

Mariana Calin[1], Supriya Bera[1], Ramasamy Parthiban[1], Mihai Stoica[1], Jürgen Eckert[2,3]

[1] IFW Dresden, Institute for Complex Materials, Dresden, Germany
[2] Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Leoben, Austria
[3] Montanuniversität Leoben, Department Materials Physics, Leoben, Austria

Materials can be tailored in structure and properties through proper alloying additions, which have been widely accepted as a means of improving mechanical properties. Bulk metallic glasses (BMGs) generally lack ductility and fail in a macroscopically brittle manner in unconstrained loading geometries. However, some BMGs are able to sustain significant plastic strain in compression at room temperature. In order to understand the different mechanical behavior of BMGs, extensive efforts are devoted to experimental and computational studies, mostly focusing on structural considerations and deformation mechanisms.

In the present work, $Ti_{40}Zr_{10}Cu_{36}Pd_{14}$ alloy was selected as a model glass to further improve its plasticity due to the change of internal structure upon partially substituting copper atoms by different contents of indium and gallium atoms [1]. $Ti_{40}Zr_{10}Cu_{36-x}Pd_{14}In/Ga_x$ (x < 8 at.%) bulk glassy alloys were produced by copper mold casting. The glass-forming ability (GFA) and thermal stability were investigated by differential scanning calorimetry. The GFA was evaluated by considering different parameters: the reduced glass transition temperature $T_{rg} = T_g/T_l$, the supercooled liquid region $\Delta T_x = T_x - T_g$ and the γ parameter defined as $T_x/(T_g + T_l)$. Structural characterization was performed by XRD and electron microscopy (TEM).

Room temperature compression tests reveal that the plastic strain of Ti-Zr-Cu-Pd BMGs can be significantly enhanced up to 8.3% via 4at.% indium addition, without compromising the high fracture strengths. In case of Ga-containing alloys, the $Ti_{40}Zr_{10}Cu_{36}Pd_{14}Ga_2$ BMG shows the most promising properties, with compressive global strain and maximum compressive strength of 4.5% and 1930 MPa, respectively. The Young's modulus of Ga-containing BMGs are 40-48% lower than that of the corresponding crystalline counterparts.

Financial support through the European Commission (FP7 VitriMetTech ITN – 607080) is gratefully acknowledged.

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Thermodynamic and dynamic studies of phosphorus containing bulk glass forming liquids

Oliver Gross*, Benedikt Bochtler, Moritz Stolpe, Ralf Busch, and Isabella Gallino

Saarland University, Chair of Metallic Materials, Campus C6.3 66123 Saarbruecken, Germany

* *corresponding author: oliver.gross@uni-saarland.de*

Phosphorous containing bulk metallic glass forming alloys (BMGs) are among the best metallic glass formers known to date [1,2]. The newly developed Ni-P-based BMGs are no exception (critical casting thickness ≥1 cm) and provide an attractive alternative to Zr-based BMGs for industrial applications due to their relatively inexpensive constituents, good processability and exceptional corrosion resistance [1]. Pt-P-based BMGs feature a large supercooled liquid region and an attractive color, which makes them highly promising for jewelry applications [3].

In this comparative study, the thermophysical properties of different phosphorus containing alloys (Ni-P, Pt-P, Pd-P) are investigated using differential-scanning calorimetry and thermal mechanical analysis for the determination of the specific heat capacity and equilibrium viscosity, respectively. The specific heat capacity data was used to calculate the enthalpy and entropy difference between the liquid and the crystalline mixture. Interestingly, the alloys differ considerably in their thermodynamic properties, whereas they show a similar behavior in the temperature dependence of their equilibrium viscosity. Hence, the data is analyzed in the framework of the Adam-Gibbs theory which aims to connect thermodynamics and dynamics. Moreover, the isothermal time-temperature-transformation (TTT) diagram of the alloys is presented. In connection with the viscosity data, these measurements are a useful tool for determining process parameters for thermoplastic forming.

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I17 - Wed 11:25-11:55 **Excit. in Liquids and Glasses** Kleiner Saal / Small Hall

Structure of liquid metals disentangled by inelastic X-ray scattering

Masanori Inui

Graduate School of integrated Arts and Sciences, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-8521, Japan

We present the results of inelastic x-ray scattering (IXS) for liquid Bi and liquid As2Se3. IXS measurements were conducted at BL35XU of SPring-8 in Japan. A highly monochromatized x-ray beam (21.747 keV) was incident on the sample, and scattered x-rays were collected by twelve analyzer crystals, with the energy resolution of approximately 1.5 meV. The *Q* resolution was set 0.4 nm^{-1} at $Q < 12$ nm^{-1}.

As crystalline Bi takes A7 structure, the structure of liquid Bi has been debated in relationship with the Peierls distortion. A recent ab initio molecular dynamics simulation for liquid Bi [1] predicted a flat-topped profile of the acoustic dispersion curve that is inconsistent with the results of inelastic neutron scattering. Our IXS results confirm the prediction and we found that linear chain model with the Peierls distortion can explain the profile [2]. The result suggests that the anomalous dispersion curve in liquid Bi arises from local anisotropy accompanying the Peierls distortion. Although by analyzing the static structure factor of liquid Bi carefully, it was reported that the local structure is intimately related to Peierls distortion [3], ambiguities of predicting three dimensional configurations from a one dimensional radial distribution function is inevitable. The atomic dynamics could provide important information on the atomic configuration in the liquid.

The rigidity theory has made great contribution to understandings of covalent glasses [4]. Recently we have studied static and dynamic structures in liquid As_2Se_3 up to 1673 K at high pressures to suppress the evaporation. The average coordination number *N* near the melting point is slightly larger than the ideal value of 2.4 that is predicted by three-fold and two fold coordinated As and Se, respectively. *N* decreases to less than 2.4 with increasing temperature [5]. We carefully investigated the Q dependence of the excitation energy of the acoustic mode and found that the energy discretely jump at approximately 3 nm^{-1} at N > 2.3. At higher temperature where N is less than 2.3, however, the energy exhibits moderate Q dependence. The results may indicate that liquid As_2Se_3 undergoes a temperature-driven stiffness transition as the composition-driven one observed in glassy As_xSe_{1-x}.

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C52 - Wed 11:55-12:15 **Excit. in Liquids and Glasses** Kleiner Saal / Small Hall

Phonon excitations in $Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ bulk metallic glass

S. Hosokawa[1], M. Inui[2], Y. Kajihara[2], A. Chiba[3], T. Ichitsubo[4], H. Kato[5], S. Tsutsui[6], and A. Q. R. Baron[7]

[1] *Kumamoto University, Department of Physics, Kumamoto, Japan*
[2] *Hiroshima University, Graduate School of Integrated Arts and Sciences, Higashi-Hiroshima, Japan*
[3] *Keio University, Department of Physics, Yokohama, Japan*
[4] *Kyoto University, Department of Materials Science and Engineering, Kyoto, Japan*
[5] *Tohoku University, Institute for Materials Research, Sendai, Japan*
[6] *SPring-8, Japan Synchrotron Radiation Research Institute, Hyogo, Japan*
[7] *RIKEN SPring-8 Center, Materials Dynamics Laboratory, Hyogo, Japan*

$Pd_{42.5}Ni_{7.5}Cu_{30}P_{20}$ is well-known to form the most excellent bulk metallic glass (BMG) with the critical cooling rate of 0.067 K/s [1]. To investigate the atomic dynamics of this BMG, we have carried out inelastic x-ray scattering (IXS) experiment using a high-energy-resolution IXS spectrometer [2] installed at the beamline BL35XU of the SPring-8. An IXS experiment was already performed by Ichitsubo et al. [3], where only the longitudinal acoustic (LA) excitations were discussed, and an elastic heterogeneity was observed as a fast sound in this BMG. In our new IXS results, the largest excitations are the LA modes at about 6-11 meV, which show the clear dispersion relation with Q, and the position of the excitation energies coincides with the previous data [3]. There are other excitations burying the hollows between the quasielatic peaks and the LA excitations at about 5 meV, which would be the transverse acoustic (TA) modes showing a slight dispersion relation with *Q*. Besides the LA and TA modes, an unknown optic-like mode at about 12 meV can be realized as a long tail at energies higher than that of the LA mode. This mode looks unchanged in excitation energy with increasing *Q*, and hidden beneath the strong LA modes. Detailed analysis of the measured IXS spectra using current-current correlation functions is now in progress.

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Transverse excitations in simple hard-sphere liquid Hg

S. Hosokawa[1], M. Inui[2], Y. Kajihara[2], A. Chiba[3], S. Tsutsui[4], and A. Q. R. Baron[5]

[1] *Kumamoto University, Department of Physics, Kumamoto, Japan*
[2] *Hiroshima University, Graduate School of Integrated Arts and Sciences, Higashi-Hiroshima, Japan*
[3] *Keio University, Department of Physics, Yokohama, Japan*
[4] *SPring-8, Japan Synchrotron Radiation Research Institute, Hyogo, Japan*
[5] *RIKEN SPring-8 Center, Materials Dynamics Laboratory, Hyogo, Japan*

Transverse acoustic (TA) phonon modes usually cannot be detected in liquids by ultrasonic or optical measurement because the shear force in the long spatial range is very weak. When the vibration wavelength in a liquid approaches the atomic nearest neighbor distance, however, there may be a solid-like cage effect on the nanometer scale that acts as a restoring force for TA modes. In the previous inelastic x-ray scattering (IXS) experiment, $S(Q,\omega)$ spectra of liquid Ga [1], Sn [2], Fe [3], and Cu [3] were measured at BL35XU of SPring-8 [4] near the melting points, and low-energy excitations were observed between the quasielastic line and the longitudinal acoustic (LA) mode. From the detailed analysis for the IXS data, the lifetime of sub-ps and the propagating length of sub-nm were estimated from the TA phonon modes in each liquid metal measured, which may correspond to the lifetime and size of cages formed instantaneously in liquid metals. Short-lived covalent bondings are contributed in liquid Ga and Sn, whereas icosahedral clusters do exist in liquid Fe and Cu. In this paper, we examine the existence of the TA mode in one of the simplest liquid metals, liquid Hg, by measuring IXS with a good statistical quality at room temperature. The LA modes are clearly seen in the measured IXS spectra at about 10-12 meV as shoulders, which are in good agreement with the previous IXS data [5]. A very interesting feature in the spectra is that in the low energy region between the LA modes and the quasielestic peak at about 5 meV, the gaps are buried or even have shoulders, which would not be reproduced by a single damped harmonic oscillator (DHO) model. Further data analysis using such as multiple DHO fittings and current-current correlation functions are now in progress.

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I18 - Wed 13:50-14:20 **Glass Transition 2** Großer Saal / Great Hall

Two glass transitions in liquid metals. Molecular modelling.

Genri E. Norman, Vasily V. Pisarev

Joint Institute for High Temperatures of RAS, Moscow, Russia

Glass transition in metals is investigated by the molecular dynamics (MD) method on the example of liquid aluminum. The transition temperature is found using several criteria based melt microstructure, diffusivity and specific heat. The dependence of glass transition temperature on cooling rate is found for each of these criteria. Two characteristic temperature ranges are found. Changes in microstructure and the self-diffusion activation energy occur in the range 820-880 K, while heat capacity changes are observed in the range 500-600 K [1]. The dependence of the "calorimetric" glass transition on cooling rate follows Bartenev's formula, while "structural" glass transition behaves according to the Vogel-Fulcher-Tammann relaxation law, which has also been found in polymer glasses [2].

Viscosity calculations are performed to find out the temperature which corresponds to the solidification of the melt [3]. Viscosity is calculated using the Green-Kubo relation which is based on the integration of shear stress autocorrelation function (SACF). The power-law decay ($t^{-\alpha}$) is found for the SACF tails, and the exponent α dependence on temperature is obtained. $\alpha=3/2$ at high temperatures and diminishes at cooling. In the range 800-900 K, α starts to deviate from the high-temperature limit, and the value $\alpha=1$ is crossed in the range 550-600 K. Therefore, the integral of the SACF diverges below 550 K, and the viscosity becomes infinite. Thus, both glass transition intervals are explained by the changes of a single parameter — SACF tail exponent.

The work is supported by the Russian Science Foundation (grant no. 14-50-00124).

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C54 - Wed 14:20-14:40 **Glass Transition 2** Großer Saal / Great Hall

Relaxation dynamics of metallic systems in the liquid/glass transition region.

Chaoren Liu[1], Eloi Pineda[1], Daniel Crespo[1]

[1] *Universitat Politècnica de Catalunya – BarcelonaTech, Department of Physics, Castelldefels, Spain*

The liquid/glass transition is controlled by structural dynamics with characteristic times changing from 10^{-2} to 10^{4} s within the $0.9T_g$-$1.1T_g$ temperature range. In metallic systems this slow dynamics is usually probed by means of calorimetric, mechanical spectroscopy and quasi-static stress relaxation measurements[1][2]. However, the accessible time window is usually restricted to 10^{-1}-10^{2} s due to limitations of the experimental techniques, instability against crystallization, physical aging or sample geometry restrictions in the case of low-GFA alloys. For instance, the characterization of the main α-relaxation in the sub-T_g region is usually estimated indirectly, assuming the response of the material maintains similarity along the whole temperature region and applying the time-temperature-superposition principle[3]. This similarity, however, is not fulfilled if aging, secondary relaxations or nonlinear response are present in the system and very few studies have been devoted to fully characterize the extremely slow α-relaxation in the sub-T_g region.

In this work we present experimental characterization and modeling of the relaxation spectrum of Mg-Cu-Y, Cu-Zr-Al, Pd-based and Fe-based metallic glass-forming alloys in the $0.9T_g$-$1.1T_g$ range. After subtracting the secondary relaxation contribution, minimizing the effect of aging and normalizing by T_g, an interesting result is that the sub-T_g α-relaxation shows common temperature and frequency dependences, while the liquid state above T_g shows different temperature behaviors as expected by the different liquid fragilities of the studied alloys. The similarity of the dynamics below T_g indicates that the nature of the microscopic mechanisms involved in the full macroscopic relaxation is similar in all metallic systems once arrested in an isoconfigurational state. The different degrees of inhomogeneity frozen in in the glassy structure, which are also known to be related to the different liquid fragilities, affect the intensity of secondary relaxations and other features of the relaxation spectrum but they seem to have little influence on the main relaxation process.

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Gauge Theory of Glass Transition: description of glass transition as a critical phenomenon

Mikhail Vasin[1, 2]

[1] *Physical-Technical Institute, Ural Branch of Russian Academy of Sciences, Izhevsk, Russia*

[2] *Institute for High Pressure Physics of Russian Academy of Sciences, Moscow, Russia*

The Gauge Theory of Glass Transition (GTGT) was recently developed [1-2]. The old idea of the gauge field description of glass transition underlies in this theory [3-5]. In GTGT is assumed that there are two key conditions for the implementation of glass transition. First of all, we believe, that the glass transition has common nature with the second order phase transition, which is spontaneous breaking continuous symmetry and starting an ordering process in the system structure. On the other hand, in contrast to the phase transition this ordering process stops because of frustration, which arises in this process. The presence of frustration is the second key condition for glass transition. The frustration gives rise to fixation of vortexes (disclinations in undercooled liquids [6, 7]) in the structure, which prevents the growth of the ordered regions. The nonequilibrium dynamics of the slowing vortex system, which takes into account the interaction of these vortexes with order parameter fluctuations, can be described in terms of the gauge field theory. This allows to get the theory analogous to the dynamical theory of phase transition [1-2], and gives the self-consistent description of glass transition, describing broad spectrum of its properties.

This work was supported by the Russian Foundation for Basic Research (Grant Nos. 13-02-00359)

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I19 - Wed 13:50-14:20 **Applications/Mater. Devel. 3** Kleiner Saal / Small Hall

Influence of nanosized admixtures on microstructure, thermophysical and mechanical properties of lead-free solder alloys

Yu. Plevachuk[1], V. Sklyarchuk[1], P. Švec[2], and A. Yakymovych[3]

[1] *Ivan Franko National University of Lviv, Department of Metal Physics, Lviv, Ukraine*

[2] *Slovak Academy of Sciences, Institute of Physics, Bratislava, Slovakia*

[3] *University of Vienna, Department of Inorganic Chemistry / Materials Chemistry, Wien, Austria*

The constant development towards miniaturization and purposeful density enhancement needs much smaller solder joints and fine-pitch interconnections for microelectronic packaging in electronic devices. The miniaturization of these electronic devices demands better solder-joint reliability, but much research is based on bulk solder properties only. However, to meet the needs of miniaturization in the electronics industry, nanoparticle reinforcements are often added to provide the mechanical integrity needed with lead-free solders, while also keeping the solder as environmentally friendly. Hence, nanoscale solder alloys have been identified as one potential route for yielding higher microstructural stability and better mechanical and thermophysical properties.

The alloys based on the Sn-Ag-Cu (SAC) and Sn-Zn systems are considered as the most promising types of lead free solder due to their excellent physical and mechanical properties. We report the impact of two type of nanosized admixtures, namely, reactive (Co, Cu, Ni) and nonreactive (ceramic powders TiO_2, ZrO_2, SiO_2, Al_2O_3) on thermophysical and mechanical properties of the basic alloys in the liquid and solid states.

Advantages and disadvantages of the composite solders SAC305, SAC387 and Sn-Zn with nanoparticles, which were prepared in the traditional bulk form, in the form of metallic ribbons (by the planar casting method), with and without flux, are analyzed. It was revealed that both metallic and ceramic nanosized admixtures in the Sn-Ag-Cu alloys results in improvement of mechanical properties (shear strength) and hardness of the solder-substrate joints. The non-reacting nanoparticles have supressing effects on the intermetallic compounds growth in the solder joint by the adsorbtion effect.

The melting characteristics of the alloys were investigated by DSC complemented by electrical resistivity and thermoelectric power measurements. The interfacial microstructures and mechanical properties of nano-composite solders reflowed between two Cu surface joints were investigated with respect to the type and amount of added nanoparticles. Scanning electron microscopy with EDS and X-ray diffraction were used to characterize the interfacial structure and morphology and to determine the chemical composition of the intermetallic compounds.

C56 - Wed 14:20-14:40 **Applications/Mater. Devel. 3** Kleiner Saal / Small Hall

Trace elements' segregation on the heterogeneous nucleation of Al alloys: A first-principles study

C. M. Fang, B. Jiang, and Z. Fan

Brunel Centre for Advanced Solidification Technology (BAST), Brunel University London, Uxbridge, Middlesex, UB8 3PH, UK

Grain refiners, such as TiB_2 have been widely used in solidification of aluminum alloys. However, only small amount of the grain-refiner particles of large sizes are effective [1,2]. Meanwhile, addition of small/trace amounts of transitional metals, such as Ti, Zr, Fe, has strong impacts on efficiency of the grain refiners [3-5]. Experiments revealed formation of a thin layer of the trace elements on the substrates [3-5]. That modifies the lattice matches between the liquids and substrate with segregated trace elements, and consequently changes the efficiency of the grain refiners, according to the epitaxial growth model [6,7]. Based on the experimental observations, different interface models are built and investigated by parameter-free first-principles approaches. Stability, local structures and chemical bonding are analyzed. Bader's charge model is also employed to investigate charges at and charge transfer between the related atoms/ions. Furthermore, first-principles molecular dynamics simulations are performed for chosen systems to understand the ordering and structures of liquid metal near the substrates at a temperature just above its melting. The simulated results are compared with the available experimental observations. The obtained information is not only useful to get insight the role of the segregated trace elements in the heterogeneous nucleation, but also helpful to understand the whole solidification processes, and further to design of new grain refiners and new alloy processes in order to control the microstructures of aluminum alloys of desired properties.

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Melt viscosity of the $Fe_{72.5}Cu_1Nb_2Mo_{1.5}Si_{14}B_9$ soft magnetic nanocrystalline alloy

Tsepelev V.S.[1], Starodubtsev Yu.N.[1,2], Konashkov V.V[1].

