ABSTRACTS

LAM–17

Lyon, 26-30 August 2019

17th International Conference on Liquid and Amorphous Metals

Welcome to the 17th International Conference on Liquid and Amorphous Metals!

The 17th International Conference on Liquids and Amorphous Metals in Lyon, August 26-30, 2019, continues a series of meetings held every three years, most recently in Beijing, China (2013), and in Bonn, Germany (2016).

In 2019, LAM-17 is hosted jointly by the Institut Lumière Matière (ILM), University of Lyon 1, INSA and CNRS in Lyon.

The aim of LAM conferences is to discuss new advances and future directions in the field of liquid and amorphous metals, by employing theoretical and simulations studies, laboratory techniques and large scale facilities such as synchrotrons and free electron lasers. The 17th edition will also include presentations on non-metallic materials, such as molecular glasses, polymers and colloids in order to encourage the interdisciplinary among different disordered materials fields.

The scientific program of LAM-17 consists of plenary sessions, parallel oral sessions with invited keynotes and contributed presentations, as well as poster sessions. Presenters were invited or selected based on their abstract submissions by the International Advisory and Program Committees and the local organizing committee. The two best posters presented by students will be awarded with the possibility to perform a short term visit in a partner laboratory.

The welcome cocktail on Monday, August 26th, at Villemanzy in the heart of the Lyon, is a first opportunity for conference participants to know each other and to network.

A boat tour of Lyon has been planned on Wednesday 28th while the conference dinner takes place on Thursday, August 29th, in the beautiful Circus Imagine at Vaulx-en-Velin. The dinner will be followed by a typical French spectacle of cabaret and circus. Both events will provide an additional important opportunity for participants for informal discussions and exchanges.

We hope you enjoy LAM-17!

Valentina Giordano and Beatrice Ruta
University Lyon 1 and CNRS

Anne Tanguy
LAMCOS, INSA Lyon

Conference Chair and Co-Chairs
Email: lam-17@sciencesconf.org
Web site: https://lam-17.sciencesconf.org/

Conference Sponsors

RATP

IDEX LYON

INSA INSTITUT NATIONAL DES SCIENCES APPLIQUÉES LYON

MANUTECH SLEIGHT Université de Lyon

INSTITUT CARNOT Ingénierie@Lyon

UCB Lyon 1

UNIVERSITÉ DE LYON

cnrs

INVESTIR L'AVENIR

iLM INSTITUTE OF LIGHT AND MATTER

SFP Société Française de Physique

ATM Association de TriboMécanique

ribori INSTRUMENTATION

VULKAM amorphous metal

Committees

International Advisory Committee

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Local Organizing Committee

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2.	Valentina Giordano	ILM, Univ Lyon 1 and CNRS
3.	Sylvie Le Floch	ILM, Univ Lyon 1 and CNRS
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6.	Aurélien Saulot	LaMCoS, INSA-Lyon
7.	Jean-Marc Pelletier	MATEIS, INSA-Lyon
8.	Damien Fabregue	MATEIS, INSA-Lyon,
9.	Valery Botton	LMFA, INSA-Lyon
10.	Remi Daudin	SIMAP, CNRS and Grenoble INP
11.	Noel Jakse	SIMAP, Grenoble INP
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13.	Gavin Vaughan	ESRF, Grenoble
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15.	Guojian Lyu	INSA-Lyon
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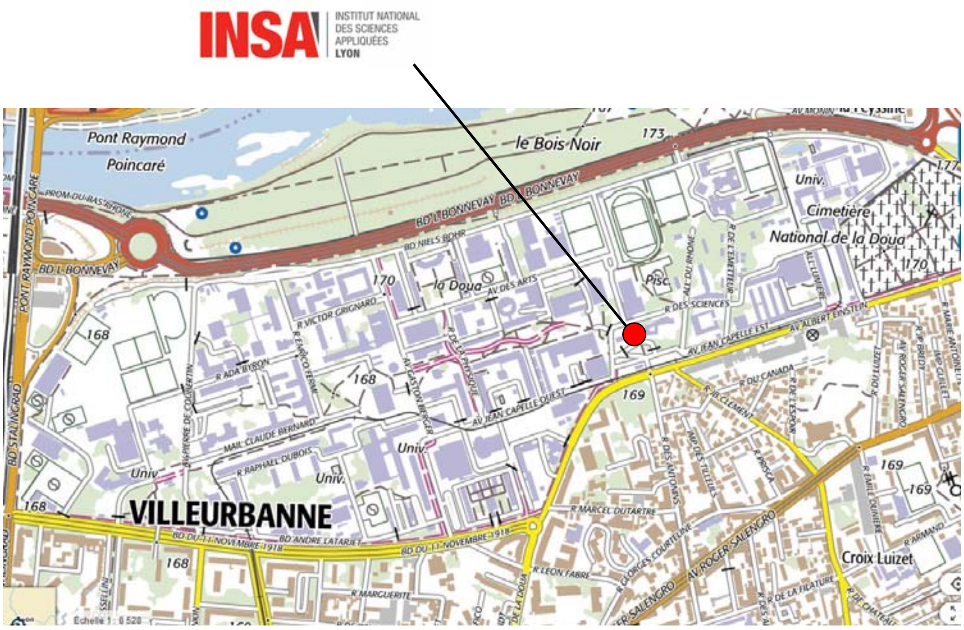
19.	Yu Shi	INSA-Lyon
20.	Dwaipayan Mallick	INSA-Lyon
21.	Paul Desmarchelier	INSA-Lyon
22.	Haoming Luo	INSA-Lyon
23.	Mohammad Hadi	ILM, Univ Lyon 1
24.	Khriscia Utria	INSA-Lyon

Practical Information

1. Venue:



The Conference is held at the INSA Lyon**,** 20, avenue Albert Einstein - 69621 Villeurbanne CEDEX

= > Interactive web map

=> MAP INSA Lyon (download)

Access by train or by plane

From Lyon-St Exupéry airport:

- Airport ↔ Lyon in less than 30 minutes : http://www.rhonexpress.fr/

From Part-Dieu train station:

- Take the T1 Tramway towards “IUT Feyssine” and get off at “INSA-Einstein”.
- or take the T4 Tramway towards "La Doua Gaston Berger" and get off at "La Doua Gaston Berger"

From Perrache train station:

- Take the Line A metro towards “Laurent Bonnevay” and get off at "Charpennes", then take :
  - the T1 Tramway towards “IUT Feyssine” and get off at "INSA-Einstein"
  - or the T4 Tramway towards La Doua Gaston Berger” and get off at "La Doua Gaston Berger"

Access from the highway (GPS: Latitude : 45.78264 | Longitude : 4.878073)

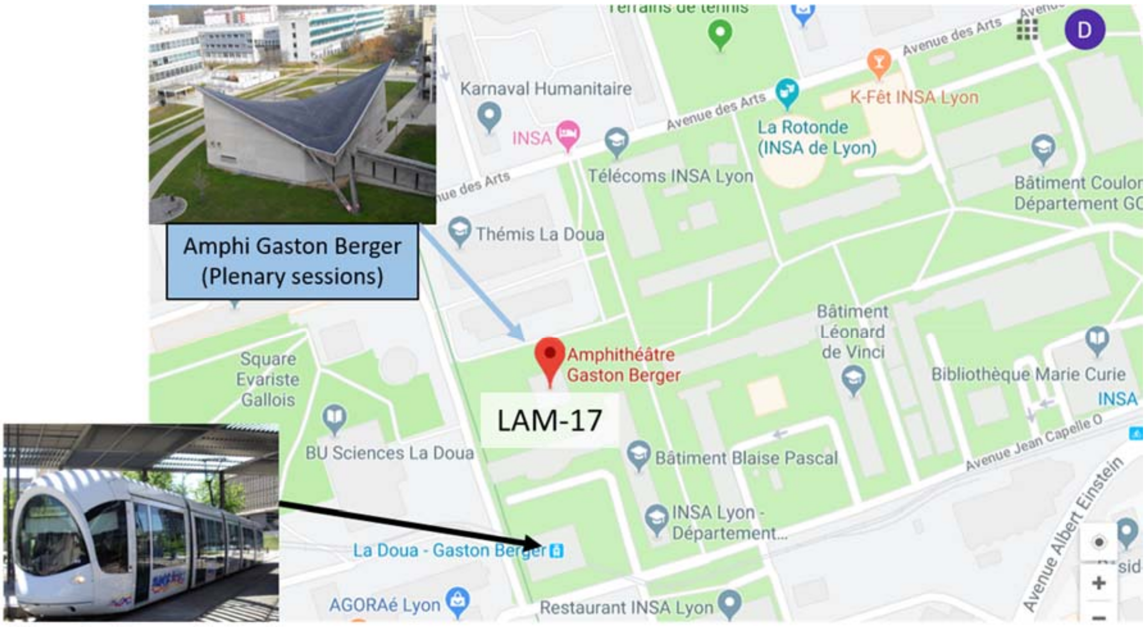
- Via "Rocade Est" ring road: exit 1B then "Croix Luizet", follow "la Doua", then "Domaine Scientifique de la Doua".
- Via the Boulevard Laurent BONNEVAY: exit 6 "Porte de Croix Luizet", then follow direction "Campus de la Doua" (road access map).