[1] *Boris Yeltzin Ural Federal University, Ekaterinburg, Russia*

[2] *Gammamet Research and Production Enterprise, Ekaterinburg, Russia*

The production of soft magnetic nanocrystalline materials implies producing alloys of a certain chemical composition, fast melt quenching with the amorphous structure being formed in the ribbon 25 μm thick and heat treatment of the ribbon to gain the magnetic properties required. It is important to determine the optimal temperature of melt heating. As such, the critical temperature of the multicomponent melt T_k [1] can be selected. With the temperature higher than the critical one, the melt properties irreversibly change, which manifests itself in the temperature hysteresis of kinematic viscosity, surface tension and other melt's characteristics.

The paper presents the results of investigation in the melt of the $Fe_{72.5}Cu_1Nb_2Mo_{1.5}Si_{14}B_9$ nanocrystalline alloy. Kinematic viscosity of melts is measured by a torsional vibration method based on measuring the vibration damping factor [2]. The kinematic viscosity has been analyzed using the Arrhenius-type equation, the Stocks-Einstein equation and the Bachinski free volume model.

The temperature curves of the melt viscosity in processes of heating and cooling differ greatly. In heating, the curve is marked off by two linear sections with the E_a = 18 kJ/mol viscous flow activation energy for the initial heated section and 61 kJ/mol for the temperature exceeding 1490 °C. In cooling, the curve is all linear over the entire temperature range studied, from 1250 up to 1650 °C, and the corresponding viscous flow activation energy in the process of cooling is 43 kJ/mol.

As in the process of cooling, the melt viscosity does not regain its initial values, the melt may be thought to have experienced irreversible changes. These changes may be attributed to the breaking of interatomic bonds influencing the melt short range order [1]. The temperature of 1490 °C may be regarded as the critical point T_k of the $Fe_{72.5}Cu_1Nb_2Mo_{1.5}Si_{14}B_9$ alloy, above which the viscous melt flow changes in accordance with the Arrhenius law with another numerical value of the viscous flow activation energy E_a.

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I20 - Thu 09:00-09:30 **Structure and Dynamics 3** Großer Saal / Great Hall

Ab initio molecular-dynamics study of structural and dynamic properties of disordered materials

Fuyuki Shimojo, Emina Ryuo, Hiroyuki Kumazoe, Masaaki Misawa, and Akihide Koura

Department of Physics, Kumamoto University, Kumamoto 860-8555, Japan

Large-scale molecular-dynamics (MD) simulation schemes on massively parallel computers, in which interatomic forces are computed quantum mechanically in the framework of the density functional theory (DFT), have been implemented and applied to high-temperature and/or high-pressure phenomena with chemical reactions.

It is known that Al particles produce hydrogen in water, which could provide a renewable energy cycle. However, its low reaction rate and poor yield hamper practical application. We have carried out large DFT-based MD simulations involving up to 16,611 atoms, and shown that orders-of-magnitude faster reactions with higher yields can be achieved by alloying Al particles with Li [1]. It was found that an abundance of neighboring Lewis acid-base pairs allows water-dissociation and hydrogen-production with very small activation energies. Negative-charge pathways across Al atoms that collectively act as a superanion facilitate these reactions, and a surprising autocatalytic behavior of bridging Li-O-Al products was seen. Furthermore, a corrosive basic solution that inhibits the formation of a reaction-stopping oxide layer on the particle surface is produced by the dissolution of Li atoms into water, thereby increasing the yield. Recent experimental findings are successfully explained by these atomistic mechanisms. Also they predict the scalability of this hydrogen-on-demand technology at industrial scales.

Silica (SiO_2) is of interest in many fields because it is one of the most abundant components of Earth, and has various polymorphs. It is well known that, when silica glass, which consists of SiO_4 units under ambient conditions, is compressed above 10 GPa, a permanent densification occurs, i.e. after decompression, silica glass maintains a densified state even under ambient conditions [2]. The density of fully densified glass is about 20 % larger than that of ordinary glass. Our DFT-based MD simulations have clarified the microscopic mechanism of the permanent densification in relation to short- and medium-range structural changes.

Stishovite, a high-pressure crystalline polymorph of silica, is one of the hardest oxide materials. Recently, a nano-structural form of stishovite is synthesized, which exhibits high fracture toughness while retaining high hardness [3]. We have revealed from DFT-based MD simulations that toughening is induced by rapid crystal-amorphous transformation under tension.

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C58 - Thu 09:30-09:50 **Structure and Dynamics 3** Großer Saal / Great Hall

Dynamic properties of liquid Ni revisited.

David J. González[1], and Luis E. González[1]

[1] *Universidad de Valladolid, Dept. Fisica Teorica, Valladolid, Spain*

Liquid Ni has been studied in past years using a variety of methods, including classical simulations with different types of interatomic potentials, ab initio simulations, and experimental techniques including inelastic neutron [1] and x-ray [2] scattering. Although some contradictory results, as the behaviour of the dynamic structure factor for $q < 1$ Å^{-1}, have already been sorted out, [2] still some discrepancies persist for larger q values among the different studies. We have performed new ab initio calculations and show in this contribution how it is possible to reconcile the differing results. This comes down to the previously unnoticed existence of two propagating modes, whose relation with transverse currents is further analyzed here. Moreover it is shown that the behavior of the transverse current spectral functions shows features which had only been observed previously for liquids under high pressure. [3]

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C59 - Thu 09:50-10:10 **Structure and Dynamics 3** Großer Saal / Great Hall

Free-volume dependent atomic dynamics in beta relaxation pronounced La-based metallic glasses

X. D. Wang[1], B. Ruta[2], L. H. Xiong[1], D. W. Zhang[1], Y. Chushkin[2], H. W. Sheng[3], H. B. Lou[1], Q. P. Cao[1], and J. Z. Jiang[1]

[1] *International Center for New-Structured Materials (ICNSM), Laboratory of New-Structured Materials, State Key Laboratory of Silicon Materials, and School of Materials Science and Engineering, Zhejiang University, Hangzhou, 310027, People's Republic of China*

[2] *ESRF - The European Synchrotron, CS 40220, 38043 Grenoble Cedex 9, France*

[3] *School of Physics, Astronomy and Computational Sciences, George Mason University, Fairfax, VA22030, USA*

The atomic dynamics and its structure dependence in a glass are fundamental issues but still little understood for decades. Through the state-of-the-art x-ray photo correlation spectroscopy (XPCS) and extended x-ray absorption fine structure (XAFS) techniques combining with reverse Monte Carlo (RMC) constrained with classic molecular dynamics simulations, we reveal that the annihilation of excess free volume in a β-relaxation pronounced La-Al-Ni metallic glass slows down the atomic motion by one order of magnitude upon annealing, which is mainly caused by the change of subatomic cavities and enhanced network structure resulting from the presence of Ni atoms, showing significant difference from a β-relaxation unpronounced La-Al-Cu glass. Our findings provide insights into the dynamics and atomic structure of La-based metallic glasses and will be helpful in understanding the microscopic dynamic behavior of metallic glasses in general.

*Corresponding author: wangxd@zju.edu.cn

C60 - Thu 10:10-10:30 **Structure and Dynamics 3** Großer Saal / Great Hall

Correlation between Dynamic Slowing Down and Icosahedral Ordering in Undercooled Liquid Alloys

Noel Jakse and Alain Pasturel

Sciences et Ingénierie des Matériaux et Procédés, UMR CNRS 5266, Grenoble Université Alpes, Grenoble, France

Understanding diffusion phenomena and relaxation dynamics in metallic liquids during undercooling is of utmost importance since they represent key parameters governing solidification and glass formation processes [1, 2]. The question of influence structural properties, *i.e.* short- and medium-range order, on these dynamic properties remains largely open [3]. We present *ab initio* based molecular dynamics simulations to study the correlation between the structure and dynamics of liquid Cu-Zr [4, 5] and Al-Ni [6, 7] alloys upon cooling, these alloys being known to possess significantly different glass-forming ability (GFA).

We show that both alloys crossover from Arrhenius to non-Arrhenius behavior around a temperature T_X located in the undercooled region, and clearly identify that this temperature corresponds to the development of dynamic heterogeneities and to the breakdown of the Stokes-Einstein relation. Our results evidence a huge increase of local icosahedral ordering for both alloys and the development of string-like domains of interconnected icosahedra and a liquid-liquid phase transition for Cu-Zr. We discuss the diffusion mechanisms and relaxation dynamics in the perspective of the mode-coupling theory, as well as the GFA of these alloys.

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I21 - Thu 09:00-09:30 **Containerless Processing** Kleiner Saal / Small Hall

Aerodynamic levitation: 20 years of experiments at synchrotron and neutron sources

Louis Hennet

CNRS-CEMHTI & University of Orleans, Orleans, France

Studies of high temperature liquids are interesting in a fundamental point of view and have technological importance since the molten state is an essential stage in various industrial processes.

At very high temperature, it is difficult to use conventional furnaces, which present various problems. In particular, the sample can react with the container and be polluted. Furthermore it is difficult to reach very high temperatures. These difficulties have led to the development of containerless techniques and their use at synchrotron and neutron sources for studying the structure and dynamics of molten materials [1].
Among the existing levitation methods [2], our group has chosen to work with the aerodynamic levitation associated with CO_2 laser heating. This method allows the design of relatively simple and compact devices that can be integrated easily into a large number of instruments at large scale facilities.

In this talk, I will present a review of the technical developments and experiments made during 20 years with aerodynamic levitation at synchrotron and neutron sources. The main results obtained during this period will be discussed.

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C61 - Thu 09:30-09:50 **Containerless Processing** Kleiner Saal / Small Hall

High resolution x-ray Compton scattering of high temperature liquids using electrostatic levitator

Junpei T. Okada[1,2], P. H. –L. Sit[3], Y. Watanabe[4], B. Barbiellini[5], T. Ishikawa[6], Y. J. Wang[5], M. Itou[7], Y. Sakurai[7], A. Bansil[5], P.-F. Paradis[6], K. Kimura[8], and S. Nanao[4]

[1] *Institute for Materials Research, Tohoku University, Sendai, Japan*
[2] *PRESTO, JST, Kawaguchi, Japan*
[3] *School of Energy and Environment, City University of Hong Kong, Hong Kong*
[4] *Institute of Industrial Sciences, The University of Tokyo, Meguro-ku, Japan*
[5] *Department of Physics, Northeastern University, Boston, USA*
[6] *Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency, Tsukuba, Japan*
[7] *Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo, Japan*
[8] *Department of Advanced Materials Science, The University of Tokyo, Kashiwa, Japan*

In the periodic table, boron (B), silicon (Si) and Germanium (Ge) belong to the group of elements situated between metals and insulators. Si and Ge, which are semiconductors in the solid state, transform into metals on melting. Some theoretical studies suggest that B could also acquire some metallic character on melting. Although transport experiments on liquid B have indicated the survival of a semiconducting behavior. To investigate the bonding properties of liquid B, we have performed high resolution x-ray Compton scattering of solid and liquid B, and Compton scattering of Si and Ge were also performed for comparison.

X-ray Compton scattering is an ideal technique for probing the ground state wave functions in materials. The Compton technique can also provide a novel spectroscopic window on the liquid state [1][2]. Since no charged particles entering or leaving the sample are detected, the technique is a genuinely bulk probe, which is not complicated by surface effects present in photoemission or electron scattering experiments. Compton profiles were measured by high energy (116keV) inelastic x-ray scattering at the BL08W beam line of SPring-8. High temperature liquids are highly reactive with most crucibles. To hold the sample without contamination, a high temperature electrostatic levitator (HTESL) was used. The HTESL levitates a spheroid sample of 2 mm diameter in a high vacuum environment (approximately 10^{-5}Pa) using electrostatic forces via a feedback computer control. The sample was heated and melted using the focused radiation of three 100W semiconductor laser beams emitting at 808nm.

Our study show covalent bond pairs clearly dominate in liquid B along with the coexistence of diffuse pairs, though diffuse pairs dominate in liquid Si and Ge.

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C62 - Thu 09:50-10:10 **Containerless Processing** Kleiner Saal / Small Hall

Atomic size effect on undercoolability of binary solid solution alloy liquids using electrostatic levitation

Geun Woo Lee[1,2], Sangho Jeon[2], Sooheyong Lee[1,2] Yun-Hee Lee[1,2] and Yong-Il Kim[1,2]

[1] *Korea Research Institute of Standards and Science, Daejon, Republic of Korea*

[2] *University of Science and Technology, Daejon, Republic of Korea*

Short range orders (SRO) affect the stability of liquids, i.e., causing supercooling. However, mixing with other elements makes the role of SRO complicate in geometric viewpoint, since the mixing gives the change of excess energy and volume. For the exact understanding of geometric contribution of SRO to the stability of liquids, in present study, we choose Zr-Ti and Zr-Hf binary solid solutions which show no heat of mixing, but atomic size difference of those elements. In this case, the excess volume can be quantified by packing density affecting excess entropy and thus mixing Gibbs free energy. Here, we studied the relationship among excess free volume, packing fraction, and undercoolability in binary metallic liquids. We used electrostatic levitation in KRISS to investigate the atomic size effect on undercoolability or stability of the liquids. Unlike Zr-Hf system having similar atomic radii, Zr-Ti liquid alloys with different atomic size showed the significant increase on undercoolability. The result show that mismatch entropy of Zr-Ti liquid alloys due to atomic size difference of Ti and Zr underlies the stability of Zr-Ti liquids.

C63 - Thu 10:10-10:30 **Containerless Processing** Kleiner Saal / Small Hall

Thermo-mechanical stability of W alloy beads solidified from electrostatically levitated melts

Y.-H. Lee[1,2], C. H. Yoo[1,3], Y.-J. Kim[1], Y. Kim[1,2], and G. W. Lee[1,3]

[1] *Division of Convergence Technology, Korea Research Institute of Standards and Science, Daejeon, South Korea*

[2] *Department of Nano Science, University of Science and Technology, Daejon, South Korea*

[3] *Department of Mechanical Engineering, Kyung Hee University, Yongin, South Korea*

Plasma-facing components (PFCs) in future fusion reactors operate under extreme environment such as high temperature and severe radiation. Plasma pulse during operation and frequent shutdowns apply significant thermo-mechanical loads on the PFCs. Thus microstructural stability and degradation resistance of plasma-facing materials are crucial issues for safety, reliability and energy conversion efficiency of the fusion reactors. In order to obtain tungsten alloys with uniform and refined microstructures we used a levitation melting technique. Tungsten alloy beads 1.0-1.5 mm in diameter are formed by melting mixed chips of W, Zr, Nb and Hf elements. Then these beads are isolated from a container or plate under high vacuum by using an electrostatic levitator (ESL). This containerless and contactless environment under high vacuum give a chance to raise temperatures of the levitated beads up to 3000 K without surface oxidation or any contamination. Deep undercooling and recalescence event are followed by solidification and radiative cooling; the deep undercooling will bring about multiple homogeneous nucleations in a levitated bead and is expected to evolve a refined microstructure. In this study, we use laser heating system in the ESL to add thermo-mechanical loads on the levitated sample; CO2 and diode lasers are focused on the bead sample levitated in the ESL chamber. Sample temperatures measured with a pyrometer increase higher than 2000 K within few seconds and rapidly decrease down to 1000 K corresponding to the laser turn-on and turn-off, respectively. This heating and cooling cycle is applied to the levitated sample more than 100 cycles and then cracks or damages formed in the sample are observed with an optical microscope. Crack density on the bead surface is discussed from the viewpoint of thermos-mechanical loading cycle and microstructural degradations of the fatigued samples are compared with the as-melted virgin sample.

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I22 - Thu 11:00-11:30 **Thermophysical Properties** Großer Saal / Great Hall

Microscopic dynamics and thermophyical properties of dense metallic melts

F. Yang[1], D. Holland-Moritz[1], M. Seidel[1], S. T. Liu[2], P. Heintzmann[1], C. C. Yuan[1], G. G. Simeoni[3], and A. Meyer[1]

[1] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), Cologne, Germany*
[2] *Institute of Physics, Chinese Academy of Sciences (CAS), Beijing, P. R. China*
[2] *Heinz Maier-Leibnitz Zentrum (MLZ) and Physics Department, Technische Universität München, Garching, Germany*

Ternary Zr-(Ni,Cu)-Al alloys are excellent bulk metallic glass formers with outstanding mechanical properties and corrosion resistance. The addition of a small amount of Al significantly enhances the glass-forming ability of the melt. However, so far, such improvement of glass forming ability has been mainly interpreted by empirical rules based on thermodynamic considerations. Another important aspect, the influence of the alloy composition on the melt properties, especially the impact by Al addition, has not been systematically studied. We thus investigated the composition dependence liquid dynamics of the Zr-based glass formers using a combination of containerless processing and quasielastic neutron scattering (QNS) [1,2]. Utilising electrostatic levitation, We also studied the macroscopic thermophysical properties of density and viscosity of theses liquid alloys. Taking the advantage of containless processing and QNS, we were able obtain precise data of liquid properties without artifacts caused by reaction and convection.

It has been shown for Ni, NiP, PdNiP, and PdNiCuP alloys that the liquid dynamics is insensitive to the drastic change of the alloy composition, as long as the packing fraction of the liquid, derived under an assumption of a hard-sphere like packing, remains unchanged [3]. We show here that these Zr-based alloys exhibit a different behaviour. For binary Zr-(Ni,Cu) melts with the same Cu/Ni content, the Cu self-diffusion in Zr-Cu is faster than corresponding the Ni self-diffusion in Zr-Ni, although the atomic radii of Ni and Cu are very similar. Nevertheless, a qualitative correlation between slower dynamics and higher packing fraction can be still observed by substituting Cu by Ni. In contrast, for ternary Zr-Ni-Al alloys, with a systematic substitution of Zr by Al from $Zr_{75}Ni_{25}$ up to $Zr_{45}Ni_{25}Al_{30}$, the average hard-sphere packing fraction remains almost constant, while the melt viscosity increases by a factor of about 8 at 1300 K. These composition dependence of the liquid dynamics indicates that apparently in these melts the dynamics is not only controlled by packing, but the influence of chemical interactions between the different alloy components needs also be considered.

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C64 - Thu 11:30-11:50 **Thermophysical Properties** Großer Saal / Great Hall

Density of liquid Ti-6Al-4V

G. Pottlacher[1], A. Schmon[1], K. Aziz[1]

[1] *Institute of Experimental Physics, Graz University of Technology, NAWI Graz, Austria*

Ti-6Al-4V is due to its high strength-density ratio a commonly used alloy in aerospace industry applications. But liquid phase data are scarce as preventing contaminations of the reactive high temperature melt during the investigation process poses a challenge. The thermophysical quantity density is of special interest since it is necessary input parameter in modern numerical casting and solidification simulations.

Liquid phase density of Ti-6Al-4V as function of temperature was determined employing a fast resistive pulse-heating technique based on the approach to avoid contaminations of the specimen by extremly reducing the experimental duration of the investigation process. The specimen material was resistively self-heated as part of an electrical discharge circuit by a current of about 5000 A. Heating rates of about 10^8 K/s reduced the experimental duration to below 50 µs. Within this time the specimen material was heated from room temperature up to the end of the liquid phase and concurrently monitored by an adapted CCD camera system working with a frame rate of 200000 images per second. The recorded images describing the thermal expansion of the specimen were evaluated to calculate the density of the specimen material. Temperature was determined pyrometrically by measuring the surface radiance emitted from the sample surface. Temperature dependent density of liquid Ti-6Al-4V was determined in a temperature range between 2050 K and 2590 K and is presented.

C65 - Thu 11:50-12:10 **Thermophysical Properties** Großer Saal / Great Hall

Thermophysical properties of SiGe melts studied in EML under microgravity conditions

Y. Luo, B. Damaschke and K. Samwer

I. Physics Institute of George-August-University Göttingen, Germany

In an electromagnetic levitator (EML) contactless investigations of melts of semiconductors $Si_{1-x}Ge_x$ were carried out under microgravity conditions. As a precondition for EML a sufficient electrical conductivity is necessary for samples and thus the processing of semiconductors is a great challenge. In cooperation with N. Abrosimov, IKZ Berlin, we prepared highly doped semiconductors $Si_{1-x}Ge_x$ by Czochralski growth [1]. The dopant used is B with a concentration of about $2\text{x}10^{20}$ at./cm^3, which corresponds to a conductivity of about $1.5\text{x}10^3\ \Omega^{-1}\text{cm}^{-1}$ at room temperature. It increases upon heating and jumps above $10^4\ \Omega^{-1}\text{cm}^{-1}$ at the melting point. The processing was performed recently in parabola flight campaigns, using spherical samples (8mm). The parabola flight provides a 20s microgravity condition ($\leq$0.05g), being more suitable for low T_l samples (Ge-rich), for which a large overheat $\Delta T > 400$°C was achieved. The temperature-dependent volume of melts was evaluated from videos recorded by high-speed cameras, giving the thermal expansion coefficient of the melts. An anormal volume expansion near T_l was observed thereby and it may be associated with a liquid-liquid phase transition regarding abrupt changes of the coordination number of neighbor atoms, as predicted by Angell et.al.[2] in a similar system. Surface tension and viscosity of the melts were determined by oscillating drop technique [3], using optic and electronic data [4]. The results demonstrate that the viscosity follows an Arrhenius temperature dependence and the surface tension is enhanced by alloying Si into Ge.

We thank DLR and Novespace for the parabola flight campaigns, the MUSC team Cologne for the help with experiments, the team partner in Leibniz-IKZ Berlin for preparation of crystals. Financial support from DLR project 50WM1036 is gratefully acknowledged.

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C66 - Thu 12:10-12:30 **Thermophysical Properties** Großer Saal / Great Hall

MD Simulation of thermotransport in Ni-Al Melts

T. Ahmed[1], A.V. Evteev[1], E.V. Levchenko[1], A. Kromik[1,2], I.V. Belova[1], and G.E. Murch[1]

[1] University of Newcastle, Department Mechanical Engineering, Newcastle, Australia
[2] The University of Applied Sciences Aalen, Aalen, Germany

In this study, the effect of thermotransport in Ni-Al melts is analyzed over a wide temperature range and concentration range. Calculations were performed by using equilibrium molecular dynamics simulation in conjunction with Green-Kubo formalism and one of the most reliable embedded-atom method potentials for this system developed by Purja and Mishin [1].

The results obtained permit the analysis of the reduced heat of transport parameter [2-4] characterizing the interdiffusion flux that is proportional to the temperature gradient. The applicability of the kinetics of solidification predicted by the Ni-Al melt models to real Ni-Al melts was also analyzed. On the basis of these calculations, it is possible to estimate the temperature and concentration gradients at the crystal-melt interface during non-equilibrium solidification of real Ni-Al alloys.

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I23 - Thu 11:00-11:30 **Modelling / Simulations 1** Kleiner Saal / Small Hall

Atomistic and continuum modeling of dynamic tensile fracture of metal melts

Alexander Mayer, and Polina Mayer

Chelyabinsk State University, Department of Physics, Chelyabinsk, Russia

Dynamic tension of metal melt takes place at fast expansion of an initially solid metal that was heated and melted by an ultra-short pulse of powerful laser [1] or high-current electron irradiation. An initial expansion is due to pressure gradients in this case, while subsequent expansion is due to inertia that leads to a tensile state with negative value of pressure. Another situation is reflection of a compression pulse from a free surface of melt, when the compression pulse transforms into a tension wave. Thermodynamic state of melt at negative pressure is unstable and decays by means of cavitations at enough high value of negative pressure.

Tensile strength of metal melts is still a question of considerable interest due to the fact that experimental data are very rare in this filed. Molecular dynamic (MD) simulations and continuum generalizations of them based on the classical nucleation theory give high values of this strength–about several gigapascals–in a wide range of strain rates–from 0.01/µs to 10/ns [2]. These results agree with the experimental data obtained for ultra-short powerful laser irradiation of thin films [1] at the strain rate about 1/ns, but contradict both the experimental data [3] for a lower strain rate–about 1/µs and the results of indirect estimations [4], which give considerably lower value of strength. It gives rise the question about factors leading to the melt strength reduction.

In this report, we present the results of MD simulations of the high-rate tension and fracture of pure metal melts and melts with both refractory and fusible inclusions. By the example of Ti and Ni inclusions in Al melt, it is shown that the refractory inclusions weakly increase the tensile strength due to the fact that tension is applied predominantly to the melt around inclusions, which effectively increases the strain rate. By the example of Mg inclusions in Al melt, it is shown that the fusible inclusions can temporally decrease the tensile strength several times, but the effect weakens together with the diffusive mixing. The continuum model based on the MD simulation results is described and applied to the large-scale problems unattainable for MD.

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C67 - Thu 11:30-11:50 **Modelling / Simulations 1** Kleiner Saal / Small Hall

Ab initio study of intrinsic profiles of liquid metals and their reflectivity.

B.G. del Rio[1], J. Souto[2], M.M.G. Alemany[3], and L.E. González[1]

[1] *Universidad de Valladolid, Dept. Fisica Teorica, Valladolid, Spain.*
[2] *University of Texas at Austin, Institute for Computational Engineering and Sciences, Austin, Texas, USA*
[3] *Universidad de Santiago de Compostela, Dept. Fisica de la Materia Condensada, Santiago de Compostela, Spain.*

The free surfaces of liquid metals are known to exhibit a stratified profile that, in favourable cases, shows up in experiments as a peak in the ratio between the reflectivity function and that of an ideal step-like profile. This peak is located at a wave-vector related to the distance between the layers of the profile. In fact the surface roughness produced by thermally induced capillary waves causes a depletion of the previous so called intrinsic reflectivity by a damping factor that may hinder the observation of the peak. The behaviour of the intrinsic reflectivity below the layering peak is however far from being universal, with systems as Ga or In where the reflectiviy falls uniformly towards the $q \to 0$ value, others like Sn or Bi where a shoulder appears at intermediate wavevectors, and others like Hg which show a minimum [1]. We have performed extensive ab initio simulations of the free liquid surfaces of Bi, Pb and Hg, that yield direct information on the structure of the profiles and found that the macroscopic capillary wave theory usually employed in order to remove the capillary wave components fails badly in some cases for the typical sample sizes affordable in ab initio simulations. However, a microscopic method for the determination of the intrinsic profile [2] is shown to be succesful in obtaining meaningful intrinsic profiles and corresponding reflectivities which reproduce correctly the qualitative behaviour observed experimentally.

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C68 - Thu 11:50-12:10 **Modelling / Simulations 1** Kleiner Saal / Small Hall

Thermodynamic properties and freezing of metastable liquid metals under tensile stresses

Konstantin V. Khishchenko

Joint Institute for High Temperatures RAS, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

Metastable states of the liquid phase under tensile stresses (negative pressures) may be realized in processes of intense pulsed influences on materials [1, 2]. Adequate description of thermodynamic properties and phase transformations of a medium is needed for analysis and numerical simulations of such processes. In this work, results of semiempirical equations-of-state modeling for some metals (aluminum, lead, tungsten) at negative pressures are presented. As distinct from the previously obtained multiphase equations of state for metals [3], a new form of expression of individual terms of thermodynamic potential Helmholtz free energy is proposed which takes greater account of thermal contribution of atoms in the liquid phase and the freezing effects at temperatures close to zero. This allows extending the thermodynamic description to cover the region of metastable liquid states at tensile stresses.

The work is supported by the Russian Science Foundation (grant 14-50-00124).

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C69 - Thu 12:10-12:30 **Modelling / Simulations 1** Kleiner Saal / Small Hall

SOUND VELOCITY AS A TOOL FOR PHASE DIAGRAM ANALYSIS UNDER PRESSURE

M. Emouna[1], Y. Greenberg[2], E. Yahel[2], and G. Makov[1]

[1] *Materials Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel*
[2] *Physics Department, Nuclear Research Centre Negev, Beer-Sheva, Israel*

The phase diagrams of binary alloys are known to vary with pressure. Within the framework of solution type models, the variation is controlled by the pressure dependence of the elemental members which is relatively well known and that of the interaction parameter which is unknown. We have developed a thermodynamic model linking the pressure dependence of the interaction parameter to the composition dependence of the density and sound velocity. The effect of composition on the sound velocity and density was studied for several binary alloys (such as Bi-Sb, Bi-Sn and Pb-Sn) and the pressure dependence of the interaction parameter in the solid and liquid phases was estimated. On this basis the pressure dependence of the binary alloy phase diagrams was calculated and found to agree well with the available data. The phase diagrams of binary alloys are known to vary with pressure. Within the framework of solution type models, the variation is controlled by the pressure dependence of the elemental members which is relatively well known and that of the interaction parameter which is unknown. We have developed a thermodynamic model linking the pressure dependence of the interaction parameter to the composition dependence of the density and sound velocity. The effect of composition on the sound velocity and density was studied for several binary alloys (such as Bi-Sb, Bi-Sn and Pb-Sn) and the pressure dependence of the interaction parameter in the solid and liquid phases was estimated. On this basis the pressure dependence of the binary alloy phase diagrams was calculated and found to agree well with the available data.

I24 - Fri 09:00-09:30 **Struct. and Prop. of Glasses** Großer Saal / Great Hall

Telluride amorphous films: structural investigation and applications

Annie Pradel[1], Andrea Piarristeguy[1], Pal Jovari[2], Ivan Kaban[3]

[1]Institut Charles Gerhardt UMR 5253 CC1503 Université de Montpellier Place E. Bataillon 34095 Montpellier Cedex 5 France
[2]Wigner Research Centre for Physics, Institute for Solid State Physics, H-1525 Budapest, POB 49, Hungary
[3]IFW Dresden, Institute for Complex Materials, PO Box 27 01 16, D-01171 Dresden, Germany

Tellurium containing materials are used for applications in diverse fields of optics and electronics. Due to their fast phase-change Ge-Sb-Te alloys serve as the information storage layer of optical and electrical storage memory, while Te-rich Ge-Te and Ge-Te-X (X= Ga; Se; I) glasses possess low absorption in the far infrared region and can be used for the development of infrared space telescopes or sensors to detect CO_2. Recently Cu-Ge-Te glasses were studied for potential application as thermoelectric materials.

In spite of the diversity and importance of applications our knowledge on the structure of binary amorphous Ge-Te alloys is much less certain than in case of other binary systems (e.g. Ge-S, Ge-Se, As-Se). The reason for this is twofold: first, Ge-Te alloys can be vitrified only in a narrow range around the eutectic point (x=15) and other compositions should be made by sputtering or thermal evaporation, which makes sample preparation long and tedious. The second difficulty follows from the structure of amorphous tellurides itself: while glassy sulfides and selenides are characterized by clear bonding tendencies – the number of homonuclear bonds is minimized - chemical ordering can be much less pronounced in telluride glasses.

In the talk, a review of our recent work on binary Ge-Te amorphous materials produced by thermal co-evaporation will be presented with an emphasis on structural characterization performed on the basis of X-ray and neutron diffraction, EXAFS measurements and RMC simulations. Reciprocal and real space properties showed singularities which could be explained in connection with topological models. These findings also pointed to a relationship with the composition dependences of some physico-chemical properties such as thermal stability and optical band gap. Onset of homopolar Ge-Ge bonds at a composition corresponding to a threshold composition for the resistance drift can be considered as a support for models pointing the breaking of homopolar Ge–Ge bonds as the main phenomenon behind the ageing of phase change materials.

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C70 - Fri 09:30-09:50 **Struct. and Prop. of Glasses** Großer Saal / Great Hall

Structure of Amorphous Aluminium-Cobalt-Rare-Earth Ribbons

Alan K. Soper[1] and Valeriy Sidorov[2],

[1] STFC Rutherford Appleton Laboratory, ISIS Facility, Harwell Campus, Didcot, OX11 0QX, UK

[2] Ural State Pedagogical University, Ekaterinburg, Russia

Alloys of aluminium with small (approximately 10 at.%) additions of transition metals and rare earth dopants have considerable potential as novel magnetic materials: they can be strong, flexible and can have excellent corrosion resistance.[1] Here, using both time-of-flight neutron total scattering and fixed wavelength x-ray total scattering, we examine the atomic structure of some $Al_{(100-x-y)}Co_xRE_y$ alloys, with x = 8 at.% for all samples, and y = 6 and 10 at.% for each of the rare-earth (RE) elements holmium and dysprosium. These rare-earth elements present considerable difficulties for total neutron scattering studies due to the presence of numerous nuclear resonances at moderate neutron energies (>~ 1 eV). The strong energy dependence of the scattering cross section that these resonances produce makes the process of putting the neutron scattering data on an absolute scale of differential cross section problematic. On the other hand for Ag K_α radiation (x-ray wavelength 0.5609 Å) the x-ray scattering is benign, so that excellent quality x-ray scattering data are readily obtainable. The combination of the two data sets plus computer simulation modeling using empirical potential structure refinement[2] (EPSR), produces powerful constraints on the possible structures of these alloys.

All alloys investigated appear perfectly amorphous, with no hint of crystallinity in the form of sharp Bragg diffraction peaks in the scattering patterns. In particular it is found that the aluminium and transition metal (Co) atoms are rather diffusely spread through the alloys while the RE atoms are well separated, producing a longer range structure. The most dominant feature of the structure is that each RE is surrounded by around 13-14 Al atoms on average at a nearest neighbour distance of approximately 3.1 Å, while the rare-earth atoms themselves have nearest neighbour distances of order 5.6 Å: direct RE-RE contacts rare. Co-Al complexes, with coordination numbers of order 8, are also present to a lesser degree.

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C71 - Fri 09:50-10:10 **Struct. and Prop. of Glasses** Großer Saal / Great Hall

The effect of a partial nanocrystallization on the transport properties of a metallic glass

A. Tlili[1, 2], S. Pailhès[1], R. Debord[1], S. Gravier[2] ,V. M. Giordano[1]

[1]Institute of Light and Matter, UMR5306 Université Lyon 1-CNRS, Université de Lyon, 69622 Villeurbanne cedex, France

[2] Science and Engineering of Materials and Processes, SIMaP, GrenobleINP, 101 rue de la physique, BP46, 38402 Saint-Martin d'Hères, France

Metallic glasses represent a novel class of amorphous alloys with excellent structural properties like high strength, high elasticity and good corrosion resistance, which make them good candidates for a myriad of applications such as fuel cells, electrodes accumulators, thermal barrier coatings, nuclear waste containers and mechanical applications.

Starting from these materials amorphous/crystalline composites can easily be prepared, where the presence of order/disorder interfaces is expected to affect elastic as well as transport properties.

In this study, we present an investigation of the transport properties of a bulk metallic glass, as cast, and partially crystallized by means of controlled thermal protocols. We will show that the dependence of the electrical resistivity on the crystalline fraction χ changes for the different thermal protocols used (linear or isothermal annealing). However, in both cases, it can still be described by a mean field approach for $\chi \leq 50\%$. Moreover, partial or complete crystallization only weakly affects the longitudinal and transverse speed of sound (and thus the elastic properties), as deduced from the phonons dispersions.

C72 - Fri 10:10-10:30 **Struct. and Prop. of Glasses** Großer Saal / Great Hall

Structures and mechanical properties of Zr-based bulk metallic glasses as a function of cobalt concentration

Y. Dong[1], H.-J. Fecht[1], J. Z. Jiang[2], and R. K. Wunderlich[1]

[1] Institute of Micro und Nanomaterials, Universität Ulm, Germany

[2] Laboratory of New-Structure Materials, Zhejiang University, China

The structure and mechanical properties of a series of Zr-based bulk metallic glass forming alloys of composition $Zr_{62-x}Ni_{10}Al_7Cu_{19}Co_x$ with x in the range of x = 3-8 at% was investigated. All compositions exhibit good glass forming ability. A pronounced change in the crystallization mode as a function of the cobalt concentration was observed in $Zr_{64-x}Ni_{10}Al_7Cu_{19}Co_x$ BMGs indicating a change in the structure of the liquid phase as a function of Co concentration. Such a structural change may also be reflected in the mechanical properties of the glassy phase. It is well known that the mechanical properties of the glassy phase can exhibit a pronounced dependence on microalloying. As such, the structural and mechanical properties of this series of bulk metallic glasses was further investigated as a function of the Co concentration.

X-Ray scattering of as cast glassy specimen indicated the formation of a new topological short range order as a function of Co concentration because of the positive mixing enthalpy between copper and cobalt (6 kJ/mol). It could, however, not be discerned if that new structure corresponds to phase separation. Because of the smaller atomic diameter compared with zirconium and the very negative mixing enthalpy between cobalt and zirconium(-41 kJ/mol), the addition of cobalt resulted in an increased bonding strength of the BMGs with concomitant increase in Young's modulus and hardness. For elastic performance, the increased both Young's modulus and maximum elastic strain lead to a pronounced increase of the stored recoverable elastic energy with increasing cobalt content. During plastic deformation, the quantity of shear bands is reduced with increasing cobalt content while more shear bands orientation form at the same time. As a result, all the alloys have Poisson's ratios of $\gamma=0.38\text{-}0.39$. The alloy with 8.3 at% cobalt exhibits the highest plastic strain $\varepsilon = 19.5\%$ because of the intersection of shear bands.

I25 - Fri 09:00-09:30 **Modelling / Simulations 2** Kleiner Saal / Small Hall

Quantum simulation of liquid metals: predicted properties and problems

Levashov P.R.[1]

[1] *Joint Institute for High Temperatures RAS, Moscow, Russia*

Properties of liquid metals are quite important for simulation of complicated processes at high pressure and temperature. Perhaps the most striking example of this kind is the numerical simulation of interaction of femtosecond laser radiation with metallic samples. In this case equation of state, thermal conductivity, complex dielectric function and electron-phonon exchange coefficient are required. Liquid metals are quite complex systems for simulation. On the one hand the structure of a liquid metal is unordered, so the theory of solid state cannot be applied directly. On the other hand, electrons are delocalized, so that classical two-particle potentials are not valid. Accurate simulation of properties of liquid metals and alloys is generally reduced to the solution of the many-body quantum problem. Only a few approaches are applicable in this case: the pseudopotential approach, Hartree-Fock method, quantum, diffusion and path integral Monte Carlo methods. However, in every case there are limitations which restrict practical applications of these methods, computational expensiveness on the first place. A good compromise between strictness and speed of computations is the so-called quantum molecular dynamics (QMD) method [1]. It is based on the Born-Oppenheimer approximation in which only the motion of ions is traced in a supercell while electrons instantly adjust their distribution to the current position of the ions. The distribution of electrons is calculated in the framework of density functional theory (DFT) which gives an approximate solution of the stationary many-body quantum problem. Quantum molecular dynamics allows one to obtain different properties for a liquid metal: mechanical, structural, thermodynamic, transport and optical. Pressure and energy of the ionic subsystem can be directly extracted from molecular dynamic results, entropy and free energy can be accurately estimated using the 2PT model. Equation of state of the electronic subsystem is available from finite-temperature DFT. Static and dynamic electrical conductivity as well as thermal conductivity can be calculated using the Kubo-Greenwood relation; the imaginary part of dynamic electrical conductivity may be restored from the Kramers-Kronig relation. A pair distribution function is calculated directly from ionic configurations and may be compared with an experimental structure factor. It is also possible to obtain ionic transport properties, such as self-diffusion coefficient and viscosity; the last one is computed from the Green-Kubo formula. The results of QMD simulation of metals and alloys will be presented in comparison with experimental data in stationary conditions, in exploding wires (foils) and shock waves. Special attention will be paid to the simulation of melting and near-critical region. Restrictions of the QMD approach together with current problems in interpretation of recent experiments will be discussed. This work is supported by the Russian Science Foundation, project No. 16-19-10700.