All the information to travel in public transports in Lyon on: www.tcl.fr

2. The Rooms:

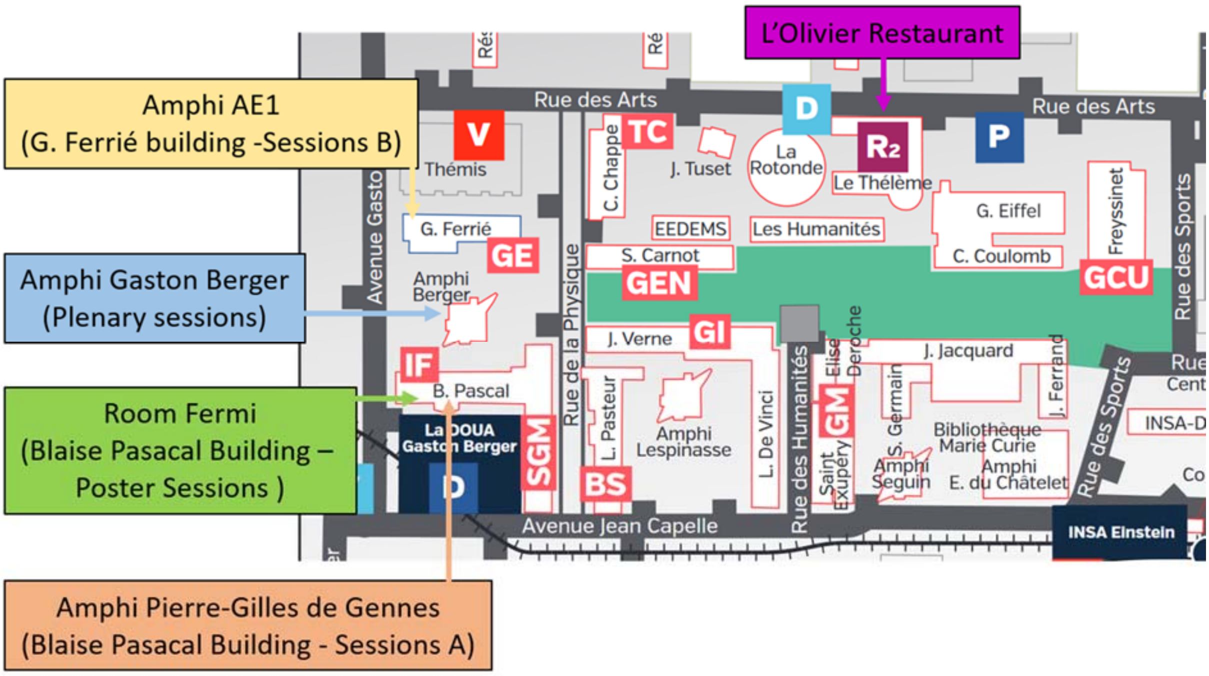
The plenary talks will take place in the Auditorium Gaston Berger, while the parallel sessions will be in the Pierre-Gilles de Gennes auditorium (Blaise Pascal Building) and AE1 auditorium (G. Ferrié Building) which are located nearby. Coffee-breaks will be served in the Blaise Pascal Building near the Auditoria, while lunches will in the campus restaurant L'Olivier located at 5 minutes' walk from the conference rooms.

Map overview



Tram Stop – La Doua – Gaston Berger

Buildings and Rooms overview



3. Registration:

All LAM-17 attendees already registered are invited to complete the check-in at the registration desk, where the conference material will be given. On-site registrations during the Conference will be at the late rates listed below.
Onsite payments are possible by credit card or cash:
800€ (regular)
600€ (student)
90€ (accompanying person)

Registration Desk

The Registration Desk will be located in the Building Blaise Pascal - ground floor. It will be open during the conference hours.

Badge Policy

When you check in at the Registration Desk, you will receive a personalized name badge. All attendees will be required to wear their name badges to enter the Conference area.

Internet Access

Wireless access will be available in the Conference area

4. Oral and Poster presentation

Oral presentation

All the oral presentations will be given in English. Speakers have been allocated the following time slots:

Plenary Speakers	40 minutes for presentation and 5 minutes for discussions
Keynote Speakers	25 minutes for presentation and 5 minutes for discussions
Contributed Talks	15 minutes for presentation and 5 minutes for discussions

All authors presenting a talk are kindly requested to show up at the beginning of their corresponding oral session.

Poster presentation

The poster size must not exceed 120 X 70 cm; dedicated tape to fix the posters will be given by the staff. The poster session will be located in the Fermi room, in front of the Auditorium Pierre-Gilles de Gennes in the Blaise Pascal Building. Although the poster session is scheduled on Tuesday 27th, all posters will be available also during all the subsequent coffee breaks, and can be removed the last day of the conference. The two best student's posters will be awarded with a short term visit in a partner laboratory. Prizes will be awarded during the conference dinner.

5. Conference Publications

Selected papers presented at the conference will be published in the peer-reviewed special issue on “*Liquids and Amorphous Metals*" of Journal of Physics: Condensed Matter.
Special issue articles are subject to the same review process and high standard as regular Journal of Physics: Condensed Matter (JPCM) articles and should be submitted in the same way. Please read the scope page for more information before submitting:
https://iopscience.iop.org/journal/0953-8984/page/liquidandamorphousmetals

The submission window will be open until 31 October 2019. JPCM is able to publish special issues incrementally. If you submit early in the period, your article will not be delayed waiting for other papers in the collection. If you are not able to meet the deadline, please let us know.

6. Social Events

Welcome Cocktail:
On monday 26th of August 7pm, we welcome you at the conference with a cocktail at the heart of the city between the Rhône and Saône, on the slopes of the Croix-Rousse hill, at the Villemanzy Residence.
You will enjoy a stunning view of the Rhone, the great Lyon and the plain of Dauphiné, drinking a good glass of wine. From this location you will be able to embark for a stroll in the Vieux-Lyon, discover the charming streets of Croix-Rousse, mix with the friendly local population, walk down the slopes and have your first feeling of Lyon.

Address: Maison Villemanzy, 21, montée Saint Sébastien, 69001 Lyon.
Website: http://www.belambra-villemanzy.fr/

Boat Tour: Visit of Lyon
On wednesday 28th of August at 4pm, enjoy a guided tour of Lyon, calmly sailing the Saone on a boat. The cruise will last 2 hours and bring you from the confluence of Saone and Rhone all along the Saone up to the wild Ile Barbe, at the gateway to the city. You will enjoy the view

of the eldest quarters of Lyon, admire the Basilica of Notre-Dame de Fourvière, and learn about Lyon's history and architecture.

The cruise will bring you back to the Confluence area, where you will be able to enjoy the shops, the little restaurants and pubs in front of the harbour, or just go back to the city centre and stroll there.