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C73 - Fri 09:30-09:50 **Modelling / Simulations 2** Kleiner Saal / Small Hall

The Thermodynamic and Kinetic Properties of Liquid Alloy by First Principles Molecular Dynamics Simulation

Jing-Yu Qin[1], Jin Wang[1], Xin-xin Li[1], Qiang Zhang[1], Saho-peng Pan[2]

[1] *Shandong University, School of Materials Science and Engineering, Jinan, China*

[2] *Taiyuan University of Technology, College of Materials Science and Engineering, Taiyuan, China*

Since the temperature of liquid alloys are generally high, and the formation enthalpy is usually much weaker than that of chemical reaction, the measurement of the formation enthalpy maybe difficult to reach high precision. The ideal mixing entropy is often employed in thermodynamics, however, how to relate the mixing entropy with the liquid structure information is an open question.

The first principles molecular dynamics simulation (FPMD) is based on the DFT theorem of electrons, and then is expected to give a proper description of electron structure, which governs the energy of materials. It is suggested that the combination of CALPHAD with the first principles calculation will have us gained substantial results [1] . We have tried to calculate the formation enthalpy of some binary liquid alloys including Al-Si, Al-Ni, Ga-Bi, Cu-Ni and etc, and then compared them with the experimental data, if feasible. By doing so, we found that poor agreement often exists between experimental data and that from FPMD. This reminds us that extra efforts should be made to improve the software of FPMD to give a better description of formation enthalpy. In addition, how to evaluate the reliability of the structure of liquid alloy remains to be discussed.

A model on configurational entropy has been provided by the author [2]. The partial coordination numbers and chemical short-range order were incorporated into such model. At random distribution, this model becomes the ideal mixing entropy, and any deviation from random distribution will reduce the mixing entropy, either clustering or segregation. Larger enhancement is found in the case of larger atoms being solved into the matrix of smaller atoms; while decrease of entropy is reached when smaller atoms enter into the matrix of larger atoms. For ordered solution at equiatomic concentration, it gives zero which is a better character of this model than that of Cluster Variation Method (CVM).The diffusion coefficients of some liquid binary alloys were also provided and discussed.

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Obtaining norm-conserving pseudopotentials for liquid metal simulations using machine learning

Andrey Sobolev, Ivan Buldashev, Alexander Mirzoev

South Ural State National Research University, Chelyabinsk, Russia

In last decades *ab initio* simulations become a standard tool for calculating various material properties. Increase in available computer power and no need in expensive experimental facilities made atomistic simulations a necessary step in constructing novel materials. Atomistic simulations typically include a numerical solution of Schrödinger equation for a system of electrons; density functional theory is the method of finding the solution to the equation as the electron density. It is represented mathematically as a linear combination of basis functions, which can be chosen arbitrarily. However, oscillations of the electronic density near atomic nuclei are reproduced with sufficient accuracy only at the price of largely expanded basis, hence, increased computational difficulties. To overcome the difficulties, pseudopotentials are used, which substitute the Coulomb repulsion of core electrons.

Finding pseudopotentials and basis sets suitable for calculating material properties is largely subject to scientific intuition. We use SIESTA [1] software; it is a software package implementing DFT, which uses atom-centered basis and norm-conserving pseudopotentials in Kleinman–Bylander form [2]. Getting right pseudopotentials is the tricky task: one can take a pseudopotential from the database maintained by SIESTA authors [3] (rather outdated, with several elements failing to converge), ask other researchers, either personally or via a mailing list, or dare to calculate it oneself. In this work we try to address the latter approach.

Machine learning is a rapidly developing computer science subfield, which deals with algorithms building models from data and making predictions out of it. Nowadays, machine learning methods are being used in all spheres, from search engines to economics and marketing. We present both a method and a code, based on machine learning techniques, that allows a simple recovery of efficient norm-conserving pseudopotentials based on the recovered properties of materials in solid and in liquid state. The test of obtained pseudopotential on the case study of iron results in increased accuracy of properties both in solid and in liquid state compared to that of Izquierdo et al [4], which is the most widely used pseudopotential for iron at the moment.

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P5 - Friday 11:00-11:40 Großer Saal / Great Hall

How Liquids and Glasses Came Into Their Own

Frans Spaepen

Harvard University, School of Engineering and Applied Sciences, Cambridge, MA 02138, USA

Of the three states of matter, the liquid state has historically been the hardest to characterize. Whereas calling a crystal *"periodic"* or a gas *"sparse"* went a long way in explaining many of their properties, no such simple label could easily be applied to a liquid. Considering it as a high-density gas, going back to Van der Waals, is theoretically sound, but leaves the problem of how the multiple positional correlations between the atoms can be simply understood. Considering it as a highly defective crystal has been tempting, but is fundamentally flawed and thermodynamically untenable due to a lack of entropy.

The insight that liquids have a structure of their own that should be considered separately from that of the other phases, grew out of key experimental observations (diffraction, undercooling, nucleation), and from the construction of physical (hard-spheres, colloid) and computer models. This talk will trace these developments, and show how the concept of *polytetrahedral* short-range order is as close as we have come to a single-word structural characterization of simple liquids.

Poster Abstracts

POSTER 01 - Tuesday 18:15-20:00hrs Foyer

Analysis of Diffusion in a Cu-Al Liquid Couple Using a Combined Interdiffusion and Self- Diffusion Formalism

I.V. Belova[1], F. Kargl[2], B. Ignatzi[2], D. Heuskin[2], G.E. Murch[1], A. Meyer[2]

[1]UCMTTEM, University of Newcastle, Callaghan, Australia
[2]Institute of Materials Physics in Space - German Aerospace Center, Cologne, Germany

Recently, a combined isotope (self- or tracer) and interdiffusion theoretical approach was developed [1] for application to solid state interdiffusion couples with an addition of an enriched isotope(s) layers. The resulting expressions allow for obtaining the self (tracer) diffusion coefficients of the atomic components corresponding to the isotopes enriched. In addition, these diffusion coefficients can be obtained as functions of composition in the diffusion zone.

In the present paper, this analysis is adapted to diffusion in the liquid state where it is then applied to the case of the liquid CuAl alloy. In this system, three experiments have been performed that are suitable for the application of this analysis. In those experiments a layer enriched in 65Cu was added between the interdiffusion couple ends. The analysis allows for a generalized treatment of the interdiffusion profile in order to obtain the total flux for one of the components. The self (tracer) diffusion coefficient of Cu is then obtainable as a function of composition in the diffusion zone. Two forms of the new analysis are in good agreement with an independently measured Cu self (tracer) diffusion coefficient at two compositions.

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POSTER 02 - Tuesday 18:15-20:00hrs Foyer

Correlation of local structure and molar volume in liquid Fe-Si alloys

Daichi Aoshima[1], Akitoshi Mizuno[1] and Masahito Watanabe[1]

[1]*Gakushuin University, Department of Physics, Tokyo 171-8588, Japan*

In recent years, since x-ray diffraction pattern and thermo-physical properties of high-temperature liquids have been accurately measured, a close correlation between the local structure and the density of the liquid has been suggested [1]. In the present study, we measured the density of the liquid Fe-Si alloys by using the electromagnetic levitation technique coupled with static magnetic field. Analyzing concentration dependence of partial molar volumes, we found that the composition dependence of the molar volume of Fe-rich region and the Si-rich region is greatly different [2]. The Fe-Si system has some intermetallic compounds such as Fe_3Si, Fe_5Si_3 and FeSi, which may have a close relation to a short range order in the liquid phase. Therefore, in order to clarify the relation of the local structure and the molar volume in the liquid Fe-Si alloys, synchrotron x-ray diffraction experiments were conducted with the use of a conical nozzle levitation technique. Liquid structure factors of the Fe-Si alloys indicate a correlation of medium range ordering with the increase of the Si content. Although the total molar volume expands with the increase of the Si content in these alloys, the concentration dependence of the average interatomic distance shows a minimum around 70 at.% Si content. To obtain more insight of liquid structure of the Fe-Si alloys, we performed structure analysis by using the reverse Monte Carlo method and the Honeycutt Andersen index (HA) method [3].

The HA analysis indicated formation of Fe atom-centered icosahedral structure in the composition range of 0-30 at.% Si. In addition, Si atom-centered tetrahedral structure can be found in the composition range of 90-100 at.% Si. The composition dependence of the local structure and the molar volume will be discussed in detail.

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POSTER 03 - Tuesday 18:15-20:00hrs Foyer

Criteria for predicting the viscosity of multicomponent liquid alloys

Jürgen Brillo[1]

[1] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany*

Viscosity is defined as the transport coefficient of momentum diffusion. There are several mathematical forms and phenomenological models describing its dependence on temperature and alloy composition. The latter models perform very differently. Depending on the materials system, a model can fail while others succeed and if the materials system is exchanged, it may be successful while the others fail. Hence, the criteria for selecting a successful model are not clarified yet.

In the present work, viscosity data is measured on pure liquid elements, binary and ternary alloys. The measurements are carried out using oscillating cup viscometry. Data is obtained as functions of temperature and, in case of alloys, of their compositions. The results are accurate within ± 20 %.

The results obtained for the pure elements are found in agreement with the Hirai law. Among the phenomenological models, the Kozlov model exhibits the best overall agreement with the measured isothermal viscosities of binary and ternary alloys. This model also works best for systems containing similar elements. In case of systems tending to demix, the Kaptay model works best and in the case of Al- based alloys with a strong attractive interaction, the Brillo/Schick model is the best choice. The majority of the investigated systems exhibit an ideal mixing behavior with respect to viscosity.

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POSTER 04 - Tuesday 18:15-20:00hrs Foyer

Multicomponent melts of metallurgical slags: computer simulation of the structure and properties

E.V. Dyuldina[1], B.R. Gelchinski[2], D.K. Belashchenko[3]

[1] *Magnitogorsk State Technical University, Magnitogorsk, Russia*

[2] *Institute of Metallurgy of UB of the Russian Academy of Science, Yekaterinburg, Russia*

[3] *Research Technological University "MISiS ", Moscow. Russia*

The casting efficiency and the ingot quality depend substantially on the correspondence between the physicochemical properties of the slags formed upon melting of slag-forming mixtures (SFMs), the chemical composition of the metal, and the casting conditions. The existing SFMs should be improved and new SFMs should be designed in order to meet the growing requirements imposed on the ingot quality and the growing range of metal grades. To solve this problem, one should have information on the dependences of the physicochemical properties and structure of a slag on the SFM chemical composition. Such information can be obtained using a microscopic theory of melts and modern computer simulation methods. Based on experimental data on the density, we performed molecular dynamics simulation of a melt of a multicomponent slag forming system at several temperatures. We are the first to perform molecular dynamics simulation of a SFM melt consisting of nine ions (Si, Ca, Al, Mg, K, Na, Fe, F, O) forming eight components (SiO_2–CaO–Al_2O_3–MgO–CaF_2–Na_2O–K_2O–FeO). The molecular dynamic simulation of multi-component melt industrial slagforming mixtures for the first time is realized. We constructed models for an eight-component SFM melt having 2001 atoms in a base cube with periodic boundary conditions at four temperatures and a fixed volume. The time step was $0.05t_0$, where t_0 is the internal time unit (7.608×10^{-14} s). The run length was 1000 steps. We calculated 50000–60000 steps to obtain time dependences of the average squared displacements of the particles. The system density was taken from our experimental data. The applicability of an ionic theory is caused by the significant difference in the electronegativities of oxygen (3.5 according to Pauling) and ordinary metals (0.9 for Na, 1.0 for Ca, 1.5 for Al, etc.). For example, for the CaO molecule, the difference in the electronegativities is ~2.5 and the ionicity is close to 76%. The ionicity of the SiO_2 molecule is ~51%. Therefore, slightly simplifying the situation, we can attribute a formal charge of $2e$ (e is the elementary charge) to an oxygen particle and formal charges of $2e$, $3e$, and $4e$ to Ca, Al, and Si particles, respectively. The interparticle interaction potentials were chosen in the Born–Mayer form, $u_{ij}(_r) = Z_iZ_je^2/r + B_{ij}\exp(-r/\rho_{ij}) + C_{ij}/r^6$, where r is the center distance, Z_i is the charge of the ith ion in units of elementary charge e, B_{ij} and ρ_{ij} are the repulsion parameters of the ionic shells of particles i and j, respectively, and C_{ij} are the parameters of the effective dipole–dipole interaction. The obtained model testifies to feeble temperature association structures of a researched melt. It is shown, that the computer model allows obtaining realistic enough pattern atomic structures of a slag melt. The developed model indicates a weak temperature dependence of the structure of the slag melt. We detected a high diffusion mobility of fluorine and sodium ions (to a lesser extent, potassium ions) as compared to other elements, and this diffusion mobility correlates with the partial pair correlation functions (PPCFs) of the corresponding oxides and fluorides. The computer model was shown to reflect the atomic structure of the slag melt: the main model parameters (PPCF peak positions and heights) agree well with the diffraction experimental data. The increased diffusive mobility of ions of fluorine and sodium (a little bit less ions of a potassium) on matching with other units which correlates with sort of the partial pair correlation functions appropriate oxides and fluorides is discovered.

POSTER 05 - Tuesday 18:15-20:00hrs Foyer

Surface tension and density of the molten thallium-lead-bismuth

R.Kh. Dadashev[1], D.Z. Elimkhanov[1], R.S. Dzhambulatov[2]

[1] Chechen State University, Grozny, Russia
[2]Chechen State Pedagogical University, Grozny, Russia

This paper experimentally studies the temperature and concentration dependence of surface tension and density of thallium-lead-bismuth melts on beam sections of Tl:Pb=1:9, 9:1. The surface tension is measured by using Pb-0000 lead, Tl-00 thallium, Bi-000 bismuth. Measurements were carried out from the liquidus temperature up to 773 K.

The researches were conducted in the combined device in which the surface tension is measured by the maximum pressure in a drop method and the density by an improved aerometer. The surface tension is defined by the maximum pressure in a drop method with high accuracy and the dispersion at the same time is 0,32 mJ/m^2.

As shown in work [1], a total error calculation of the surface tension measurement at 0,95 confidential probability are respectively 0,8%. The possible spread of experimental points for this device is caused by the measurement error of the density and the height of a metal column. The height of the column is measured repeatedly, the variation coefficient of this size is 0,1%. The density measurement error is 0,2%. Therefore, the spread of the experimental points received by one device should not exceed 0,3%.

The temperature dependence of the surface tension of the thallium-lead-bismuth ternary system is linear with a negative temperature coefficient.

The surface tension isotherms on the investigated sections of the concentration triangle are characterized by smooth curves without special points. With increasing bismuth content, the surface tension monotonously decreases. Bismuth is surface-active both in thallium and lead and in thallium-lead melts. However, its maximum surface activity in thallium is much more than in lead and increases linearly in the melts by replacing lead with thallium.

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POSTER 06 - Tuesday 18:15-20:00hrs Foyer

Aerodynamic-Electrostatic Hybrid Levitator

P. Fopp[1], D. Bräuer[1], J. Drescher[1], C. C. Yuan[1,2], and F. Kargl[1,3]

[1] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany*
[2] *Southeast University, School of Materials Science & Engineering, 211189 Nanjing, P. R. China*
[3] *Foundry-Institute, RWTH Aachen University, Intzestraße 5, 52072 Aachen, Germany*

An aerodynamic-electrostatic hybrid-levitator developed at DLR is presented. The levitator is designed to enable measurements of viscosity, surface tension and density of refractory and highly reactive liquid metal alloys, e. g. Al-Ti, in the laboratory. Electrostatic levitation (ESL) has several benefits compared with other levitation techniques regularly used at DLR for measuring thermophysical properties of liquids at high temperatures: i) compared with electromagnetic levitation in ESL no strong-fluid flow and sample distortions are present; ii) compared with aerodynamic levitation (ADL) the entire sample is visible.

However, ESL systems at DLR operate under high-vacuum conditions. Due to the environment conditions a large number of alloy systems, like those with low vapour pressure, are precluded from the measurement due to concomitant charge-loss. The same holds for many alloy systems with solid state phase transformations that typically lead to a sudden change of surface-charge and subsequently a loss of the sample.

A potential way to overcome this is to operate the ESL system under pressure and to melt the material before initiating ESL. A way to achieve both aims is to use a hybrid ADL-ESL system. For levitating oxides the Japanese Aerospace Agency (JAXA) has already developed such a system [1,2].

To this end we designed a new electrode system [3] for the hybrid ADL-ESL based on former in-house developments at DLR [4,5]. In first experiments it turned out that the Paschen law is only a rough approximation for high-voltage operation under a 5 bar Argon 5.0 atmosphere. For operation of standard-sized spheres of 2mm diameter a high voltage of up to 20kV is required. Electrical breakthrough occurs already at around 12kV, much lower than the theoretically predicited value using the Paschen law. The experiments predict a high-voltage breakthrough resistance of 20kV at 15 bar pressure for Argon.

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POSTER 07 - Tuesday 18:15-20:00hrs Foyer

Disorder trapping by rapidly moving phase interface in an undercooled liquid

P.K. Galenko[1], D.A. Danilov[2], I.G. Nizovtseva[1,3], K. Reuther[1] and M. Rettermayr[1]

[1] *Friedrich-Schiller-Universität Jena, Physikalisch-Astronomische Fakultät, D-07743 Jena, Germany*
[2] *Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany*
[3] *Ural Federal University, Laboratory of Multi-Scale Mathematical Modeling, 620000 Ekaterinburg, Russian Federation*

Disorder trapping is a known non-equilibrium phenomenon occurring during transformations of congruently melting ordered intermetallic compounds [1,2]. Especially, this phenomenon occurs during rapid crystallization of undercooled melts of intermetallics with a superlattice crystalline structure [3]. In such systems, the phase interface propagation is very sluggish at small undercoolings. The atomic attachment of atoms from the liquid to the phase interface needs short-range atomic diffusion since atoms have to sort them out to find the proper lattice place in the superlattice structure. If undercooling increases the non-equilibrium effect of disorder trapping leads to the formation of a metastable disordered structure. Experimental evidence of disorder trapping has been demonstrated by *in situ* diffraction studies using synchrotron radiation on levitation-processed samples, in which a transition from ordered to disordered growth at critical undercooling was unambiguously shown [4].

In the present work, using the approach to fast phase transformations [5], a diffuse interface model is developed on the basis of hyperbolic Allen-Cahn-type equations to describe (*i*) the rapid interface motion and (*ii*) the transition from ordered to disordered crystalline lattices formed from undercooled liquids. In the solutions of the model, pronounced disorder trapping by direct exchange of dissimilar atoms between sublattices is found at high interface velocities and large undercoolings. We show that a steep increase of the interface velocity exists at a critical undercooling connected with a sharp decrease of the order parameter that is consistent with previous experimental observations [4]. A discussion on trapping of anti-site lattice defects and vacancies at high interface velocity [6] is given.

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POSTER 08 - Tuesday 18:15-20:00hrs Foyer

Transition to amorphous structure and properties of Pd-based glass forming melts

P.K. Galenko(1), S. Koch(2,3), W. Dreier(2), M. Rettenmayr(1), D.M. Herlach(3),
M.V. Zamoryanskaya(4), A.V. Egorov(5), A.S. Senchenkov(5), E.V. Kharanzhevskii(6)

[1] *Friedrich Schiller University, Jena (Germany)*
[2] *German Aerospace Center, Cologne(Germany)*
[3] *Ruhr-University, Bochum (Germany)*
[4] *Ioffe Physical-Technical Institute, Russian Academy of Science, Saint-Petersburg (Russia)*
[5] *Federal Space Agency, Moscow (Russia)*
[6] *Udmurt State University, Izhevsk (Russia)*
Peter.Galenko@uni-jena.de

Experiments were performed to investigate the freezing of undercooled melts of Pd-based bulk glass forming alloys to the glassy state. Samples of Pd-based melts were studied to obtain the influence of cooling rate on the transition to the amorphous state. Processed in a multi zone electromagnetic vacuum furnace, the obtained samples were characterized by calorimetric methods and with respect to chemical inhomogeneity (microsegregation) and mechanical properties of the amorphous phases and nano-crystalline solid states. Temperature Time Transformation (TTT) diagrams are constructed which give the critical cooling rate to bypass crystallization and to solidify an amorphous alloy. The results are analyzed using models of nucleation and crystal growth. The work has been done within cooperative partnerships of ESA-European Space Agency (Project “MULTIPHAS”) and ROSKOSMOS-Russian Space Agency (Project “KINETIKA”). Financial support by the DLR Space Management within contract 50WM1140 is gratefully acknowledged.