Conference dinner:
On Thursday 29th August at 6:30 pm, the conference dinner will take place at IMAGINE CIRCUS. Unique in France, this Circus makes up a show where the traditional arts of French Cabaret mix with the Circus arts in a cosy atmosphere.
You will enjoy a surprising evening full of events, from the aperitif accompanied by some magic show, through the dinner in the baroc tent, to the Cabaret-Circus Show after dinner, with artists exhibiting just a few meters from your table. And if you are not tired, disco dance will be open until 1am.

Programme at glance

- ⬜ Blaise Pascal (Hall)
- 🟦 Amphi. Gaston Berger
- 🟧 Amphi. Pierre-Gilles de Gennes (Blaise Pascal building)
- 🟨 Amphi. AE1 (G. Ferrié building)
- 🟩 Fermi Room (Blaise Pascal building)
- 🟪 L'Olivier Restaurant

Monday 26th August

14h30	Registration	
15h00	**Introduction**	
15h20	**Plenary** Hajime Tanka	
	Sess. A1	**Sess. B1**
16h10	D. M. Louzguine-Luzgin	E. Pineda
16h30	F. Spieckermann	L. Guojian
16h50	E. Kirova	B. Shang
17h10	V. Sidorov	E. Yahel
18h30 21h30	**Welcome Cocktail** **(Villemanzy – Downtown)**	

Tuesday 27th August

9h00 9h45	**Plenary** Wang Wei-Hua	
	Sess. A2	**Sess. B2**
9h50	R. Bruening	X. Wang
10h10	C. Yuan	F. Caporaletti
10h30	M. Bokova	N. Amini
10h50	Coffee Break	
	Sess. A3	**Sess. B3**
11h20	K. Nishio	R. Busch
11h40	K. Khishchenko	M. Stiehler
12h00	G. Makov	B. Issenmann
12h20	Lunch Break	
	Sess. A4	**Sess. B4**
14h00	**Invited** R.L. Maas	**Invited** R. Torchio
14h30	P. Derlet	L.E. Gonzales
14h50	C. Bernard	L.A. Haozhe
15h10	G. Kermouche	S. Menshikova
15h30	Coffee Break	
	Sess. A5	**Sess. B5**
16h00	D. Fleita	B. Grosdidier
16h20	S. Ayrinhac	A. Polyakov
16h40	P. Galenko	
17h 19h	**Poster Session**	

Wednesday 28th August

9h00 9h45	**Plenary** Jörg Löffler	
	Sess. A6	**Sess. B6**
9h50	F. Zontone	S. Gravier
10h10	B. Sarac	B. Bochtler
10h30	Q. Cao	E. Guérin
10h50	Coffee Break	
	Sess. A7	**Sess. B7**
11h20	A. Lu Anh Khoa	S. Koch
11h40	O. Gross	N. Neuber
12h00	E. S. Osman	B. Lavisse
12h20	Lunch Break	
	Sess. A8	**Sess. B8**
13h50	**Invited** I. Gallino	**Invited** Y. Fomin
14h20	A. Kao	J.G. Gasser
14h40	M. Frey	D. Fabrègue
15h00 ----	**Social Activities**	

Thursday 29th August

9h00 9h45	**Plenary** Alfred Baron	
	Sess. A9	**Sess. B9**
9h50	J.F. Wax	B. Adam
10h10	S. Hosokawa	L. Ruschel
10h30	H. Luo	D. Holland-Moritz
10h50	Coffee Break	
	Sess. A10	**Sess. B10**
11h20	T. Usuki	E. Babic
11h40	L. Kamaeva	I. Balyakin
12h00	A. Sobolev	A. Kuball
12h20	Lunch Break	
	Sess. A11	**Sess. B11**
14h00	**Invited** B. Riechers	**Invited** Q. Zeng
14h30	G. Lohöfer	S. Ohmura
14h50	Y. Chushkin	X. Wang
15h10	S. Lee	B. Gelchinski
15h30	Coffee Break	
	Sess. A12	**Sess. B12**
16h00	**Invited** K. Martens	**Invited** F. Yan
16h30	D. Vandembroucq	S. Sandro
16h50	T. Albaret	N. Klongvessa
18h30 ----	**Gala Dinner**	

Friday 30th August

9h00 9h45	**Plenary** Fernando Lund	
	Sess. A13	**Sess. B13**
9h50	T. Bryk	S.S. Riegler
10h10	F. Demmel	A. F. Garcia
10h30	M. Vasin	M. Kageshima
10h50	Coffee Break	
	Sess. A14	
11h20	Y. Kajihara	
11h40	N. Dubinin	
12h00	**Conclusions**	
12h20	Lunch	

Sessions List

Monday 26th August

Sess. A1: Crystallization and glass transition I
Sess. B1: Stress Relaxation and Rheological behaviour

Tuesday 27th

Sess. A2: Metallic glass formers characterization I
Sess. B2: Diffusion and relaxation processes in liquids and glasses I
Sess. A3: Local and medium range order in liquids and amorphous I
Sess. B3: Dynamical and Phase Transitions in the liquid state I
Sess. A4: Plasticity and mechanical behaviour I
Sess. B4: Extreme conditions and metastability I
Sess. A5: Phase transitions and Phase Diagram
Sess. B5: Local and medium range order in liquids and amorphous II

Wednesday 28th

Sess. A6: Thin Materials
Sess. B6: Functional Materials I – (funded by Institut Carnot@Lyon)
Sess. A7: Local and medium range order in liquids and amorphous III
Sess. B7: Functional Materials II – (funded by Institut Carnot@Lyon)
Sess. A8: Crystallization and glass transition II
Sess. B8: Functional Materials III – (funded by Institut Carnot@Lyon)

Thursday 29th

Sess. A9: Thermal, transport properties and dynamics I
Sess. B9: Metallic glass formers characterization II
Sess. A10: Local and medium range order in liquids and amorphous IV
Sess. B10: Thermo-Physical characterization of metallic alloys
Sess. A11: Novel experimental approaches
Sess. B11: Extreme conditions and metastability II
Sess. A12: Plasticity and mechanical behaviour II
Sess. B12: Diffusion and relaxation processes in liquids and glasses II

Friday 30th

Sess. A13: Thermal, transport properties and dynamics II
Sess. B13: Plasticity and mechanical behaviour III
Sess. A14: Dynamical and Phase Transitions in the liquid state II

LAM-17 Conference Full program

Day 1 - Monday 26th August 2019

14:30 - 15:00	**Coffee break and Registration in the Blaise Pascal Hall**		
15:00 – 15:20	**Welcome/Introduction**	*Organisers*	
15:20 – 16:05	**Plenary Talk:** Auditorium Gaston Berger Structural origin of slow glassy dynamics and glass-forming ability	**Hajime Tanaka** *Tokyo University, Japan*	**PL1**
16:10 – 17:30	**Session A1: Auditorium Pierre-Gilles de Gennes** *Crystallization and glass transition I*	Chair: D. Fabregue	
16:10 – 16:30	Crystal nucleation- and crystal growth-controlled type bulk metallic glasses and the nature of incubation period before crystallization	**Dmitri V Louzguine-Luzgin** *Tohoku University, Japan*	**O1**
16:30 – 16:50	Reduced glass transition in amorphous Cu64Zr36/Cu64Hf36 metallic nanolayers	**Florian Spieckermann** *Montanuniversität Leoben, Austria*	**O2**
16:50 – 17:10	Morphological aspect of crystal nucleation and glass transition in supercooled metallic melt	**Elena Kirova** *National Research University, Russia*	**O3**
17:10 – 17:30	Peculiarities in crystallization of Al- and Co-based amorphous alloys.	**Valeriy Sidorov** *Ural State Pedagogical University (USPU), Russia*	**O4**
16:10 – 17:30	**Session B1: Auditorium AE1** *Stress Relaxation and Rheological behaviour*	Chair: I. Gallino	
16:10 – 16:30	Determination of the slow dynamics of metallic glasses by stress relaxation	**Eloi Pineda** *Universitat Politècnica de Catalunya (UPC), Spain*	**O5**
16:30 – 16:50	Study of dynamic mechanical behavior of Cu64Zr36 metallic glass investigated by atomistic simulations	**Guojian Lyu** *MATEIS INSA Lyon, France*	**O6**
16:50 – 17:10	Local viscoelastic spectrum in a supercooled liquid near the glass transition by molecular dynamics	**Baoshuang Shang** *Beijing Computational Science Research Center, China & LiPhy, France*	**O7**
17:10 – 17:30	Liquid Ga-In alloys: Thermo-physical measurements, liquid transformations and pressure dependent phase diagram	**Eyal Yahel** *Ben Gurion University, Israel*	**O8**
18:30 – 21:30	**Welcome Cocktail (Villemanzy - Downtown)**		

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Day 2 - Tuesday 27th August 2019

09:00 – 09:45	**Plenary Talk:** Auditorium Gaston Berger *Slow Dynamics and Ultrastability of Metallic glasses*	**Wei-Hua Wang** *Chinese Academy of Science, Beijing*	**PL2**
09:50 – 10:50	**Session A2: Auditorium Pierre-Gilles de Gennes** *Metallic glass formers characterization I*	Chair: N. Jakse	
09:50 – 10:10	Molecular Dynamics Simulation of Low-Energy Deposition of Amorphous Nickel Phosphide	**Ralf Brüning** *Mount Allison University, Canada*	**O9**
10:10 – 10:30	Impact of hybridization on metallic-glass formation and design	**Chenchen Yuan** *Southeast University, Nanjing, China*	**O10**
10:30 – 10:50	Relationships between glass structure and properties in single and mixed thallium and/or silver thiogermanate glasses	**Maria Bokova** *Univ. du Littoral Côte d'Opale, France*	**O11**
09:50 – 10:50	**Session B2: Auditorium AE1** *Diffusion and relaxation processes in liquids and glasses I*	Chair: F. Yang	
09:50 – 10:10	Structural signature of beta-relaxation in La-based metallic glasses	**Xiaodong Wang** *Zhejiang University, China*	**O12**
10:10 – 10:30	A microscopic look at the Johari-Goldstein relaxation in a hydrogen-bonded liquid.	**Federico Caporaletti** *University of Trento, Italy*	**O13**
10:30 – 10:50	Microscopic and macroscopic characterization of the relaxation processes in metallic glasses	**Narges Amini** *Deutsches Zentrum für Luft- und Raumfahr, Köln, Germany*	**O14**
10:50 – 11:20	**Coffee break - Blaise Pascal Hall**		
11:20 – 12:20	**Session A3: Auditorium Pierre-Gilles de Gennes** *Local and medium range order in liquids and amorphous I*	Chair: M. Brunelli	
11:20 – 11:40	Entropy-driven docosahedral short-range order in simple liquids and glasses	**Kengo Nishio** *Nat. Inst. of Advanced Industrial Science & Technology, Japan*	**O15**
11:40 – 12:00	Thermodynamic properties and freezing of metastable liquid niobium at negative pressures	**Konstantin Khishchenko**	**O80**
12:00 – 12:20	Short range order in liquids? quasi-crystalline model	**Guy Makov** *Ben Gurion University, Israël*	**O17**

11:20 – 12:20	**Session B3: Auditorium AE1** *Dynamical and Phase Transitions in the liquid state I*	Chair: H. Tanaka	
11:20 – 11:40	Liquid-liquid transitions in bulk metallic glass forming liquids	**Ralf Busch** *Saarland University, Germany*	**O18**
11:40 – 12:00	Caught in the act: The glass transition in undercooled metallic liquids observed in-situ by synchrotron X-ray diffraction	**Martin Stiehler** *Cranfield University, United Kingdom*	**O19**
12:00 – 12:20	Viscosity of supercooled water under pressure and two-state interpretation of water anomalies	**Bruno Issenmann** *ILM, Université Lyon 1, France*	**O20**
12:20 – 14:00	**Lunch at L'Olivier**		
14:00 – 15:30	**Session A4: Auditorium Pierre-Gilles de Gennes** *Plasticity and mechanical behaviour I*	Chair: K. Martens	
14:00 – 14:30	**Invited Keynote:** Deformation-induced structural dynamics in metallic glasses	**Robert L. Maas** *University of Illinois, USA*	**KL1**
14:30 – 14:50	Collective plasticity in a model binary glass spanning five orders of magnitude strain rate.	**Peter Derlet** *Paul Scherrer Institute, Switzerland*	**O21**
14:50 – 15:10	Influence of the presence of crystalline defects in bulk metallic glasses on cracking and plasticity	**Cédric Bernard** *IRDL, Université de Bretagne Sud, France*	**O22**
15:10 – 15:30	A new long-term nanoindentation relaxation method to characterize the time-dependent behavior of thin ZrNi metallic glass films	**Guillaume Kermouche** *LGF, Ecole des Mines de St Etienne, France*	**O23**
14:00 – 15:30	**Session B4: Auditorium AE1** *Extreme conditions and metastability I*	Chair: Q. Zeng	
14:00 – 14:30	**Invited Keynote:** Liquid 3d metals under extreme conditions	**Raffaella Torchio** *ESRF, Grenoble, France*	**KL2**
14:30 – 14:50	Ab initio study of the properties of liquid uranium for temperatures up to 2050 K.	**Luis E. Gonzalez** *Universidad de Valladolid, Spain*	**O24**
14:50 – 15:10	Metallic glasses and melt under high pressure conditions	**Arthur Haozhe Liu** *Center for High Pressure Science & Technology Advanced Research, China*	**O25**
15:10 – 15:30	Structure of the glass-forming Al-Y-Ni alloys formed from liquid upon high pressure solidification	**Svetlana Menshikova** *Federal State Budgetary Institution of Science, Russia*	**O26**
15:30 – 16:00	**Coffee break - Blaise Pascal Hall**		

16:00 – 17:00	**Session A5: Auditorium Pierre-Gilles de Gennes** *Phase transitions and Phase Diagram*	Chair: A. Tanguy	
16:00 – 16:20	The singularity of four-point correlation functions at the phase transition point of copper/nickel melt	**Dmitrii Fleita** *Joint Institute for High Temperatures of the RAS, Russia*	**O27**
16:20 – 16:40	Thermodynamic properties of heavy alkali liquid metals measured by picoseconds acoustics	**Simon Ayrinhac** *IMPMC, Sorbonne Université, France*	**O28**
16:40 – 17:00	Traveling waves in the field approach to fast phase transformations: a case of melt freezing to glassy states	**Peter Galenko** *Friedrich-Schiller-University Jena, Germany*	**O29**
16:00 – 17:00	**Session B5: Auditorium AE1** *Local and medium range order in liquids and amorphous II*	Chair: F. Yuri	
16:00 – 16:20	Alloy order revisited: Calculation of the radii and order parameter of the layers for binary alloys with spherical symmetry	**Benoit Grosdidier** *LCP-A2MC, Université de Lorraine, France.*	**O30**
16:20 – 16:40	The three-dimensional fractals of stars with icosahedral symmetry	**Alexander Polyakov** *South Ural State University, Russia*	**O32**
17:00 – 19:00	**Poster Session (Blaise Pascal building)**		

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Day 3 - Wednesday 28th August 2019

09:00 – 09:45	**Plenary Talk:** Auditorium Gaston Berger *Metastable phase identication and discovery of novel phase-transition pathways via ultrafast calorimetry*	**Jörg Löffler** *ETH Zurich, Switzerland*	**PL3**
09:50 – 10:50	**Session A6: Auditorium Pierre-Gilles de Gennes** *Thin Materials*	Chair: R. Daudin	
09:50 – 10:10	Structural relaxations in metallic glass membranes stimulated by in-situ hydrogenation	**Federico Zontone** *ESRF, Grenoble, France*	**O33**
10:10 – 10:30	Hydrogen storage in Pd-based metallic glass nanofilms via electrochemical methods	**Baran Sarac** *Erich Schmid Institute, Austria*	**O34**
10:30 – 10:50	Mechanical behaviors of metallic glassy thin films	**Qingping Cao** *Zhejiang University, China*	**O35**