POSTER 09 - Tuesday 18:15-20:00hrs Foyer

Ionic structure and atomic transport properties of liquid iron, nickel and iron-nickel alloys: a molecular dynamics investigation

N. Harchaoui[1], S. Hellal[1], O. Haddag[1], B. Grosdidier[2], and J. G. Gasser[2,*]

[1] *Laboratoire de Physique et Chimie Quantique (LPCQ), Département de Physique, Faculté des Sciences, Université Mouloud Mammeri, 15010 Tizi-Ouzou, Algérie*

[2] *Laboratoire de Chimie et Physique-Approches Multiéchelles des Milieux Complexes (LCP-A2MC). Institut de Chimie, Physique et Matériaux Université de Lorraine 1Bd Arago57070 Metz France*

To investigate the static structures and the atomic transport properties of 3-d band liquid transition metals, we carried out classical molecular dynamics simulations based on pseudopotential-derived interatomic forces. The calculated ionic structures of pure liquid iron and nickel and of Fe-Ni molten alloys are rather well described in comparison with existing X-ray or neutron diffraction experimental structures. We also reported the calculated temperature dependences of transport coefficients within the Green-Kubo formalism. The simulation results of shear-viscosity are also very close to available experimental values. Concerning the self-diffusion coefficients for pure liquid metals and the inter-diffusion one for molten alloys, and due to the lack of experimental results, our computer simulations can only be compared to other theoretical predictions.

Keywords: model pseudopotentials, molecular dynamics, liquid transition metals and alloys, atomic transport properties, shear viscosity, self-diffusion, inter-diffusion, Green-Kubo relationship

*Corresponding author: jean-gorges.gasser@univ-loraine.fr, Tel: + 33 (0)3 87 31 58 59, Fax+ 33 (0)3 87 31 58 84

POSTER 10 - Tuesday 18:15-20:00hrs Foyer

The possibility of ab initio molecular dynamics for predicting the properties of liquid s-, s-p, d- metals including extreme states

Boris R. Gelchinski, Anatoly A. Yuryev

Institute of Metallurgy of UB of the Russian Academy of Sciences, Ekaterinburg, Russia

For the development of modern technology requires information about various properties of substances. Of particular interest are the calculations for the case of extreme states of matter, where the experimental data are difficult to obtain or even impossible. Considerable progress in theoretical studies of liquid metals in recent years related to the method of ab initio molecular dynamics, Car and Parrinello proposed [1]. Significant progress has been achieved through the use of supercomputers and parallel computing technology. In this research simulations were performed using the SIESTA program [2], based on the basis of atom-orbitals, which was used earlier [3,4]. It should be noted that unlike classical molecular dynamics, ab initio approach immediately calculated forces on individual atoms, and thus, there is no problem with the construction of the pair potentials. Additionally, the uniqueness of our approach is that it works in a wide range of temperatures and pressures, in particular alkali metal density may vary more than 10 times that allows to study how much compressed state and supercritical fluids. The test objects were selected by molten metals belonging to different groups: the alkali Na and Cs, polyvalent Pb and Bi, and transition Cu and Ti metals. It was built supercell containing 250-500 atoms, and calculate the total energy, pressure, radial distribution function of the atoms, the self-diffusion coefficient, density of electronic states, modeling was carried out over a wide temperature and pressure range, including extreme. The results are compared with experimental data.

The work was performed as part of the State job IMET UB RAS, theme N 0396-2015-0080, as well as with the financial support of the RFBR, the project 15-03-04182, the Program for Basic Research, UB RAS, project 15-7-3-15.
Our work was performed using «Uran» supercomputer of IMM UB RAS.

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POSTER 11 - Tuesday 18:15-20:00hrs Foyer

An ab-initio molecular dynamics study of several static and dynamic properties of liquid palladium and platinum.

M.R. Molla[1,2], A.Z.Z. Ahmed[1], G.M. Bhuiyan[1], L.E. González[3] and D.J. González[3]

[1] *University of Dhaka, Department of Theoretical Physics, Dhaka, Bangladesh*
[2] *University of Dhaka, Department of Mathematics, Dhaka, Bangladesh*
[3] *Universidad de Valladolid, Dept. Fisica Teorica, Valladolid, Spain*

Several static and dynamic properties of liquid Pd and Pt at thermodynamic states near their respective melting points have been calculated by ab-initio molecular dynamics simulations. The calculated static structure shows a very good agreement with the available experimental data [1]. As for the dynamic properties, results are reported for both single and collective dynamics. The calculated dynamic structure factors show side peaks which point to the existence of collective density excitations. Finally, several transport coefficients have also been evaluated and compared with the corresponding experimental data available [2].

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POSTER 12 - Tuesday 18:15-20:00hrs Foyer

Orbital-free *ab initio* molecular dynamics study of the free liquid surface of Sn. From pseudopotential generation to structural and dynamic properties.

Beatriz G. del Rio[1] and Luis. E. González[1]

[1] *Universidad de Valladolid, Dept. Fisica Teórica, Valladolid, Spain*

We report results of an orbital-free *ab initio* molecular dynamics (OF-AIMD) study of the free liquid surface of Sn at 1000K and 600K. A key ingredient in the OF-AIMD method is the local ionic pseudopotential describing the ions-valence electrons interaction. We have developed a force-matching method [1] to derive a local ionic pseudopotential suitable to account for a rapidly varying density system, such as a free liquid surface. We obtain very good results for structural properties, such as the reflectivity and the characteristic shoulder it presents in X-ray experiments. We study the origin of this shoulder through the intrinsic density profile. Moreover we have been able to study *ab initio* for the first time the evolution in some dynamical properties as we move from the central region where the system behaves like the bulk liquid, to the free liquid surface.

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POSTER 13 - Tuesday 18:15-20:00hrs Foyer

Theoretical and experimental investigations of electrical resistivity of molten BiMn alloy

J. Ataati[1], B. Grosdidier[2], M. Mayoufi[3], S. M. Osman[4] and A. Ben Abdellah[1,2,5]

[1] Innovation and Management of Industrial Systems, Abdelmalek Essaadi University, College of Sciences and Techniques of Tangier , P.O. Box 416, Postal code 90000, Tangier Morocco.
[2] Laboratoire de Chimie Physique – Approche Multi-Echelle des Milieux Complexes,
Institut Jean Bariol, Université de Lorraine, Institut de Chimie, Physique et Matériaux 1 Bd Arago 57078 Metz Cedex 3, France.
[3] Laboratoire de Chimie des Matériaux Inorganiques, Faculté des Sciences, Université Badji-Mokhtar Annaba, BP 12 Annaba 23000, Algérie.
[4] Physics Department, College of Science, Sultan Qaboos University, P.O. Box 36, Postal Code 123,
Al-Khod, Muscat, Sultanate of Oman.
[5] Université Internationale de Rabat, Parc Technopolis Rabat-Shore, 11100 Sala El Jadida, Moroc.

We present the experimental and theoretical results of the electrical resistivity of liquid BiMn alloy at wide range of temperatures. First, we present results of resistivity measurements of pure liquid bismuth and five liquid alloys $Bi_{(1-x)}Mn_x$, (x = 0.1, 0.2, 0.3, 0.4 and 0.5). The resistivity value increases from $127.78\ \mu\Omega \cdot cm$ for pure bismuth, (x=0.0), to $210.79\ \mu\Omega \cdot cm$ for the alloy $\mathrm{Bi_{0.50}Mn_{0.50}}$. We measured the Resistivity-Temperature coefficient, $d\rho(T)/dT$, at $T = 1060\ °C$. The shift of $d\rho(T)/dT$ is found to be at Mn concentrations between $20\,\%\,\mathrm{at.\,Mn}$ and $30\,\%\,\mathrm{at.\,Mn}$. For all five alloys under investigation, the electrical resistivity does not display anomaly. We proposed theoretical model to calculate the resistivity of these alloys based on neutron scattering observations that manganese could exist in different spin states with effective spin of manganese atoms can be averaged around 1.2 in $Bi_{(1-x)}Mn_x$ for all values of *x*. Consequently, $Bi_{(1-x)}Mn_x$ alloys are treated as five spin components alloys. In the present theoretical calculations of resistivity suggest that the original Faber Ziman formula, originally designed for binary alloy to be extended to five-component formalism. The theoretical predictions for resistivity are in extremely good agreement with our experimental values.

POSTER 14 - Tuesday 18:15-20:00hrs Foyer

Liquid-solid interface confinement and its effect on the crystallization kinetics: Linking molecular-dynamics simulation and phase-field modeling

M. Guerdane[1]

[1] Karlsruher Institut für Technologie, Institut für Angewandte Materialen (IAM-CMS), Karlsruhe, Germany

One of the central challenges in multiscale modeling, consists of how to bridge the gap among atomistic and macroscopic approaches in order to ensure that the descriptions at all levels are quantitatively consistent with each other. In our work, we carry out this task for the hierarchical coupling approach that combines molecular dynamics (MD) with phase-field (PF) modeling. The consistency analysis is achieved by detailed comparisons of quantitative predictions of the considered modeling methods for the kinetics of crystal growth from the melt. The latter is a typical multiscale problem in materials physics. The MD simulations provide the physical quantities needed for the construction of the multiscale model. Of central importance are the free-energy values of the bulk liquid and of the solid-liquid interface. In particular, we link MD to PF modeling in order to estimate quantitatively the influence of the solid-liquid interface confinement (reduced diffusion in liquid) and of the 'in-plane' solid-liquid interface ordering on the growth kinetics. These issues will be illustrated for the binary alloy NiZr. Our observations provide evidence for a strong link between the interface ordering and the short-range order in the bulk liquid. These findings are of relevance for the alloy-growth kinetics as well as for the fundamental issue of local (atomic) structure of metallic liquids.

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POSTER 15 - Tuesday 18:15-20:00hrs Foyer

Thermodynamic properties of liquid Zr-Ni alloys

P. Heintzmann[1], F. Yang[1], S. Schneider[1], F. Kargl[1], B. Schillinger[2], T. Unruh[2] and A. Meyer[1]

[1] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany*

[2] *Forschungsneutronenquelle Heinz Maier-Leibnitz (FRMII), Technische Universität München, 85747 Garching*

In order to understand glass formation in metallic melts a precise knowledge of structural as well as dynamical properties, such as structure factors, diffusion coefficients and viscosity, of these melts is a prerequisite. Typically bulk metallic glass (BMG) formers consist of several components, exhibiting a high complexity. For studying multicomponent glass forming melts such as Vit1/Vit4 the binary Zr-Ni system has evolved as a model system, since dynamics are comparable to these BMGs and the structure can be described by experimental accessible partial structure factors.

Complementing experimental partial structure factors [1] as well as self-diffusion measurements of Zr [2] and Ni [3] we have determined interdiffusion coefficients of Zr-Ni alloys utilizing neutron and X-ray radiography. With this we have obtained a full set of diffusion coefficients for two Zr-Ni compositions. Our data show an increasing inter- to self-diffusion coefficient ratio with increasing Zr content, while the thermodynamic factor is decreasing. This can be explained by an increase of cross correlations. We are able to show that the empirical Darken equation overestimates the interdiffusion in the analyzed systems. For dense liquids it seems that the cross correlation contribution to the kinetic coefficient may not be neglected due to the highly cooperative nature of the mass transport processes. Our data confirm results of mode coupling theory calculations [4] using experimental structure factors as input.

We have studied the composition dependence of the viscosity of liquid Zr-Ni alloys using the oscillating drop technique with ground based electrostatic levitation (ESL). For the analyzed alloys our results show an increasing viscosity with decreasing Zr content. Unlike the ternary Zr-(Co,Ni)-Al melts, here an average molar volume (packing fraction) can capture the composition dependence of the liquid viscosity qualitatively. With a systematic analysis of the oscillating drop technique using ESL we can show that reliable viscosity data can be obtained as long as internal viscous damping of a single oscillation mode of a levitated drop dominates external perturbations yielding a measurement range of viscosity of ~ 10 – 250 mPa s.

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POSTER 16 - Tuesday 18:15-20:00hrs Foyer

Effect of Antimony addition on thermal properties of GeTe glasses

L. Heireche[1,2], M. Belhadji[2], M. M. Heireche[2,3] .

[1]*Département de physique, Ecole préparatoire en sciences et techniques d'Oran, Oran, Algeria.*
[2]*Département de physique, faculté des sciences exactes appliquées Université d'Oran 1 Ahmed Ben Bella, Oran, Algeria.*
[3]*Département des sciences exactes, Ecole normale supérieure d'Oran,Oran, Algeria.*

Abstract:

Glass chalcogenide have become the subject of intensive research because of their potential applications in technologies [1, 2]. Several studies have developed to understand their properties [3,5], the thermal properties are very important which are based on thermoanalytical techniques such as differential thermal analysis DTA, or differential scanning calorimetry DSC. In general the chalcogenide glasses are based on three chalcogen elements Se,Te,S in conjunction with more electropositive elements as As, Sb and Bi [6].The effect of antimony Sb addition on GeTe glasses are experimentally studied using Differential Scanning Calorimetry (DSC) under non-isothermal conditions at different heating rate (5, 7, 10 °C/min). The thermal properties, such as glass transition temperature, average coordination number and thermal stability are evaluated using different methods [7,8], the glass transition temperature and peak crystallization temperature are found to increase with increasing heating rate. The dimensionalities of growth m and activation energy of crystallisation Ec have been determined from Matusita model [9]. The role of Sb in glass formation of GeSbTe chalcogenide systems are presented and discussed in detail.

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POSTER 17 - Tuesday 18:15-20:00hrs Foyer

The dispersion relation of the acoustic mode in liquid Ca and liquid Cd

Masanori Inui[1], Yukio Kajihara[1], Koji Kimura[2,*], Kazuhiro Matsuda[2], Tetsu Miyatake[2],
Ayano Chiba[3], Shinya Hosokawa[4], Satoshi Tsutsui[5], and Alfred Q. R. Baron[6,5]

[1] *Graduate School of integrated Arts and Sciences, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-8521, Japan*

[2] *Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan*

[3] *Department of Physics, Keio University, Yokohama 223-8522, Japan*

[4] *Department of Physics, Graduate School of Science and Technology, Kumamoto University, Kumamoto 860-8555, Japan*

[5] *Japan Synchrotron Radiation Research Institute, SPring-8, Sayo-gun, Hyogo 679-5198, Japan*

[6] *Materials Dynamics Laboratory, RIKEN SPring-8 Center, Sayo-gun, Hyogo 679-5148, Japan*

We have investigated the atomic dynamics in liquid Ca and liquid Cd, by utilizing inelastic x-ray scattering (IXS). The strong chemical corrosion and high vapor pressure of liquid Ca, and a very large absorption cross section of ^{113}Cd for neutron make inelastic scattering measurements for these liquids difficult. However our sample cells developed for x-ray scattering measurements of supercritical metallic fluids overcame the experimental difficulties, and the dynamic structure factors $S(Q,E)$ with reasonable statistics were obtained for these divalent liquid metals. IXS measurements were conducted at BL35XU of SPring-8 in Japan. A highly monochromatized x-ray beam (21.747 keV) was incident on the sample, and scattered x-rays were collected by twelve analyzer crystals, with the energy resolution of approximately 1.5 meV. The Q resolution was set 0.4 nm^{-1} at low Q. For both liquids, $S(Q,E)$ at low Q exhibits a central peak with a shoulder or small hump clearly visible on each side, and the inelastic excitation disperses with increasing Q. The $S(Q,E)$'s were deconvoluted using the model function composed of Lorentzian and the damped harmonic oscillator functions, and the excitation energy of the acoustic mode was determined. We compared the present results with the previous ones of liquid alkaline earth elements obtained experimentally [1,2] and theoretically [3]. We will discuss the dispersion relation of the acoustic mode in divalent liquid metals.

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**present address: Nagoya Institute of Technology, Nagoya 466-8555, Japan*

POSTER 18 - Tuesday 18:15-20:00hrs Foyer

Inelastic x-ray scattering measurements of liquid water-glycerol mixtures

Y.Kajihara[1], N.Shibata[1], M.Inui[1], K.Matsuda[2], S.Tsutsui[3]

[1]*Graduate School of Integrated Arts and Sciences, Hiroshima University, Higashi-Hiroshima 739-8521, Japan*

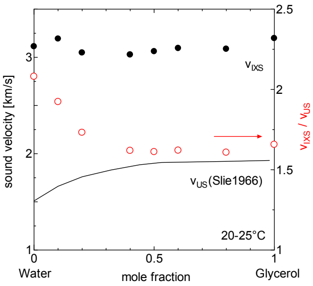
[2]*Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan*

[3]*Japan Synchrotron Radiation Research Institute, SPring-8, Sayo, Hyogo 679-5198, Japan*

Liquid water-monohydric alcohol mixtures exhibit many thermodynamic anomalies [1]. For example, a maximum appears at around 10-20% alcohol mole fraction in the concentration dependence of the ultrasonic sound velocity (v_{US}, frequency is MHz) [2,3]. The anomalies have been believed to arise from structural origin [1] and special clathrate structure at the composition was proposed [4], but there has been no direct experimental observation and the discussion has not been concluded.

We have studied liquid water-ethanol and water-methanol mixtures [5] by using inelastic x-ray scattering (IXS) technique at BL35XU/SPring-8 in Japan and obtained sound velocities (v_{IXS}, THz). In both alcohol systems, there is no peak or anomaly in composition and temperature dependences of v_{IXS}. Here we focus on a parameter, the ratio of the two sound velocities (v_{IXS} / v_{US}), which we name the strength of "fast sound [6]". It shows smaller value (about 1.3) at alcohol-rich region but rapidly increases with decreasing alcohol concentration especially below 20% and reaches to about 2. The result indicates that the intensity of the relaxation in the mixtures is largest at pure water. Thus we have concluded that the anomaly of v_{US} in the mixture does not arise from structural anomaly at the composition, but originates from the anomalous slowing down of v_{US} in pure water itself.

In the present study, we have carried out IXS measurements for water-glycerol mixtures. Glycerol is a trihydric alcohol, and the mixtures do not show a maximum in the composition dependence of v_{US} [7] (line in the figure). Consequently, the relationship between the water-glycerol and water-monohydric alcohols mixtures has not been discussed before. The obtained v_{IXS} is almost constant, being independent of the composition (closed circles), and the strength of fast sound (open circles) becomes the largest at pure water and gradually decreases with increasing mole fraction of glycerol. This result is similar to those of water-monohydric alcohol mixtures, and indicates that our interpretation is also applicable to this system.



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POSTER 19 - Tuesday 18:15-20:00hrs Foyer

Quasicrystal nucleation in an intermetallic glass-former

R. Kobold[1,2a], W. Hornfeck[1b], M.Kolbe[1c] and D.M. Herlach[1,2d]

[1] *Institute of Materials Physics in Space, German Aerospace Center DLR, 51147 Köln, Germany*

[2] *Institute of Experimental Physics IV, Ruhr-Universität Bochum, 44780 Bochum, Germany*

The solidification of the intermetallic, congruently melting binary alloy NiZr is studied in a temperature regime of the undercooled melt between the melting and the glass transition temperature. The NiZr system is well known as a good glass former in a broad concentration range of 30 to 70 at.% Zr. We use electrostatic levitation technique to melt and undercool samples with a diameter of 3 - 4 mm under ultra-high-vacuum conditions. Containerless processing is an effective tool for undercooling metallic melts far below their equilibrium melting temperatures since heterogeneous nucleation on container walls is completely avoided. During crystallization the release of the heat of fusion leads to a rapid increase of the temperature at the solid-liquid interface. This makes the solidification front visible by optical observation. The rapid propagation of the solidification front is recorded by using a high-speed camera with a frame rate of 10.000 (1024x744 pixels) frames per second. At high undercoolings the solidification front of NiZr shows features, which make the investigation of its solidification behavior particularly interesting. We observed the growth of a solidification front with 10-fold symmetry at large undercoolings of approximately 300 K and a cooling rate of 35 K/s. A detailed picture of the solidification process was gained, correlating the macroscopic decagon-shaped growth front to the microscopic dendrite growth into a tenfold twinned microstructure and eventually to the crystal structure, whose metrical properties explain the mechanism of twinning, at the atomic scale.

An atomistic twin model is proposed which has the potential to represent a missing link connecting quasicrystals and multiple twinned structures shedding light on intermediate states of order between glasses, crystals and their twins, and quasicrystals.

Funding by Deutsche Forschungsgemeinschaft, under grant HE1601/28 is gratefully acknowledged.

POSTER 20 - Tuesday 18:15-20:00hrs Foyer

Pressure dependence of the static structure of liquid GeTe based on *ab initio* molecular dynamics simulations

Akihide Koura[1] and Fuyuki Shimojo[1]

[1] *Department of Physics, Kumamoto University, Kumamoto 860-8555, Japan*

Germanium tellurides are interesting materials because of its electronic properties and the fast phase transition feature, e.g., $Ge_2Sb_2Te_5$. At room temperature, crystalline GeTe has an A7 structure, which is obtained by distorting a rocksalt (fcc) structure in the (111) direction. This structural change is known as Peierls distortion. When the temperature increases up to around 700 K, the Peierls distortion is dissolved and the structure changes to rocksalt. With increasing temperature further, crystalline GeTe melts at about 1000 K and the Peierls-type distorted structure appears again in the liquid state [1].

On the other hand, the compression also induces the structural change of crystalline GeTe. When pressure increases up to around 3 GPa, GeTe changes from the A7 to rocksalt structure. It has been suggested that, under further compression, GeTe eventually becomes bcc (CsCl-type) structure at 40-50 GPa, through several structural changes [2]. The pressure dependence of the structure of the liquid state was also reported by X-ray diffraction measurement [3], which suggests that the structural change in the liquid state is different from that in the crystalline state. However, the details are not clarified yet.

In this study, we investigate the pressure dependence of the structure of liquid GeTe based on *ab initio* molecular dynamics simulations, in which the electronic structure is calculated in the framework of the density functional theory with the generalized gradient approximation. The temperature and pressure ranges are from 1000 to 4000 K and from 0 to 250 GPa, respectively.

The pressure dependence of the calculated static structure factors is in excellent agreement with experimental results [3]. Our simulation shows that the structure of liquid changes in two stages under pressure. In the first stage below 12 GPa, the Peierls-type distortion in the liquid state was completely dissolved. In this pressure range, the nearest neighbor (NN) distance becomes longer, and the semiconducting properties are maintained. It seems that semiconductor-metallic transition occurs at approximately 12 GPa. In the second stage above 12 GPa, the NN distance shortens. The coordination number reaches about 13.7 at 250 GPa, which is quite similar to that of CsCl-type crystalline state with taking the second neighbor into account.

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POSTER 21 - Tuesday 18:15-20:00hrs Foyer

Investigation of electrical properties of amorphous $AgGe_{1+x}As_{1-x}(S+CNT)_3$ composites on AC

Kurochka K. V. and Melnikova N. V.

Ural Federal University, Institute of natural science, Ekaterinburg, Russia

Multicomponent silver chalcogenides are widely applied now in various electronic devices such as elements of operational and nonvolatile memory, solar cells, etc. The addition of carbon nanotubes leads to improvement in microhardness and electronic characteristics of materials [1-3].

In this work the electrical properties of glassy $AgGe_{1+x}As_{1-x}(S+CNT)_3$ x = 0.4; 0.5; 0.6 composites containing carbon nanotubes (CNT) have been considered. Synthesis and attestation of these materials are described in [2, 4].

In this report the influence of electrode materials on the impedance of the cell with glassy $AgGe_{1+x}As_{1-x}(S+CNT)_3$ x = 0.4; 0.5; 0.6 materials were studied. Investigations were carried out at room temperature in a wide range of frequencies (from 1 Hz to 32 MHz) of AC electric field in cells with copper, graphite, silver and gold electrodes by using of amplitude-phase analyzer Solartron 1260A.

Furthermore, studies of electrical properties were performed at temperature range from 10 to 300 K in the cell with silver electrodes. The temperature intervals corresponding to the beginning of an appreciable ion transport as well as features in the behavior of the electrical properties have been established.

The study was supported by the Foundation for Assistance to Small Innovative Enterprises in Science and Technology and by the Russian Foundation for Basic Research, projects 16-02-01137 and 16-02-00857.

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POSTER 22 - Tuesday 18:15-20:00hrs Foyer

Effects of thickness on structure and magnetic property of Fe-Y-B thin films

S.Y. Liu[1], Q.P. Cao[1,*], X.D. Wang[1], D.X. Zhang[2], Q.M. Su[3], G.H. Du[3] and J.Z. Jiang[1,*]

[1] International Center for New-Structured Materials (ICNSM) and State Key Laboratory of Silicon Materials, Zhejiang University and Laboratory of New-Structured Materials, School of Materials Science and Engineering, Zhejiang University, Hangzhou, People's Republic of China

[2] State Key Laboratory of Modern Optical Instrumentation, Zhejiang University, Hangzhou, People's Republic of China

[3] Key Laboratory of the Ministry of Education for Advanced Catalysis Materials, Institute of Physical Chemistry, Zhejiang Normal University, Jinhua, China

Iron-based amorphous alloys have been widely investigated because of their excellent soft magnetic properties, high mechanical properties, strong corrosion resistance and low prices [1-3]. Recently, bulk-sized ternary Fe-X-B (X=Sc, Y, Dy, Ho, Er) amorphous alloys, with minor addition of rare earth elements, were successfully developed, and Fe-Y-B possessed the relatively high potential in industrial applications due to low cost [4,5]. However, little research has been done into its film counterpart, which may be used in MEMS and NEMS. The influences of film thickness on structure and magnetic property of Fe-Y-B thin films, deposited on Si substrate by DC magnetron sputtering, was systematically investigated. The 283 nm-thick film was in fully amorphous state, and nanocrystals gradually appeared in the amorphous matrix with increasing thickness. The increase in the thickness makes Fe-Y-B thin film magnetically softer, with the decreased coercivity and increased magnetic permeability, and the increased conductivity, resulting in the reduction of skin depth and consequently the enhanced MI effect. The increase of magnetic softness and MI effect with the film thickness could be associated with the annealing effect during the sputtering process and the presence of nanograins. This work may be of benefit to development of micro-sized magnetic actuators.

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POSTER 23 - Tuesday 18:15-20:00hrs Foyer

Short range order peculiarities and thermal expansion of liquid metals

I. Shtablavyi, U. Liudkevych, S. Mudry

Ivan Franko National University of Lviv, Department of Metal Physics, Lviv, Ukraine

It is well known that the structure of densely packed metals and their alloys in liquid state little differs from the structure in the crystalline state. On other hand, melting of loosely packed metals is accompanied by some compaction of the structure, leading to the reduction of interatomic distances at temperatures close to the melting point. Further heating leads to a decrease in the density of the alloy that is the result of thermal expansion of melt.

For crystalline metals a measurements of its crystal lattice parameter at different temperatures can be used for calculation of thermal expansion coefficient. Similarly, the coefficient of thermal expansion could be investigated for liquid metals. But contrary to crystals in which atomic distribution is determined by lattice parameters, in liquid state there is a set of values of interatomic distances in the first coordination sphere, distribution of which is determined by profile of the pair correlation function first peak. Moreover, as was established by means of diffraction and computer simulation methods, increase of temperature in many cases is accompanied by a decrease of interatomic distances and coordination numbers. Such structural changes are associated with increasing of free volume beyond the first coordination sphere.

In this work the structural changes of fusible liquid metals and their alloys are investigated in a wide temperature range by means of X-ray diffraction method and reverse Monte Carlo method. It was revealed nonmonotonous changes of interatomic distances and coordination numbers for bismuth and indium, while their alloys are characterized by monotonous decrease of these parameters. For a more detailed study of the distribution of free volume in the investigated melts, reverse Monte Carlo method has been used.

POSTER 24 - Tuesday 18:15-20:00hrs Foyer

Neutron and X-ray scattering Study of Isotope Enriched Glassy $Sm_4Ti_9O_{24}$

Kenji. Maruyama[1], Yasutomo Arai[2], Satoshi Hiroi(Sato)[3], Mayumi Sanada[1], and Keiji Itoh[4]

[1] Department of Chemistry, Faculty of Science, Niigata University, Niigata, JAPAN
[2] ISAS, Japan Aerospace Exploration Agency, Tsukuba, Ibaraki, JAPAN
[3] Toyota Technological Institute, Nagoya, JAPAN
[4] Graduate School of Education, Okayama Univ., Okayama, JAPAN

The high refractive-index glass $Sm_4Ti_9O_{24}$ is one of key elements for downsizing digital cameras, an endoscope and etc. In order to obtain the structural information of the coordination structure of oxygen atoms around metal atoms, Ti and Sm, is required. Recently, the total neutron scattering measurements for glassy $Sm_4Ti_9O_{24}$ were performed with the high intensity total scattering spectrometer NOVA (BL21 at J-PARC) [1]. Three independent structure factors $S_{ij}(Q)$ for $Sm_4Ti_9O_{24}$ were able to be obtained with isotope substituted samples. However, the local structure around Sm atoms contained large uncertainty because of small scattering lengths of Sm isotopes.

In this study the structural data from X-ray scattering measurements were also combined with neutron scattering data In order to compensate this weak point. After performing the reverse Monte Carlo modeling all six partial structure could be obtained. The local structure analyzed with the 3D structure model will be reported

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POSTER 25 - Tuesday 18:15-20:00hrs Foyer

Molecular dynamics study on AgI-AgPO$_3$ glass and its melt

Shigeki Matsunaga

National Institute of Technology, Nagaoka College, Division of General Education, Nagaoka, Japan

The superionic conducting glasses have attracted much attention for many years as a promising candidate for the application to solid state batteries or indication devices. Above all, a lot of examinations have been performed on the silver iodide – silver phosphate series, (AgI)x(AgPO3)1-x, because of some advantages. For example, the glass transition temperature is low, which varies from 350K to 430K as x increases. The ionic conductivity at room temperature is about 10^{-2} S cm^{-1}, which is comparable to that of liquid electrolytes.

Neutron scattering experiment and Reverse Monte-Carlo (RMC) analysis have revealed that the large structure change has occurred around the glass transition temperature. The tetrahedral structure PO$_4$ exists on the glass state. The infinite random chain of PO$_4$ tetrahedra is formed in the glass state, with Ag+ ions embedded in the PO$_4$ network. Ag+ ions are expected to hop one Ag-O bond to another. Ag-Ag correlation is also observed in the glass state.

The molecular dynamic (MD) simulations have also been adopted to simulate the glass transition of the AgI based conducting glass. By means of MD, not only the structure of glass state, but also the transport properties of ions can be discussed. The BMH type potentials have been adopted for this purpose. For (AgI)x(AgPO3)1-x glass, however, no MD simulation has been performed, to the best of our knowledge. In this study, we wish to show the MD simulation results for (AgI)x(AgPO3)1-x in their molten and glass state. The structure and transport properties will be discussed.

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POSTER 26 - Tuesday 18:15-20:00hrs Foyer

Shear Viscosity of Liquid Potassium and Cesium: a Simulation Study

N. Meyer[1], H. Xu[1] and J.-F. Wax[1]

[1] *University of Lorraine-Metz, Laboratoire de Chimie Physique-A2MC, Metz, FRANCE*

The shear viscosity as a function of temperature and density is studied for liquid potassium and cesium. Calculating the stress autocorrelation function by equilibrium molecular dynamics simulations and using Green-Kubo formula, the shear viscosity value is obtained. The interionic interactions are calculated using Fiolhais potential [1]. They are validated by comparison between simulation and available experimental data along the liquid-gas coexistence curve. Then the viscosity behavior is studied for each metal along three different isochoric lines and one isotherm. We observe that the relation proposed by Meyer et al. [2] for Na reproduces qualitatively and quantitatively well the behavior of the viscosity for K and Cs over a wide range of the liquid phase.

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POSTER 27 - Tuesday 18:15-20:00hrs Foyer

First-principles study of amorphization of stishovite under tension

Masaaki Misawa[1], Fuyuki Shimojo[1], Aiichiro Nakano[2], Rajiv K. Kalia[2] and Priya Vashishta[2]

[1] *Department of Physics, Kumamoto University, Kumamoto, Japan*

[2] *Collaboratory for Advanced Computing and Simulations, University of Southern California, Los Angeles, USA*

Stishovite, a high-pressure crystalline polymorph of silica, is one of the hardest oxide materials [1]. Such a hard ceramic made from Earth-abundant material has a high potential of providing sustainable supply for mechanical and structural applications. Unfortunately, its brittleness has hindered practical application of stishovite so far. Recently, Nishiyama *et al*. synthesized a nano-structural form of stishovite named nano-polycrystalline stishovite (NPS) [2]. NPS exhibits high fracture toughness while retaining high hardness. The toughening mechanism has been hypothesized to originate from crystal-amorphous transformation. Under high tensile stress near a crack tip, metastable stishovite undergoes structural transformation to amorphous silica with a large volume expansion. The expanded amorphous silica covers crack tip and prevents crack extension. It was reported that the toughening mechanism is effective even if a crack length is on the order of nm [3]. The hypothetical amorphization-induced toughening relies critically on rapid amorphization to catch up with fast crack propagation. However, crystal-amorphous transformation dynamics under tension elusive.

We performed first-principles molecular dynamics simulations of single-crystalline stishovite with isotropic volume expansion in order to investigate the crystal-amorphous transformation dynamics under tension. In the simulations, rapid amorphization was observed within 1.5 ps. To understand structural and energetic properties of amorphous phase, the energy-volume relation and the coordination number of Si and O atoms were investigated. Furthermore, we also study reaction coordinates along the phase transformation by using the nudged elastic band method to understand the amorphization pathway. The amorphization-induced toughening mechanism found here is likely to operate in various other materials.

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POSTER 28 - Tuesday 18:15-20:00hrs Foyer

Containerless processing of BMG forming binary alloys

Akitoshi Mizuno[1*], Takeshi Harada[1], Daichi Aoshima[1], Masahito Watanabe[1]

[1] *Gakushuin University, Department of Physics, Tokyo, Japan*

It was empirically known that multicomponent alloys with three or more elements should be prepared to produce bulk metallic glasses (BMGs). However, recent experimental studies have shown that BMGs can be formed even from binary alloys as shown in Zr-Cu system [1]. In addition, it was reported that the glass-forming ability (GFA) of several Zr-based alloys can be improved by controlling the oxygen content in the alloy [2]. Recently, we succeeded in producing binary Zr-Cu BMG at peculiar compositions for spherical samples with a diameter of about 2 mm by using an aerodynamic levitation (ADL) technique. In the present study, therefore, we have investigated the influence of oxygen content on the GFA of Zr-Cu alloys in the containerless solidification process. The doping level of oxygen from 0.2 to 0.7 at.% affected the undercoolings and hence the GFA of the liquid Zr-Cu alloys. Slight amount of oxygen in Zr about 0.3 at.% enhanced the GFA of the alloys and BMG samples were made over wider composition range. In addition, the critical cooling rate for producing BMG by containerless processing was reduced when the oxygen content increased from 0.2 to 0.3 at.%. To obtain more insight into the GFA of Zr-Cu BMGs, we conducted in-situ synchrotron x-ray diffraction experiments during containerless processing using the ADL technique. We performed millisecond order time-resolved x-ray diffraction measurements with a two-dimensional detector to observe relative variations of structure during the solidification from the undercooled liquid. In the case of 0.2 at.% oxygen content, the B2 and the metastable fcc-Zr_2Cu phases precipitated during solidification of the $Zr_{53}Cu_{47}$ alloy. Subsequently, the martensitic transformation from the B2 phase to the B19' phase was observed with decreasing temperature. In contrast, fully vitrification was observed of the $Zr_{53}Cu_{47}$ alloy with the oxygen content of 0.3 at.%. The relation between the amount of oxygen and the GFA will be discussed from the statistical thermodynamic point of view.

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** Present address: National Institutes of Technology, Hakodate College*

POSTER 29 - Tuesday 18:15-20:00hrs Foyer

Structure of Liquid Rhodium

Junpei T. Okada[1,2], Y. Watanabe[3], T. Ishikawa[4], S. Kohara[5], P.-F. Paradis[4], and S. Nanao[3]
[1] *Institute for Materials Research, Tohoku University, Sendai, Japan*
[2] *PRESTO, JST, Kawaguchi, Japan*
[3] *Institute of Industrial Sciences, The University of Tokyo, Meguro-ku, Japan*
[4] *Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency, Tsukuba, Japan*
[5] *Synchrotron X-ray group, National Institute for Materials Science, Hyogo, Japan*
[6] *Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo, Japan*

Levitation and containerless methods enable experiments on high-temperature liquids without contamination effects from containers. The structure factor S(Q) and the pair distribution function g(r) has been measured for liquid rhodium at 2300K using a high temperature electrostatic levitator (HTESL). The HTESL levitates a spheroid sample of 2 mm diameter in a high vacuum environment (approximately 10^{-5}Pa) using electrostatic forces via a feedback computer control. The sample was heated and melted using the focused radiation of three 100W semiconductor laser beams emitting at 808nm. The temperature was controlled with an accuracy of 15K and measured by pyrometry at wave lengths of 0.96 nm. The experiments were performed at the BL04b2 beamline of SPring-8 and S(Q) was obtained in the Q range of 1-16 Å^{-1}.

POSTER 30 - Tuesday 18:15-20:00hrs Foyer

Velocity Autocorrelation Function in Supercooled Liquids: Long-time tails and Anomalous Shear-wave Propagation

H. L. Peng[1], H. R. Schober[2], and Th. Voigtmann[1,3]

[1] *Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln, Germany*

[2] *Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany*

[3] *Department of Physics, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany*

One of the simplest parameters measuring liquid dynamics is diffusion coefficient, which can be evaluated from mean square displacement or single particle's velocity fluctuation through Green-Kubo relation [1]. In dilute fluids, where the sequence of binary collision can be neglected, velocity autocorrelation function (VAF) decays exponentially with time, which can be validated from kinetic theory and brownian dynamics [1]. It came as a surprise when Alder and Wainwright the first time reported the long-time tail of VAF decays algebraically as $t^{-D/2}$ (D is the dimensionality of the system), attributed to the well-known hydrodynamic vortex, or backflow [2].

At high density, the initial direction of movement is soon reversed on average as it feels the surrounding neighbours, then develops a negative region. The reverse of velocity direction has been reported in Lorentz gas as $-t^{-5/2}$ decay [3], and the same algebraic decay in hard-sphere fluid [4].

In order to address this question in atomic liquids, we perform molecular dynamic computer simulation for Lennard-Jones potential. The new physics exposed by this work include: (1) Strong system size dependence for the long-time tail of VAF is discovered on simulation, which is found due to long-time lived transverse wave in supercooled liquids; (2) The negative long-time tail of VAF is found as $t^{-5/2}$ decay in supercooled liquids; (3) Through the generalized Maxwell model for shear wave propagation, the negative long-time tail of VAF is reproduced, but in a slower algebraic decay: t^{-2}.