09:50 – 10:50	**Session B6: Auditorium AE1** *Functional Materials I - funded by Institut Carnot Ingéniérie@Lyon*	Chair: M. Brunelli	
09:50 – 10:10	Vulkam presentation	**Sébastien Gravier** *Vulkam Inc. Amorphous metal micro casting, Grenoble, France*	**O36**
10:10 – 10:30	The influence of minor additions of sulfur in Zr- and Cu-based bulk metallic glass forming liquids	**Benedikt Bochtler** *Saarland University, Germany*	**O37**
10:30 – 10:50	Study of surface crystallization during the elaboration of a ZrCoAl bulk metallic glass.	**Eliott Guérin** *SIMaP, CNRS, Univ. Gre. Alpes, France*	**O38**
10:50 – 11:20	**Coffee break - Blaise Pascal Hall**		
11:20 – 12:20	**Session A7: Auditorium Pierre-Gilles de Gennes** *Local and medium range order in liquids and amorphous III*	Chair: D. Hallon-Moritz	
11:20 – 11:40	Short- and medium-range order in Cu-Zr metallic glasses analyzed using the p3 code	**Augustin Lu Anh Khoa** *Advanced Institute for Materials Research, Tohoku Univ., Japan*	**O39**
11:40 – 12:00	Signatures of structural differences in Pt-P- and Pd-P-based bulk glass-forming liquids	**Oliver Gross** *Saarland University, Germany*	**O40**
12:00 – 12:20	Structural Properties of Expanded Liquid Carbon C60	**El Sayed Osman** *Sultan Qaboos University, Muscat, Oman*	**O41**
11:20 – 12:20	**Session B7: Auditorium AE1** *Functional Materials II - funded by Institut Carnot Ingéniére@Lyon*	Chair: M. Brunelli	
11:20 – 11:40	Thermophysical properties of undercooled liquid Zr-Cu-x alloys under microgravity	**Stefanie Koch** *Friedrich-Schiller-University Jena, Germany*	**O42**
11:40 – 12:00	The role of Ga addition on the thermodynamics, kinetics, and tarnishing properties of the Au-Ag-Pd-Cu-Si bulk metallic glass forming system	**Nico Neuber** *Saarland University, Germany*	**O43**
12:00 – 12:20	Metallic glasses micro-parts molding and determination of the alloy properties by an experimental inverse analysis.	**Bruno Lavisse** *SIMaP, CNRS, Univ. Gre. Alpes, France*	**O44**
12:20 – 13:50	**Lunch at L'Olivier**		

13:50 – 15:00	**Session A8: Auditorium Pierre-Gilles de Gennes** *Crystallization and glass transition II*	Chair: D. Fabrègue	
13:50 – 14:20	**Invited Keynote:** Vitrication kinetics versus atomic mobility in metallic glass-formers studied by fast scanning calorimetry	**Isabella Gallino** *Saarbrucken University, Germany*	**KL3**
14:20 – 14:40	Convective effects in undercooled liquids during dendritic crystallization	**Andrew Kao** *University of Greenwich, United Kingdom*	**O45**
14:40 – 15:00	The fragility of bulk metallic glass forming liquids studied via modulated DSC	**Maximilian Frey** *Saarland University, Germany*	**O46**
13:50 – 15:00	**Session B8: Auditorium AE1** *Functional Materials III – funded by Institut Carnot Ingéniérie@Lyon*	Chair: F. Demel	
13:50 – 14:20	**Invited Keynote:** Supercritical metal-based liquiids: dynamical crossover and metal - nonmetal transition	**Yuri Fomin** *Russian Academy of Sciences, Russia*	**KL4**
14:20 – 14:40	Electronic transport in solid Ni64-Zr36. alloy (amorphous and recrystallized). Effect of temperature and time.	**Jean-Georges Gasser** *Laboratoire de Chimie et Physique, Univeristé de Lorraine, France*	**O47**
14:40 – 15:00	Yttria precipitates formation in a Cu-based amorphous alloy to improve mechanical properties.	**Damien Fabrègue** *MATEIS -INSA Lyon, France*	**O48**
15:00 – 18:00	**Social activities – Visit Lyon**		

LAM-17 Conference

Day 4 - Thursday 29th August 2019

09:00 – 09:45	**Plenary Talk:** Auditorium Gaston Berger The Landau-Placzek plateau in liquid iron via sub-meV resolution inelastic x-ray scattering at sub-nm-1 momentum transfers	**Alfred Baron** *Materials Dynamics Laboratory, Sayo, Hyogo, Japan*	**PL4**
09:50 – 10:50	**Session A9: Auditorium Pierre-Gilles de Gennes** *Thermal, transport properties and dynamics I*	Chair: A. Baron	
09:50 – 10:10	On the existence of two contributions from collective excitations to the transverse dynamics of liquid metals	**Jean-François Wax** Université de Lorraine, France	**O49**

10:10 – 10:30	Phonon excitations in liquid Au	**Shinya Hosokawa** *Kumamoto University, Japan*	**O50**
10:30 – 10:50	Phonons attenuation in a 2D nanocomposite	**Haoming Luo** *LaMCoS-INSA Lyon, France*	**O51**
09:50 – 10:50	**Session B9: Auditorium AE1** *Metallic glass formers characterization II*	Chair: C. Martinet	
09:50 – 10:10	Characterization of a novel titanium based bulk metallic glass in the quaternary	**Bastian Adam** *Saarland University, Germany*	**O52**
10:10 – 10:30	Development of novel bulk glass-forming alloy compositions in the Ti(Zr)-Ni-Cu-S system	**Lucas Ruschel** *Saarland University, Germany*	**O53**
10:30 – 10:50	On the relationship between short-range structure and atomic dynamics in melts of glass-forming metallic alloys	**Dirk Holland-Moritz** *German Aerospace Center, Köln, Germany*	**O54**
10:50 – 11:20	**Coffee break – Blaise Pascal Hall**		
11:20 – 12:20	**Session A10: Auditorium Pierre-Gilles de Gennes** *Local and medium range order in liquids and amorphous IV*	Chair: G. Vaughan	
11:20 – 11:40	Glass structure and characteristic connectivity of mobile ions in fast ion-conducting chalcogenide glasses	**Takeshi Usuki** *Faculty of Science, Yamagata University, Japan*	**O55**
11:40 – 12:00	Structure and properties of Al-Cu-Fe and Al-Cu-Ni melts	**Larisa Kamaeva** *Udmurt Federal Research Center of Ural Branch RAS, Russia*	**O56**
12:00 – 12:20	The factors affecting the carbide formation in ternary iron-chromium-carbon system close to the melting point	**Andrey Sobolev** *South Ural State University, Russia*	**O57**
11:20 – 12:20	**Session B10: Auditorium AE1** *Thermo-Physical characterization of metallic alloys*	Chair: V. Sidorov	
11:20 – 11:40	Transition from high-entropy to conventional alloys in amorphous and crystalline systems	**Emil Babic** *Department of Physics, Faculty of Science, University of Zagreb, Croatia*	**O58**
11:40 – 12:00	Partial pair correlation functions of liquid VZrNbHfTa high-entropy alloy	**Ilya Balyakin** *Institute of Metallurgy Ural Branch of Russian Academy of Science, Russia*	**O59**
12:00 – 12:20	Thermo-physical characterization of sulfur-bearing bulk metallic glasses	**Alexander Kuball** *Saarland University, Germany*	**O79**

12:20 – 14:00	**Lunch at L'Olivier**		
14:00 – 15:30	**Session A11: Auditorium Pierre-Gilles de Gennes** *Novel experimental approaches*	Chair: S. Le Floch	
14:00 – 14:30	**Invited Keynote:** Dielectric and Mechanical Response beyond the Linear Regime	**Birte Riechers** *Arizona State University, USA*	**KL5**
14:30 – 14:50	High resolution inductive electrical resistivity measurement of electromagnetically levitated liquid metal droplets	**Georg Lohöfer** *German Aerospace Center, Germany*	**O61**
14:50 – 15:10	X-ray photon correlation spectroscopy for probing slow atomic scale relaxations in glasses and supercooled liquids.	**Yuriy Chushkin** *ESRF, Grenoble, France*	**O62**
15:10 – 15:30	Unraveling non-equilibrium thermal relaxation in semiconductors using ultrafast x-ray diffuse scattering measurement at PAL-XFEL	**Sooheyong Lee** *Korea Research Institute of Standards and Science, South Korea*	**O63**
14:00 – 15:30	**Session B11: Auditorium AE1** *Extreme conditions and metastability II*	Chair: R. Tochio	
14:00 – 14:30	**Invited Keynote:** Pressure-induced structure and properties tuning of metallic glasses	**Qiaoshi Zeng** *HPSTAR, Shangai*	**KL6**
14:30 – 14:50	Pressure-induced structural change of liquid sulfur from polymeric liquid to simple liquid	**Satoshi Ohmura** *Hiroshima Institute of Technology, Japan*	**O64**
14:50 – 15:10	Behaviors of disordered alloys under various thermodynamic conditions	**Xiaodong Wang** *Zhejiang University, China*	**O65**
15:10 – 15:30	Comparative estimation of the properties of liquid metals at high temperatures and pressures using the methods of classical and first-principle molecular dynamics	**Boris Gelchinski** *Institute of Metallurgy of Ural Branch of the Russian Academy of Sciences, Russia*	**O66**
15:30 – 16:00	**Coffee break – Blaise Pascal Hall**		
16:00 – 17:10	**Session A12: Auditorium Pierre-Gilles de Gennes** *Plasticity and mechanical behaviour II*	Chair: A. Tanguy	
16:00 – 16:30	**Invited Keynote:** Characterising residual stress states of athermally driven glasses	**Kirsten Martens** *LiPhy, Univ. Grenoble Alpes, France*	**KL7**
16:30 – 16:50	Plasticity of amorphous materials: from atomic to mesoscopic scale	**Damien Vandembroucq** *PMMH, Sorbonne Université, France*	**O67**

16:50 – 17:10	Full decomposition of plasticity in terms of Eshelby inclusions in amorphous solids studied with molecular dynamics	**Tristan Albaret** *ILM, Université Claude Bernard, Lyon, France*	**O68**
16:00 – 17:10	**Session B12: Auditorium AE1** *Diffusion and relaxation processes in liquids and glasses II*	Chair: T. Bryk	
16:00 – 16:30	**Invited Keynote:** Mass transport and structural relaxation in glass-forming alloy melts	**Fan Yang** *Deutsches Zentrum für Luft und Raumfahrt, Köln, Germany*	**KL8**
16:30 – 16:50	Self-diffusion in Mercury investigated with quasi-elastic neutron scattering	**Sandro Szabo** *MLZ, Technical University of Munich, Germany*	**O69**
16:50 – 17:10	From supercooled to glass: opposite effects of weak self-propulsion on relaxation	**Natsuda Klongvessa** *ILM, Université Claude Bernard, Lyon, France*	**O70**
17:10-18:30	**Free time**		
18:30 – xxx	**Gala Dinner**		

LAM-17 Conference

Day 5 - Friday 30th August 2019

09:00 – 09:45	**Plenary Talk:** Auditorium Gaston Berger *Strings in Glasses---Metallic and Otherwise*	**Fernando Lund** *Universidad de Chile, Santiago, Chile*	**PL5**
09:50 – 10:50	**Session A13: Auditorium Pierre-Gilles de Gennes** *Thermal, transport properties and dynamics II*	Chair: J.F. Wax	
09:50 – 10:10	Specific features of dynamics in expanded liquid mercury in the region of metal-nonmetal transition: Ab initio study	**Taras Bryk** *Institute for Condensed Matter Physics, Ukraine*	**O71**
10:10 – 10:30	The Stokes-Einstein relation of a simple liquid metal and its relationship to changes in the microscopic dynamics with increasing temperature	**Franz Demmel** *ISIS Facility - Rutherford Appleton Laboratory, United Kingdom*	**O72**
10:30 – 10:50	To understanding of slow and non-monotonic relaxation processes in liquid eutectics	**Mikhail Vasin** *Institute for High Pressure Physics of the RAS, Russia*	**O73**

09:50 – 10:50	**Session B13: Auditorium AE1** *Plasticity and mechanical behaviour III*	Chair: F. Lund	
09:50 – 10:10	Investigations on the annealing-induced structural changes in the Zr48Cu36Al8Ag8 bulk metallic glass and their effects on the kinetic and mechanical properties	**Sascha S. Riegler** *Saarland University, Germany*	**O74**
10:10-10:30	Control of microstructural evolution of bimetallic Janus particles	**Alberto Fraile Garcia** *Czech Technical University in Prague, Czech Republic*	**O75**
10:30 – 10:50	Casimir Effect as a Complex Response of Near-Critical Binary Liquid Mixture Analyzed with Atomic Force Microscopy	**Masami Kageshima** *Osaka Electro-Communication Univ., Japan*	**O76**
10:50 – 11:20	**Coffee break – Blaise Pascal Hall**		
11:20 – 12:00	**Session A14: Auditorium Pierre-Gilles de Gennes** *Thermal, transport properties and dynamics III*	Chair: N. Jakse	
11:20 – 11:40	Density fluctuations of supercooled liquid Te	**Yukio Kajihara** *Hiroshima University, Japan*	**O77**
11:40 – 12:00	Thermodynamic perturbation theory: Mon's correction in terms of pair potentials	**Nikolay Dubinin** *Ural Federal University, Russia*	**O78**
12:00 – 12:15	**Conclusions**	*Organisers*	
12:20 – 14:00	**Lunch at L’Olivier**		

Plenary Lectures

Abstracts

PL 1

Structural origin of slow glassy dynamics and glass-forming ability

Hajime Tanaka*[1], Hua Tong[1], Seiichiro Ishino[1], Rui Shi[1], Flavio Romano[2], and John Russo[3]

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[3]University of Bristol (Univ Bristol) – Bristol BS8 1 TW, United Kingdom

Abstract

If a liquid is cooled with a certain cooling rate, it will be either crystallized or vitrified depending upon the rate. However, it has been unclear what physical factors control the fate of the liquid. Upon cooling structural order develops in a supercooled liquid. If it is compatible with crystal symmetry, it acts as precursor for crystal nucleation and thus also plays an important role in the selection of polymorphs. On the basis of this physical picture, we study the glass-forming ability of liquids with competing orderings, where an increase in the glass forming ability is signaled by a depression of the melting temperature towards its minimum at triple or eutectic points. We find that the enhancement of glass-forming ability is caused by an increase in the structural contrast between liquid and crystal: stronger competition in orderings towards the melting point minimum makes a liquid structure less similar to crystalline structures. This increase in the liquid-crystal structural difference leads to a rapid increase of the free-energy barrier for crystallization towards the glass-forming region.

Even if structural order is not compatible with crystal symmetry, it still grows its size upon cooling, which leads to slow glassy dynamics. We introduce a set of new structural order parameters characterizing sterically favored structures with high local packing capability, and then access structure-dynamics correlation by a novel nonlocal approach. The fast beta process is controlled by the instantaneous order parameter field locally, resulting in short-time particle-scale dynamics. Then, the mobility field progressively develops with time, following the initial order parameter field from disorder to more ordered regions. This clearly indicates that the particle mobility is under control of the static order parameter field.

These results suggest that structural order developed in a supercooled liquid controls not only the glass-forming ability but also glassy dynamics.

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*Speaker

PL 2

Slow Dynamics and Ultrastability of Metallic glasses

Weihua Wang[*][†][1]

[1]Institute of Physics, Chinese Academy of Sciences (IPCAS) – Beijing 100190, China

Abstract

Relaxations in glassy state involve wide timescales and rich dynamic modes. As a model glass system, metallic glasses were studied with complementary approaches. The low temperature heat capacity associated with the anomalous atomic vibration (i.e., boson peak) was found following exactly the structural relaxation and showing memory effect, revealing the direct link between the slow structural relaxation and the fast boson peak dynamics. Long time stress relaxation experiments unveiled the two-step process, indicating the existence of a new relaxation decoupling and distinct dynamic process in glassy state. Slow vapor deposition of metallic glass on room temperature cold substrate was found to enable accessing the extremely low energy states and creating ultrastable metallic glasses with _˜60 K enhanced Tg, which highlights the key role of surface dynamics in ultrastable glass formation and suggests that it could be much faster-than-expected at low temperatures. These observations provide new insights for understanding the glassy dynamics and pave a way for controllable fabrication of unique and sophisticated nanostructure in glasses to realize the properties modification.