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POSTER 31 - Tuesday 18:15-20:00hrs Foyer

Viscosity of copper-aluminum melts

N.Konstantinova[1)], A.Kurochkin[2)], A.Borisenko[2)], V.Filippov[3)], P.Popel[1)], B.Rusanov[1)], E.Baglasova[1)]

[1)]Ural State Pedagogical University, Yekaterinburg, Russia
[2)] Ural Institute of State Fire Service, Yekaterinburg, Russia
[3)]Institute of Metallurgy of the Ural Division RAS, Yekaterinburg, Russia

The most detailed results of viscometric investigation of copper-aluminum liquid alloys were obtained before by N.Konstantinova at all. [1] using crucible oscillation method. Unfortunately, the authors had not reliable data about density ρ of the melts and they were forced to use linear interpolation between corresponding ρ values of pure aluminum and pure copper. From one side, this fact has lowered accuracy of kinematic viscosity determination and, from the other one, it excluded the opportunity of dynamic viscosity η calculation. The very reliable density data were obtained recently by A.Kurochkin at all. [2]. Using the gamma absorption method they have demonstrated that discrepancies between real and interpolated density values can be as much as 15%. It makes necessary using the real density values [2] to correct previous viscosity date [1] and to calculate the corresponding dynamic viscosity values. This is the aim of the present report.

We have compared results of calculation of the copper-aluminum melts viscosity using the exact decision of corresponding hydrodynamic equation performed by V.Beskachko and results of more simple iteration procedure proposed before by E.Shvidkovsky. The obtained results were practically co-incited . That is why we used the last method. Density values are necessary for introduction of a level of the investigated melt in the crucible into the kinematic viscosity calculation and for determination of dynamic viscosity. We introduced the values into the calculation as the parameters of linear approximation of temperature dependences [2] because the accuracy of the approximation and precision of density measurements were identical.

As a result, we have obtained corrected temperature and concentration dependences of kinematic viscosity and the corresponding dependences of dynamic one. The ν values at fixed temperatures were obtained as a result of quadratic spline approximation of the $\nu=\nu(T)$ curves and dynamic viscosity at the same temperatures was calculated as $\eta=\rho\nu$. Comparison of the ν with the results of [1] shows significant (from 13 to 22%) accuracy improvement.

Consequently, one can use our values as a reference data with accuracy of 2% declared before by the authors [1].

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POSTER 32 - Tuesday 18:15-20:00hrs Foyer

Electronic structure and properties of (TiZrNbCu)$_{1-x}$Ni$_x$ high entropy amorphous alloys

Katica Biljaković[1], György Remenyi[2], Ignacio A. Figueroa[3], Ramir Ristić[4], Damir Pajić[5], Ahmed Kuršumović[6], Damir Starešinić[1], Krešo Zadro[5] and Emil Babić[5]

[1] Institute of Physics, Bijenička cesta 46, P. O. Box 304, HR-10001 Zagreb, Croatia

[2] Institut Neel, Universite Grenoble Alpes, F-38042 Grenoble, France

[3] Institute for Materials Research-UNAM, Ciudad Universitaria Coyoacan, C.P. 04510 Mexico D.F., Mexico

[4] Department of Physics, University of Osijek, Trg Ljudevita Gaja 6, HR-3100 Osijek, Croatia

[5] Department of Physics, Faculty of Science, Bijenička cesta 32, HR-10002 Zagreb, Croatia

[6] Department of Materials Science & Metallurgy, University of Cambridge ,27 Charles Babbage Road, Cambridge CB3 0FS, UK

Comprehensive study of selected properties of four (TiZrNbCu)$_{1-x}$Ni$_x$ ($x \le 0.25$) amorphous high entropy alloys (a-HEA) has been performed. These alloys, depending on the cooling rate, form either amorphous or crystalline (mostly two phase [1]) structure. This offers unique opportunity to study the impact of amorphisation on properties of HEA. The samples were ribbons about 20 μm thick and their fully amorphous state was verified by X-ray diffraction. The surface morphology, the actual composition and the distribution of components were studied with SEM equipped with EDX. The properties selected were the low temperature specific heat (LTSH), the magnetic susceptibility χ_{exp} and the Youngs modulus (E). Whereas LTSH and χ_{exp} were measured at the as-cast samples, E was measured both at as-cast and relaxed (short anneal [2] close to glass transition temperature [1]) samples. LTSH revealed that the electronic density of states at the Fermi level, N(E$_F$), decreases with increasing x, whereas the Debye temperature (Θ_D) increases with x. This is similar to what observed in binary and ternary amorphous alloys of early transition metals (TE) with late transition metals [2] and indicates that N(E$_F$) is dominated with d-electrons of TE. Accordingly, the free-electron like paramagnetic contribution to χ_{exp} also decreases with x, whereas E increases with x indicating stronger interatomic bonding. The applicability of the rule of mixture to these and other HEA is briefly discussed.

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POSTER 33 - Tuesday 18:15-20:00hrs Foyer

Microscopic mechanism of permanent densification of silica glass based on *ab initio* molecular dynamics simulations

Emina Ryuo[1], Daisuke Wakabayashi[2], Akihide Koura[1], and Fuyuki Shimojo[1]

[1] *Department of Physics, Kumamoto University, Kumamoto 860-8555, Japan*

[2] *Institute of Materials Structure Science, High Energy Accelerator Research Organization, Tsukuba 305-0801, Japan*

The structure of silica glass consists of SiO_4 units under ambient conditions. These tetrahedral units form three-dimensional networks by sharing corner oxygen atoms. Under pressure, silica glass is densified with structural relaxation. It has been well known that a permanent densification occurs above 10 GPa [1], i.e. after decompression, silica glass maintains a densified state even under ambient conditions. The density of fully densified glass is about 20 % larger than that of ordinary glass. Although it is expected that the permanent densification is due to intermediate structural changes in the SiO_4 network structure, the details have not been clarified yet.

In this study, the microscopic mechanism of the permanent densification of silica glass is investigated by *ab initio* molecular-dynamics simulations, in which the electronic states are calculated using the projector-augmented-wave method within the framework of density functional theory. To obtain densified glassy states under pressure in a range from 10 to 40 GPa, a liquid state at each pressure is cooled down to room temperature under isobaric condition. The obtained compressed glass is depressurized to atmospheric pressure gradually to reproduce a permanently densified state under ambient conditions. The density of permanently densified silica glass obtained theoretically is in good agreement with experimental results [2] irrespective of pressure used in the generation processes.

We emphasize that it is important to comprehensively relax the structure in the liquid state under pressure to obtain the correct density under ambient conditions. When the normal glass was compressed to a certain pressure at an insufficiently high temperature, the density after decompression was somewhat different from the experimental value due to finite simulation time.

In this presentation, we will discuss the microscopic mechanism of the permanent densification in relation to short- and medium-range structural changes.

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POSTER 34 - Tuesday 18:15-20:00hrs Foyer

Sound velocity measurements of liquid water-methanol mixtures

N. Shibata[1], Y. Kajihara[1], K. Nukumizu[1], M. Inui[1], S. Tsutsui[2]

[1]*Graduate School of Integrated Arts and Sciences, Hiroshima University, Higashi-Hiroshima 739-8521, Japan*

[2]*Japan Synchrotron Radiation Research Institute, SPring-8, Sayo, Hyogo 679-5198, Japan*

Liquid water–alcohol mixtures have been known to show various thermodynamic anomalies [1]. One of them is that the concentration dependence of the ultrasonic velocity (v_{US}, frequency is MHz) of a liquid water–ethanol mixture shows a maximum at the ethanol concentration of about 15% [2]. It has been thought to be attributed to particular clathrate structures [3]. On the other hand, the sound velocity measured by inelastic X-ray scattering (IXS) (v_{IXS}, THz) doesn't show the maximum and is faster than v_{US} [4]. It was already concluded in liquid water that a large difference between v_{US} and v_{IXS} arises from a huge frequency dependence of sound velocity by relaxation phenomena [5]. Thus the ratio of the two sound velocities (v_{IXS}/v_{US}) is a good measure of the intensity of the relaxation. In water-ethanol mixtures, the ratio rapidly decrease with increasing ethanol concentration in the water rich region. The result indicates that the anomalous concentration dependence of v_{US} arises from large slowdown of v_{US} in the water rich region, not from the speed-up of v_{US} at the concentration of approximately 20% alcohol.

In the present study, we measured v_{US} and v_{IXS} of water-methanol mixtures. IXS measurements were carried out at BL35XU/SPring-8 in Japan. These experiments were performed in the whole liquid temperature region. The concentration dependence of v_{US} showed a maximum at the methanol concentration of 10-30%. By contrast, that of v_{IXS} didn't show a maximum and v_{IXS} increased almost linearly with decreasing methanol concentration. As the water-ethanol mixture, v_{IXS}/v_{US} was large at the low methanol concentration. This result supports the view that the anomalous concentration dependence of v_{US} is due to slowing down of v_{US} of pure water. The temperature dependences of the ratios of the water rich samples increased with decreasing temperature but those of the methanol rich samples were almost constant. We think this result indicates that large slowdown of v_{US} of water arises from the liquid-liquid phase transition of water at the supercooling region.

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POSTER 35 - Tuesday 18:15-20:00hrs Foyer

Crystallization of Al-TM-REM amorphous alloys

Valeriy Sidorov[1], Peter Svec Sr.[2], Peter Svec[2], Dusan Janickovic[2], Sofiya Petrova[3], Anastasiya Palitsina[1]

[1] *Ural State Pedagogical University, Ekaterinburg, Russia*

[2] *Institute of Physics SAS, Bratislava, Slovakia*

[3] *Institute of Metallurgy UD RAS, Ekaterinburg, Russia*

Nowadays Al-TM-REM amorphous alloys are used as protecting materials in the devices working in corrosive medium. These alloys exhibit good mechanical characteristics combining high strength and plasticity. Further improvement in the mechanical properties has been reached by partial crystallization of amorphous structures, forming a precipitation of nanometer-sized fcc-Al phase in the amorphous matrix. However, their crystallization pass depends on nature of TM (3d-transition metal) and REM (rare-earth element) and their content in the alloy.

In this work we investigated crystallization kinetics of amorphous alloys containing 2 - 10 at. % of Ni(Co) and 4 - 10 at. % of Ce (Sm, Dy, Gd, Ho) by the high temperature X-ray diffraction, DSC and electrical resistivity measurements. The amorphous ribbons were prepared by the standard planar flow method in argon atmosphere. The DSC curves were obtained at heating rates of 10, 20 and 40 K/Min.

Two stages of crystallization with big heat effects were detected for Al-Co-REM alloys. For high concentration of TM and REM elements the formation of $Al_3Dy(Ho)$ or $Al_{11}Ce_3$ compounds is going at the first stage, whereas crystallization of aluminum matrix takes place at the second stage. The appearance of Al_9Co_2 compound starts at T > 750 K and is accompanied by a small heat effect, but is fixed on resistivity curves. With the decrease of TM (REM) content the situation is vice versa: aluminum matrix crystallizes at the first stage and all the compounds appear at the second and third stages. For Al-Ni-REM alloys crystallization always starts with the formation of nanosized Al particles and several stable or metastable ternary compounds can appear with temperature increase.

The influence of REM nature and concentration on temperatures and energies of activation is discussed. It is shown, in particular, that in order to increase the stability of amorphous state it is better to use the alloy with big REM content and the alloys with nickel are preferable than the alloys with cobalt.

The work is partially supported by the Ministry of Education and Science of the Russian Federation (Project no. 4.1177.2014/K).

POSTER 36 - Tuesday 18:15-20:00hrs Foyer

Statistics and Thermodynamics of Fe-Cu Alloys at High Temperatures

L.D.Son[1], N.N.Katkov[2], V.E.Sidorov[1]
[1] *Ural Federal University, Ekaterinburg, Russia*

[2] *Ural State Pedagogical University, Ekaterinburg, Russia*

Fe-Cu system is a binary system with limited miscibility of the components. Most of such systems correspond to the eutectic or monotectic type of the concentration – temperature phase diagram, but Fe-Cu system demonstrates eutectoid triple point [1] and strong microheterogeneity in the liquid state [2].

In [3], we suggested the model of binary systems with limited miscibility, which is based on the local state representation of condensed matter statistics and thermodynamics. It was shown, that the model reproduces eutectics and monotectics rather well. In the present work, we modify the model to describe the iron-copper system. Besides, we apply the correction introduced in [4] to describe nonergodic microheterogeneity in Fe-C melts.

We discuss our results in comparison with thermodynamic calculations carried by standard technique [5].

The work was supported by Russian Ministry of Science and Education (Government job 2014/392 projects 2391 and 1177), and by Goverment of the Russian Federation, act 211 contract № 02.A03.21.0006.

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POSTER 37 - Tuesday 18:15-20:00hrs Foyer

Thermal effects on structural and magnetic properties of $Fe_{78}B_{13}Si_9$ amorphous ribbon

M.L. Soltani[1], A. Mansri[1], T.A.M. Aboki[2]

[1] LPS, Dpt. of Physics -Annaba University, Route d'El Hadjar BP 12, Annaba, Algérie ;
[2]GMS-LPCS UMR 7045, Chimie Paristech, 11 rue Pierre et Marie Curie, F-75231 Paris Cedex 05, France

The crystallization behavior of amorphous $Fe_{78}Si_9B_{13}$ ribbons was examined by the Differential Scanning Calorimetry (DSC) measurements to study the thermal effect on structural and magnetic evolution of soft magnetic $Fe_{78}Si_9B_{13}$ amorphous ribbons. Annealing of the as-purchased ribbon that contains some amount of bcc-αFe during various times at 420°C results in crystallization of the remaining amorphous phase confirmed by X-rays diffraction (XRD) patterns.

We discuss some aspects related to the thermomagnetic treatment of structural relaxation, which, following the development of amorphous, improves through the hysteresis loop, macroscopic magnetic properties. We study the influence on magnetic properties of the iron-based amorphous in as-quenched and annealed state, and evaluation of magnetic losses are studied using a high-resolution fluxmeter.

Another aspect related to the use for applications will be examined by experimental estimate of losses and confrontation Bertotti model of the magnetic loss distribution. Results have been found which confirm the high accuracy in the use of high-resolution fluxmeter and give good concordances,with the Bertotti model of losses and helps to explain the distribution of magnetic losses, particularly through interaction with the microstructure. Previous experiments on Fe-Si polycrystals confirm the validity of the method.

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POSTER 38 - Tuesday 18:15-20:00hrs Foyer

Thermal effect on structural and magnetic properties of Fe78B13Si9 annealed amorphous ribbons

M.L. Soltani[1]*, A. Touares[1], T.A. Aboki[2] and J-G. Gasser[3]

[1] LPS, Dpt. of Physics -Annaba University, Route d'El Hadjar BP 12, Annaba, Algérie
[2]GMS-LPCS UMR 7045, Chimie Paristech, 11 rue Pierre et Marie Curie, F-75231 Paris Cedex 05, France
[3]LCP –A2MC Institut de Chimie, Physique et Matériaux, Université de Lorraine, 1 bd Dominique François Arago 57078, Metz Cedex 3, France

In the present work, we study the influence of the structure formed in thermal and thermomagnetic treatment in amorphous of iron. on the macroscopic magnetic properties of as- quenched and thermo-magnetically treated amorphous FeBSi. The crystallization behavior of amorphous and thermo-magnetically treated Fe78Si9B13 ribbons was revisited examining the Differential Scanning Calorimetry DSC measurements; X-ray diffraction (XRD) is used to confirm the thermal effect on structural and magnetic evolution of soft magnetic $Fe_{78}Si_9B_{13}$ amorphous ribbons. Samples were heated in the resistivity device until 700°C and annealed at 420°C during 1, 3, 5 and 8 hours. The chosen annealing temperature corresponds to the end of the stress relaxation maximum that contains also the stable Curie temperature on the DSC curve. In as-quenched sample, two transitions points occur about 505°C and 564°C but in relaxed sample, the transition points have been found about 552°C and 568°C, that are related respectively to the onset and the completion of the crystallization. Kinetics of crystallization were deduced for all studied samples.

The effect of annealing time of the samples is characterized by a significant decrease in activation energies, from the first crystallization step, while a low increase of activation energies occurs from the second step of crystallization. Annealing of the as-purchased ribbon that contains some amount of bcc-αFe during various times at 420°C results in crystallization of the remaining amorphous phase highlighted by X-ray diffraction (XRD) patterns. The effects on magnetic properties were pointed out by relating the structural evolution of the samples. The thermomagnetic treatments and annealing change the coercive magnetic field values. The heat treatment shows that the crystallization has greatly altered the shape of the cycles and moved the magnetic saturation point of the samples. Another finding: the effect of treatment on the anisotropy is not clearly demonstrated.

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POSTER 39 - Tuesday 18:15-20:00hrs Foyer

Sound velocity of water-methanol mixtures: Molecular dynamics

Y. Tachibana and S. Munejiri

Graduate School of Integrated Arts and Sciences, Hiroshima University.

It has been reported that for water-methanol mixtures the experimental ultrasonic velocity takes a maximum value at methanol concentration of around 20 molar percentage [1]. Similar phenomena were also observed for water-ethanol mixtures [2] and for water-propanol mixtures [3]. However, the microscopic mechanism of these features has not yet been revealed.

The purposes of this work are to calculate sound velocity of the water-methanol mixtures by molecular-dynamics simulations and to investigate methanol concentration dependence of sound velocity when their wave-lengths are much smaller than those of ultrasonic wave. Furthermore, we also investigate the wave-length dependence of the sound velocity of these systems.

The SPC-E model and the OPLS-AA model were employed for the interaction potentials of water and methanol, respectively. The molecular-dynamics simulations were carried out for the systems of methanol concentration of from 0 to 100 percentage in steps of 20 percentage using GROMACS package (version 5.1). All the simulations were performed with 10000 molecules in the NVT ensemble at room temperature (298.15K). The volume of each system was determined by isothermal-isobaric molecular-dynamics simulation. The sound velocity was calculated from the longitudinal current correlation functions.

Main findings of this study are as follows: (1) When the wavelength is shorter than about 2nm, the sound velocity does not show the maximum but varies almost linearly from the sound velocity for the pure water to that for the pure methanol. (2) With increasing wave-length of the sound, the methanol concentration dependence of the sound velocity changes and show maximum at methanol concentration from 20 to 40 percentage for the wave-length over 2nm.

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POSTER 40 - Tuesday 18:15-20:00hrs Foyer

Ionic conductivities of molten CuI-AgI mixtures

Shuta Tahara[1], Hironori Shimakura[2], Satoru Ohno[2], and Takanori Fukami[1]

[1] *University of the Ryukyus, Faculty of Science, Okinawa, Japan*

[2] *Niigata University of Pharmacy and Applied Life Sciences, Faculty of Pharmacy, Niigata, Japan*

AgI and CuI are well known as superionic conductors. In these materials, Ag and Cu ions can migrate through the interstitial space of the sublattice formed by I ions in high temperature solid phase under the melting point [1-3]. It is also known that the AgI-CuI mixtures form solid solutions, and both Ag and Cu ions can migrate through the anion sublattice in the high temperature solid phase [4,5]. Although the structure and ionic conductivity of AgI-CuI solid solutions have been investigated by several scholars by using experimental and simulation techniques so far [5-7], those of molten AgI-CuI mixtures have not been investigated yet. In the present study, we measure the temperature and concentration dependences of ionic conductivities of molten (AgI)$_{1-x}$(CuI)$_x$ mixtures as shown in Fig. 1. In the presentation, we will report the detailed information on ionic conduction including activation energies obtained by the temperature dependence of ionic conductivities.

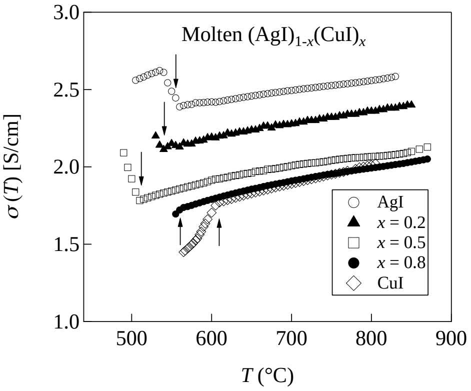

Fig. 1. Ionic conductivities of molten AgI-CuI mixtures. Arrows show the melting point.

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POSTER 41 - Tuesday 18:15-20:00hrs Foyer

Structure and ionic diffusion in molten NaI-RbI system

Shuta Tahara[1,2], Koji Ohara[2], Hironori Shimakura[3], and Takanori Fukami[1]

[1] *University of the Ryukyus, Faculty of Science, Okinawa, Japan*
[2] *Research and Utilization Division, Japan Synchrotron Radiation Research Institute (JASRI, SPring-8), Hyogo 679-5198, Japan*
[3] *Niigata University of Pharmacy and Applied Life Sciences, Faculty of Pharmacy, Niigata, Japan*

The intermediate-range ordering (IRO) of cations in several simple molten salt mixtures has been predicted by molecular dynamics (MD) simulations, for example LiF-KF, LiCl-KCl [1] systems. It has been suggested that the IRO in these mixtures is induced by differences in cationic size.

In the present study, we are interested in molten NaI-RbI mixtures, because there is a large difference in cationic size between Na and Rb. Structure factors $S(Q)$ for pure NaI, RbI and their mixtures are measured by high-energy X-ray diffraction (HEXRD) at BL04B2 in SPring-8 as shown in Fig. 1. The first sharp diffraction peak (FSDP) is not observed in $S(Q)$ for molten $(RbI)_{0.3}(NaI)_{0.7}$ mixture, indicating that the IRO is not formed in the mixture. We also carried out the MD simulations by using Born-Mayer pair potentials. The MD results well reproduced experimental $S(Q)$, and information on the ionic transport properties is also obtained. In the presentation, we will report the detailed experimental and simulation results.

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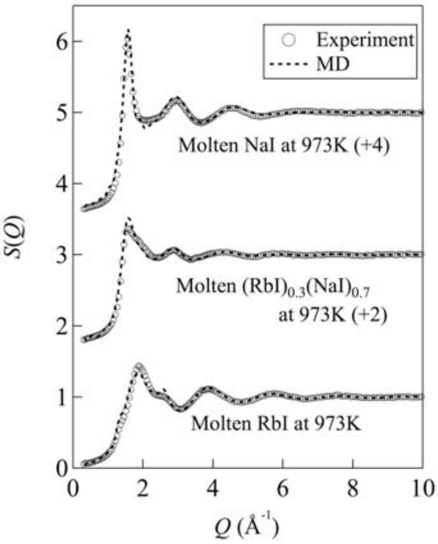

Fig. 1. Structure factors for molten NaI, RbI, and their mixture obtained by HEXRD and MD.

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Structural analysis of molten $NaNO_3$ by molecular dynamics simulation

Shuta. Tahara[1], Hiroshi. Toyama[1], Hironori. Shimakura[2], and Takanori. Fukami[1]

[1] *University of the Ryukyus, Faculty of Science, Okinawa, Japan*
[2] *Niigata University of Pharmacy and Applied Life Sciences, Faculty of Pharmacy, Niigata, Japan*

$NaNO_3$ is well known as a component of the explosive. Recently, molten $NaNO_3$ has also been used for a component of heat storage material in the process of solar power generation. The microscopic atomic configuration and diffusion in molten $NaNO_3$ have been investigated by Adya et al. [1] by means of X-ray diffraction measurement and molecular dynamics (MD) simulation, and partial structure factors and partial pair distribution functions have been reported. In the present study, we carried out the MD simulation for molten $NaNO_3$ by using pair potentials reported by Adya et al., and new information on the atomic configuration is deduced by analyzing the atomic configuration obtained by the MD simulation. For example, Fig. 1 shows the statistical positions of Na ions around a $NaNO_3$ molecule. Na ions are gathered around O ions due to Coulomb attraction. On the other hand, Na ions are not observed in a region around N ion due to Coulomb repulsion. In the presentation, we will report other structural information obtained in our study.

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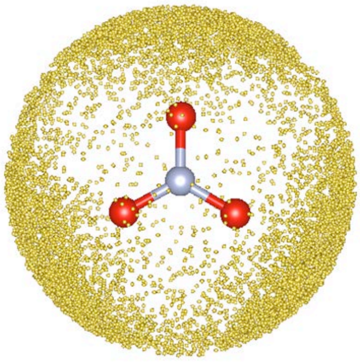

Fig. 1. Statistical positions of Na ions around a NO_3 molecule.

POSTER 43 - Tuesday 18:15-20:00hrs Foyer

Brittle to ductile transition and homogeneous flow of amorphous silicon micro pillars

Yuecun Wang [1], Lin Tian [1, 2], Zhi-Wei Shan [1] , Ju Li [1, 3] & Evan Ma [1, 4]

[1] *Center for Advancing Materials Performance from the Nanoscale (CAMP-Nano) & Hysitron Applied Research Center in China (HARCC), State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China*

[2] *Institut für Materialphysik, Universität Göttingen, Göttingen 37077, Germany*

[3] *Department of Nuclear Science and Engineering and Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

[4]*Department of Materials Science and Engineering, Johns Hopkins University , Baltimore, Maryland 21218, USA .*

As a typical covalent network material, amorphous silicon (a-Si) has been intensively studied with regard to structural and mechanical properties. Simulation work suggests that there are two distinct atomic environments in a-Si, solidlike and liquidlike. Liquidlike clusters in a-Si have higher density and larger coordination number and they contribute to homogeneous deformation in this amorphous material. Increasing the population of liquidlike clusters could lead to the brittle to ductile transition (BDT) in amorphous materials. While BDT has been reported in submicron to nanoscale metallic glass, it has not been studied in a-Si. Using in-situ compression technique in electron microscope, deformation behavior of a-Si pillars with size from 80 nm to 1400 nm has been studied. It was found that BDT occurs when reducing the sample size to around 400 nm. This large transition size also allows us to study the homogeneous flow in a-Si.

POSTER 44 - Tuesday 18:15-20:00hrs Foyer

Structure modeling of AlAg-doped CuZr bulk metallic glasses

Takeshi Usuki[1], Toshio Nasu[2] and Wei Zhang[3]

[1] *Faculty of Science, Yamagata University, Yamagata, Japan*

[2] *Faculty of Education, Art and Science, Yamagata University, Yamagata, Japan*

[3] *Institute for Materials Research, Tohoku University, Sendai, Japan*

It has been reported that minor additions of other elements can dramatically improve glasses forming ability (GFA) of binary metallic glasses. For example, the addition of Al and Ag elements significantly improve the GFA of $Cu_{50}Zr_{50}$ binary alloys and leads to an increase of critical sample diameters at $x = 16$ for $(Cu_{0.5}Zr_{0.5})_{100-x}(Al_{0.5}Ag_{0.5})_x$ glasses [1]. On the other hand, a transition from plasticity to brittleness happens with increasing Al and Ag contents [2]. The atomic origins of the GFA and transition from plasticity to brittleness have not yet been well understood. In this study, the atomic structure of the $(Cu_{0.5}\ Zr_{0.5})_{100-x}(Al_{0.5}Ag_{0.5})_x$ glasses was investigated with a help of the reverse Monte Carlo (RMC) simulations..

The HEXRD experiments were carried out at BL04B2/SPring-8. The RMC simulation was performed on an ensemble of 3,000 particles. The starting configuration was created using hard sphere Monte Carlo (HSMC) simulations with closest atom-atom approach constraints that were determined to avoid unreasonable spikes in the pair correlation functions. The coordination number, angular and ring distributions were calculated to discuss the detailed structure of the present glasses.

The results show that the Al and Ag atoms make relatively shorter bonds with Cu and Zr, and therefore the addition of these atoms improves the packing efficiency and the GFA of BMGs. The atomic configuration model also supports the notion that the chemical short-range order of paired and chained Al and Ag atoms were widely observed in the system, implying that the atomic scale inhomogeneity plays a key role on the transition from plasticity to brittleness in Cu-Zr-based BMGs by addition of Al and Ag. The sum of coordination numbers of Al, Ag and Cu atoms around Zr shows maximum at $x = 16$, which might be strongly related to the GFA of the present BMGs.

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POSTER 45 - Tuesday 18:15-20:00hrs Foyer

Local atomic arrangements in amorphous carbon

Rud A.D[1], Kirian I.M.[1], Lakhnik A.M.[1], and Vasin M.G.[2]

[1]*G. V. Kurdyumov Institute for Metal Physics of the NAS of Ukraine, Kyiv, Ukraine*

[2] *Physicotechnical Institute of the UB of the RAS, Izhevsk, Russia*

It is shown that quasi-continuous structural transformation from the crystalline to amorphous state takes place in graphite during ball-milling (BM). The quantitative characteristics of a short- and a medium-range orders in carbon nanomaterials structure are determined by a combined application of X-ray diffraction, reverse Monte Carlo modeling and Voronoi diagram method. High resolution TEM images revealed formation of disordered carbon materials. The parameters of a short-range order (coordination numbers, radius of the first coordination sphere and bond angle distribution) and a medium-range order (rings distribution) are established for amorphous carbon. The 1-st coordination number is increased during BM what indicates the formation of a more close-packed structure in contrast to the pristine graphite.

The Voronoi polyhedra (VP), constructed for simulated atomic configurations of ball-milled graphite, have an extraordinary variety in their topological and metric characteristics and contain a lot of 5-fold faces. The analysis of VP sphericity coefficient K_{sph} (Fig. 1) enables a conclusion about changing local atomic arrangement in a structure of ball-milled carbon from graphite-like to typical for disordered tetrahedral network and random systems of points (atoms), proper for amorphous state [1]. The Voronoi polyhedra for amorphous carbon, obtained after 10 hrs of BM, are characterized by substantially higher sphericity coefficient (K_{sph}) compared to original crystalline graphite. It has bimodal distribution: one sub-peak corresponds to the structure with a disordered tetrahedral network which is specific to diamond-like carbon and the second one belongs to disordered system of points, proper to amorphous materials. So, we propose to apply K_{sph} of the VP as a parameter of the topological order to quantitative estimation of disordering degree in amorphous structures [2].

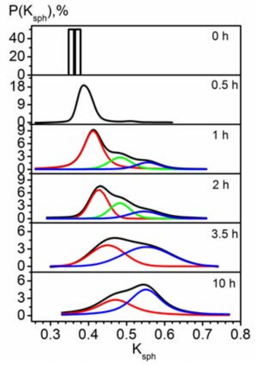

Fig. 1. Distributions of sphericity coefficient of Voronoi polyhedra for ball-milled graphite.

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POSTER 46 - Tuesday 18:15-20:00hrs Foyer

Theoretical description of slow non-monotonic relaxation processes in Al-Y melts

Vasin M.G.[1, 2], Menshikova S.G.[1], Ivshin M.D.[1]

[1] *Physical-Technical Institute, Ural Branch of Russian Academy of Sciences, Izhevsk, Russia*

[2] *Institute for High Pressure Physics of Russian Academy of Sciences, Moscow, Russia*

The slow non-monotonic relaxation processes, which have been recently fixed in Al-Y melts [1-3], are described theoretically. The theoretical description is based on the Cahn-Hilliard theory and functional methods of non-equilibrium dynamics. In terms of the suggested approach the reasons of this relaxation kinetics are non-linearity of the system near to the liquidus line, which sharply increases with Y concentration, and strong initial heterogeneity of the melt on the concentration of Y atoms [4]. According to our analysis one can conclude that the non-monotonic temporal dependence of viscosity is caused by the Ostwald ripening processes in the rich in yttrium areas.

This work was supported by the Russian Scientific Foundation (grant RNF 14-12-01185)

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POSTER 47 - Tuesday 18:15-20:00hrs Foyer

Microstructure and thermal property of Fe based amorphous alloy during heating

A.Yamada[1], Y.Sato[1]

[1] *Tohoku University, Graduate School of Environment Studies, Sendai, Japan*

Atomic structure of amorphous alloy obtained by rapid quenching from the liquid state is thermally unstable because the structure is in a metastable state. Many investigations on the crystallization of amorphous alloys have been carried out. However, the relationship between microstructure and thermal property does not appear to have been extensively studied.

The purpose of this study is to make clear the relationship between microstructure and thermal property of Fe based amorphous alloy annealed in a variety of heating conditions. Fe based amorphous alloys (Metglas 2605SA1) are annealed in various conditions by using electric furnace. Microstructure and thermal property of annealed amorphous alloys are examined in detail by TEM and DSC, respectively. The relationship between microstructure and thermal property has been discussed by using these results examined.

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Glass forming ability, thermal stability and soft magnetic property of $Fe_{76}Si_9B_{10}P_5$ metallic glass

Noriharu Yodoshi[1], Rui Yamada[2], Akihiro Makino[1], and Akira Kawasaki[3]

[1] *Institute for Materials Research, Tohoku University, Sendai, Japan*

[2] *Frontier Research Institute for Interdisciplinary Science, Tohoku University, Sendai, Japan*

[3]*Department of Materials Processing, Graduate School of Engineering, Tohoku University, Sendai, Japan*

The urgent worldwide demand of energy saving requires miniaturized electrical equipment with improved energy efficiency [1]. Fe-based amorphous materials including metallic glasses have recently attracted much attention due to their high magnetic susceptibility, very low coercivity and high electrical resistance, combined with exceptionally high fracture strength. In this study, we aim to prepare $Fe_{76}Si_9B_{10}P_5$ metallic glassy particles with high homogeneity, and a low content of nucleation sites by the container-less solidification process called pulsated orifice ejection method (POEM), and to investigate the glass or amorphous forming ability, thermal stability and soft magnetic properties.

Monodispersed $Fe_{76}Si_9B_{10}P_5$ particles with a high sphericity were successfully prepared by the pulsated orifice ejection method. All obtained monodispersed particles, with various diameters, were identified to be a single glassy or amorphous phase by X-ray diffraction and DSC thermal analysis. The critical average cooling rate to form the fully amorphous phase could be estimated in less than 550 K/s by a model based on Newton's law of cooling. Soft magnetic properties of as-quenched and heat treated particles were evaluated by VSM measurement with a single particle. Fig. 1 show the B-H curves of a single particle after and before demagnetizing field correction with *N*=1/3, powder, and ribbon sample. In case of as-quenched single particle, the relationship between magnetic field and magnetization showed straight liner just before the saturation. Saturation magnetization was increased up to 1.64 T as a maximum by optimum annealing. It can be concluded that the $Fe_{76}Si_9B_{10}P_5$ has good soft magnetic properties as well as sufficient inherent glass forming ability under restrained nucleation conditions.

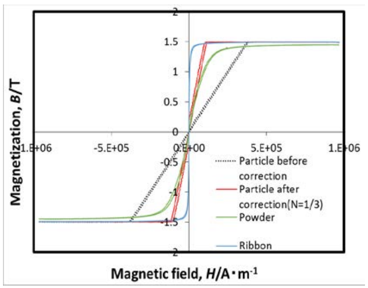

Fig. 1 B-H curves of a single particle after and before demagnetizing field correction with N=1/3, powder, and ribbon sample.

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POSTER 49 - Tuesday 18:15-20:00hrs Foyer

Self-Diffusion, density, and viscosity in liquid $Ni_{66.7}B_{33.3}$

Sarah Zimmermann[1], Fan Yang[1], Zach Evenson[2] and Andreas Meyer[1]

[1] *Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Materialphysik im Weltraum, Cologne, Germany*
[2] *Technische Universität München, Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany*

Binary Ni-B and multicomponent Ni-B based alloys are an important class of metallic glasses which exhibit extremely high mechanical strength and very promising soft magnetic properties. Solidification of these melts are of great scientific and technological interest in order to understand the glass formation and glass forming ability of the alloys. For modeling of such processes and studies of the underlying physical mechanism, it is of great importance to gain knowledge of material parameters like density, self-diffusion coefficients, or viscosity. However, for these highly reactive alloy melts precise data, especially in the undercooled state, is barely available.

The crystal growth velocity of the undercooled melt of the transition-metal semi-boride $Ni_{66.7}B_{33.3}$ alloys has been studied over a wide range of undercooling, which shows a characteristic of a diffusion controlled growth dynamics [1]. We therefore investigated liquid properties of the alloy over a broad temperature range. The liquid density and viscosity $Ni_{66.7}B_{33.3}$ have been measured using electrostatic levitation technique. This advanced containerless processing technique allows measuring thermophysical properties in undercooled melts, since heterogeneous nucleation sites are absent. The self-diffusion coefficient of nickel D_{Ni} in this binary alloy is obtained from a quasielastic neutron scattering experiment (QNS) on the time-of-flight spectrometer TOFTOF at FRM II. One of the great benefits of the QNS measurement is that the liquid dynamics is probed on microscopic time scales where convection does not affect the results.

It is found that both the Ni self-diffusion coefficient and the viscosity of the $Ni_{66.7}B_{33.3}$ melt are identical to that of liquid $Zr_{64}Ni_{36}$ within the experimental uncertainties. Furthermore, the Ni self-diffusion and the melt viscosity of $Ni_{66.7}B_{33.3}$ exhibit a similar temperature dependence. The equation $D \cdot \eta = \mathrm{const.}$, where D is the self-diffusion coefficient and η the viscosity, applies to $Zr_{64}Ni_{36}$, in contradiction to the Stokes-Einstein relation [2]. Such correlation between D and η will be investigated for $Ni_{66.7}B_{33.3}$. The macroscopic density of the melt was used to derive the packing fraction of liquid $Ni_{66.7}B_{33.3}$. It was found that this is slightly lower for $Ni_{66.7}B_{33.3}$ than for $Zr_{64}Ni_{36}$. Whether this is due to the small atomic size of B-atoms or the chemical interaction between Ni- and the metalloid B-atoms still needs to be clarified with structural studies.

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POSTER 50 - Tuesday 18:15-20:00hrs Foyer

Mechanical stress-corrosion interactions in Zr-based bulk metallic glass

P.F. Gostin[1], D. Geissler[2], D. Grell[3], M. Uhlemann[2], E. Kerscher[3], J. Eckert[4] and A. Gebert[2]

[1] *University of Birmingham, School of Metallurgy and Materials, Birmingham, United Kingdom*

[2] *Leibniz-Institute for Solid State and Materials Research, IFW Dresden, Dresden, Germany*

[3] *University of Kaiserslautern, Working Group of Materials Testing, Kaiserslautern, Germany*

[4] *Erich Schmid Institute of Materials Science, Austrian Academy of Sciences (ÖAW) and Montanuniversität Leoben, Department Materials Physics, Leoben, Austria*

Unlike conventional crystalline alloys which may strain harden when plastically deformed, metallic glasses strain soften locally within shear bands upon yielding resulting in an observed almost complete lack of ductility in tension. However, they may possess high fracture toughness which is due to the formation and multiplication of shear bands at notch tips. Still, the environment can cause superimposing (electro) chemical reactions at stably propagating crack tips leading to stress corrosion cracking phenomena. Investigations of these phenomena in metallic glasses are scarce. Stress corrosion cracking investigations are carried out on the bulk glassy Zr52.5Cu17.9Al10Ni14.6Ti5 alloy (Vit 105) by means of three-point bending at constant deformation in chloride-containing electrolytes with an in-house designed setup which enables in situ polarisation control and measurement. Potentiostatic experiments during static mechanical loading are performed at several anodic potentials. Typically, under static loading, after a certain incubation time, the current starts to increase suggesting the initiation of localized corrosion first. Only at a later point, the stress also starts to decrease gradually indicating stress corrosion cracking with stable crack propagation. In the end, unstable crack propagation is observed, which is due to overload of the remaining load-bearing section. Microscopic analysis of fracture surface revealed a clear distinction between the two modes of crack propagation. Stress corrosion cracking is perpendicular to the major tensile stress component. This is accompanied by minor crack branching and very limited shear banding.

Funding from the DFG in the framework of SPP-1594 under grant number GE 1106/11 is acknowledged.

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DLR
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für Luft- und Raumfahrt
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Institut für Materialphysik im Weltraum

Köln-Porz
Linder Höhe
51147 Köln

Telefon: +49 2203 601-3330
Fax: +49 2203 61768

http://www.dlr.de/mp