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[*] Speaker

PL 3

Metastable phase identification and discovery of novel phase-transition pathways via ultrafast calorimetry

Jörg F. Löffler*†1

1Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich (ETHZ) – 8093
Zurich, Switzerland

Abstract

I will report on various thermophysical phenomena that have been identified via fast differential scanning calorimetry (FDSC), which allows measurements at rates of more than 10,000 K/s. For an Au-based glass [1] and other metallic systems we observe that solid-solid phase transitions can occur via intermediate (metastable) melting. By investigating the sequences of metastable phase formation upon melt solidification we also identified, for an Mg-based alloy, the primary nucleation of a transient quasicrystal phase which transforms into an equilibrium phase upon further solidification [2]. Because this phase-transition path minimizes the free-energy barrier for nucleation it is likely to occur in many metallic systems. Using FDSC it is also possible to interrupt rapid cooling after a transition and then to "up-quench" the frozen structure via heating at ultrafast rates. In this way we have been able to completely melt metastable phases and thus to determine their thermophysical properties, with the intent of constructing complete metastable phase diagrams. Finally we show via FDSC that metallic glass-forming alloys can have multiple critical cooling rates that generate different types of monolithic glass with distinctly different short-range orders [3]. This reveals the need to classify monolithic glasses into two types, which we term "self-doped glass" (SDG) and "chemically homogeneous glass" (CHG). As opposed to common belief, CHG exhibits similar critical heating and cooling rates and a tendency towards stochastic nucleation, underlining the novelty of this glass state. In general, I will show that novel FDSC experimental possibilities allow us to identify hidden transient phases, and thus to discover and thermophysically describe new metastable materials that are potentially useful for novel structural and functional applications.

-[1] S. Pogatscher, *et al.*, *Nat. Commun.* **7**, 11113 (2016).

-[2] G. Kurtuldu, K.F. Shamlaye, J.F. Löffler, *PNAS* **115** (2018) 6123.
-[3] J.E.K. Schawe, J.F. Löffler, *Nat. Commun.* **10**, 1337 (2019).

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*Speaker

PL 4

The Landau-Placzek plateau in liquid iron via sub-meV resolution inelastic x-ray scattering at sub-nm-1 momentum transfers.

Alfred Q.r. Baron*†1

1Materials Dynamics Laboraotry, RIKEN SPring-8 Center (MDL RSC) – 1-1-1 Kouto, Sayo, Hyogo, 679-5148, Japan

Abstract

Following investigations of water [1], inelastic x-ray scattering (IXS) has become the method of choice for investigating dynamics of disordered materials in the mesoscopic region where the crossover from continuum to atomistic behavior occurs. However, the method is limited by the increasing difficulty of getting clean data at small momentum transfers with sufficient resolution. At the RIKEN Quantum NanoDynamics beamline (BL43LXU) [2] of SPring-8, T-gradient analyzers allow _˜0.8 meV resolution at 25.7 keV [3] while a combination of a Soller slit and analyzer masks [4] allow efficient data collection at sub-nm-1 momentum transfers. Iron was placed in a single crystal sapphire cell [5] and heated to a liquid state in a new chamber using a carbon-composite heater [6]. High-quality data at momentum transfers, Q, down to 0.771 nm-1 show the acoustic mode dispersion changes from "fast" sound at higher Q to the hydrodynamic value at low Q, while the Landau-Placzek ratio plateaus at a value substantially lower than expected from the known high specific heat ratio, hinting at a mesoscale region where the liquid behavior is *semi*-hydrodynamic [7].

-[1] F. Sette, et al., Phys. Rev. Lett. 75 (1995) 850 and Phys. Rev. Lett. 77 (1996) 83.
-[2] A.Q.R. Baron SPring-8 Inf. Newsl. 15, 14–19. http://user.spring8.or.jp/sp8info/?p=3138 and in Synchrotron Light Sources and Free-Electron Lasers, edited by E.J. Jaeschke, et al., pp. 1643–1757. Cham: Springer. See also https://arxiv.org/abs/1504.01098
-[3] D. Ishikawa, et al., J. Synch. Rad. 22 (2015) 3–8. DOI: 10.1107/S1600577514021006.
-[4] A.Q.R. Baron, et al., AIP Conf. Proc. 2054 (2019) 20002. DOI: 10.1063/1.5084562.
-[5] K. Tamura, et al., Rev. Sci. Instrum. 70 (1999) 144.
-[6] A.Q.R. Baron, et al., unpublished
-[7] A.Q.R. Baron, M. Inui, D. Ishikawa, Y. Kajihara, Y. Nakajima, K. Matsuda, et al., In Preparation.

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*Speaker

PL 5

Strings in Glasses—Metallic and Otherwise

Fernando Lund*†[1]

[1]Universidad de Chile (UC) – Santiago, Chile

Abstract

For quite some time, there have been indications of string-like behavior at intermediate scales in glasses: Schober (1993) identified vibrational modes in a soft-sphere simulation well below the glass transition temperature that involve atoms arranged in a string-like pattern. Donati et al. (1998) identified string-like cooperative motion in a supercooled Lennard-Jones liquid. Zhang et al. (2015) also identified string-like cooperative behavior in a molecular dynamics simulation of Cu-Zr liquid alloys. Novikov and Surotsev (1999) showed that Raman scattering data from glasses could be explained by vibration eigenmodes localized along a one-dimensional spatial geometry. Yu et al. (2013) have rationalized the behavior of β-relaxation in a variety of supercooled liquids and glasses in terms of string-like configurations. Concustell et al. (2011) have induced elastic anisotropy (as characterized by resonant ultrasound spectroscopy-RUS) in a bulk metallic glass, with a result that is consistent with an alignment of string-like atomic arrangements. Can these various aspects of string behavior be linked together? A specific coupling of strings to acoustic waves in glasses was proposed by Lund (2015), leading to a qualitative relation between normal modes of oscillation in the THz range (blamed on string normal modes) with the attenuation and dispersion of acoustic waves in the same frequency range. Recently, using a generalized elastodynamics formulation of the acoustic wave-string interaction, a quantitative expression has been derived for a string-based dynamical structure factor S(q,w) that does not use a damped harmonic oscillator (DHO) parametrization. The resulting expressions are in satisfactory agreement with inelastic x-ray scattering (IXS) data for glycerol glass and for silica glass.

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*Speaker

Keynotes Lectures

Abstracts

KL 1

Deformation-induced structural dynamics in metallic glasses

Robert Maass*[1]

[1]University of Illinois at Urbana-Champaign (UIUC) – 1304 West Green Street, 61801 Urbana, IL,
United States

Abstract

Subjecting a metallic glass to increasing temperature is known to induce thermally-activated structural dynamics, also referred to as aging. This type of far-field stimulus causes an increase of relaxation times with increasing waiting time at a given temperature. Here we focus on the structural dynamics induced by deformation in the elastic and plastic regime. We use x-ray photon correlation spectroscopy (XPCS) to reveal this structural activity, with a focus on the dynamics in the pre-yield regime and in regions of strain localization due to shear bands. It is found that stresses in the nominally elastic regime induce highly non-monotonous changes in the time-dependent relaxation behavior, which we attribute to microplasticity that is localized in space and time. As a function of temperature, we observe monotonous aging in both the as-cast material and the material that has undergone strain localization, with significantly faster dynamics near shear bands. The faster dynamics found near a shear band has a distinctly different aging behavior, as characterized by temperature-specific scaling functions. Our new insights are discussed in the context of pre-yield structural excitations that either lead to structural relaxation or rejuvenation, as well as the mesoscopic effects of shear banding during plastic flow.

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*Speaker

KL 2

Liquid 3d metals under extreme conditions

Raffaella Torchio[*][†][1]

[1]European Synchrotron Radiation Facility (ESRF) – ID24 beamline, HPLF-I – 71 avenue des Martyrs
GRENOBLE CEDEX, France

Abstract

In the last 20 years, a lot of experimental and theoretical efforts have been focused on the evaluation of the equation of state of liquid iron and iron alloys, with important implications in geophysics and material science.
Despite this, the knowledge of short range and electronic structure of liquid Fe as well as of the other 3d metals at high pressure (g(r), first neighbor distance, coordination number, density...) remains quite limited, in particular from the experimental point of view.

This is certainly not due to the lack of interest in the topic, but rather to the challenging experimental conditions which have only recently started to be surmounted, allowing to obtain first reliable melting curves and first structural information on the melts.

3d metals melts under extreme compression can be obtained in a static or in a dynamic way. The static approach relies on the laser heated diamond anvil cell, enabling to reach up to few Mbar and thousands of kelvin range. The dynamic approach consists of laser inducing shock waves in the metal allowing to reach more extreme states typically in the multi Mbar and few eV range, depending on the laser energy. Laser shocks can bring the matter to exotic states such as the Warm Dense Matter, somehow in between solids and plasmas, which are still hard to describe by theoretical models.

We show here novel results coming from both approaches coupled to X-rays Absorption obtained on beamline ID24 at the ESRF.

In particular, the first determination of the 1st neighbor distance compression in pure cobalt and nickel melts up to 100 GPa and first observation of ns-lived equilibrium states of WDM Fe. Moreover, comparison to ab-initio calculations gives novel insights on the physical phenomena taking place at the atomic scale in the molten phases.

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[*] Speaker

KL 3

Vitrification kinetics versus atomic mobility in metallic glass-formers studied by fast scanning calorimetry

Isabella Gallino*[1]

[1]Saarland University (Chair of Metallic Materials) – Campus C6.3, 66123 Saarbruecken, Germany

Abstract

This work shows that the vitrification process of metallic glasses can take place according to the atomic mobility of processes different from the alpha-relaxation process. The evidence is based on an exhaustive study by fast scanning calorimetry (FSC) of vitri?cation kinetics and atomic mobility using an Au-based alloy [1].The kinetics of vitri?cation is characterized for 5 decades of cooling rates in terms of the limiting ?ctive temperature, Tf, at which a glass that was formed after cooling at a given rate, would be at equilibrium. Additionally, through a step response analysis, FSC provided information on the atomic mobility connected to the structural alpha-relaxation process via the temperature and frequency dependence of the complex speci?c heat, resulting in relaxation time data for the so-called dynamic glass transition temperature, Tg(dyn), in the range from 0.001 to 1 s. These latter data are found in agreement with atomic relaxation time data based on dynamic mechanical analysis (DMA) and x-ray photon correlation spectroscopy (XPCS) at deeper undercooling [2] and are representative of an highly fragile liquid in terms of kinetic fragility. The process of vitrification, as identified by Tf, follows a milder temperature dependence than that of the alpha-process. The separation of these two aspects of the glassy dynamics becomes more pronounced at larger undercooling, suggesting a larger contribution of additional dynamical processes to the vitrification process, which are not connected to the alpha-process. The observed heterogeneity of vitrification kinetics hints toward the existence of multiple relaxation mechanisms, which are observed during aging experiments [3-4].

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-[2] S. Hechler et al., Phys. Rev. Mat. 2 (2018) 085603.
-[3] I. Gallino et al., Acta Mater. 144 (2018) 400.
-[4] I. Gallino, R. Busch, JOM 69 (2017) 2171.

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*Speaker

KL 4

Supercritical metal-based fluids: dynamical crossover and metal - nonmetal transition

Yury Fomin*[1], Elena Tsiok , Kostya Trachenko , Valentin Ryzhov , and Vadim Brazhkin

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Abstract

Supercritical fluids based on metals are of great interest for both fundamental science and technological applications. Of special interest is metal to nonmetal transition [1]. However, investigation of their behavior meets an obvious problem: it requires extremely high temperatures which makes experimental studies very difficult. Because of this it is of particular importance to find a relation of the properties of supercritical fluids based on metals to the one of other liquids which are easier to study. In the present paper we discuss a concept of dynamical crossover in liquids which takes place along the so called Frenkel line [2,3]. This crossover is related to a qualitative change of microscopic dynamics of liquid upon heating. It leads to several important consequences. In particular, the isochoric heat capacity along the Frenkel line is about 2k_B per particle [2,3] and the Gruneisen parameter is nearly constant along the Frenkel line [4]. Moreover, in our recent paper we proposed that the Frenkel line can be related to metal - nonmetal transition in supercritical fluids based on metals [5]. Similar conclusion was obtained in a recent experimental work by studying metal - nonmetal transition in lead [6].

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*Speaker

KL 5

Dielectric and Mechanical Response beyond the Linear Regime

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Abstract

The linear dielectric response of polar molecular glass-formers is based on reorientational processes that show the characteristics of nearly constant loss, as well as primary and secondary processes. Thus, linear dielectric data bears similarities to the linear response patterns of structural glass-formers as perceived by mechanical spectroscopy. For high excitation intensities, mechanical data suggests the existence of local shear events subject to long-range correlation (avalanches) that occur even at moderate excitation intensities and evolve towards an overall plastic, serrated response with increasing mechanical load. By comparison, the application of high electric fields to polar materials results in nonlinear contributions to the response signal. The origins of the occurring nonlinearity are discussed in terms of saturation, chemical effects, energy absorption, or the electro-rheological effect, depending on material, measurement parameters, and the implementation of high-field excitation. Instantaneous changes in the dielectric response signal as perceived for mechanical excitation in terms of avalanches are not observed, despite the very good resolution of the technique. This is attributed to the difference in the energy introduced by high-field excitation, which is clearly beyond thermal energy kT in case of mechanical high-field experiments, but remains far below kT even for highest electric fields applied.

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*Speaker

KL 6

Pressure-induced structure and properties tuning of metallic glasses

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Abstract

With many properties superior to the conventional crystalline metals, metallic glasses (MGs) are currently at the focus of intense research efforts worldwide. However, MGs are "disordered" systems that lack identifiable symmetry in their atomic arrangement, which makes a theoretical description of their atomic structure in detail very challenging. On the other hand, without the strict constraints of a well-defined crystalline symmetry and substantial energy barriers separating different states in crystals, MGs are expected to be more flexible and tunable in structures and properties. Over the last few decades, intense efforts have been made to modulate the structures of MGs to obtain desired properties, primarily focusing on different synthesis routes or post-fabrication treatments. However, effectively modulating the structure of MGs especially to distinct states has shown to be rather challenging. By employing high-pressure (up to tens or hundreds of GPa) as a unique tuning parameter, the structure and properties of MGs can be effectively modified in a controllable way. Many interesting transitions have been observed using multiple in situ high-pressure diffraction,imaging and spectroscopy techniques, e.g., glass to glass, glass to crystal transitions, etc., which opens a new avenue towards accessing the unexplored phase space and provide valuable constraints from experiments for the better understanding of the structures and their relationship with properties of MGs.

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*Speaker

KL 7

Characterising residual stress states of athermally driven glasses

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Abstract

In this talk I will adress the question of residual stress states that are created in athermally sheared disordered materials when brought to rest from a flowing regime. The non-trivial relaxation dynamics will depend on the initial driving rate and the deformation history. The resulting mechanical properties of the final states are encoded not only in the locally stored residual stresses but also in the potential energy landscape that is reached in the partial relaxation process. We propose microscopic structural observables that can characterise the relaxation dynamics and the typical final mechanical state, which enable us to derive a meso-scale picture for the relaxation dynamics and the mechanical properties of pre-sheared soft glassy materials.

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*Speaker

KL 8

Mass transport and structural relaxation in glass-forming alloy melts

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Abstract

We study mass transport and structural relaxation in metallic glass-forming melts. Knowledge of the relations between these melt properties are essential to understand the dynamics in disordered media. Employing containerless processing techniques combined with large-scale facilities at synchrotron and neutron sources, the structure and dynamics of a number metallic glass-forming liquids are investigated in details on the basis of accurate experimental data. We show that in these alloys the self-diffusion coefficients and the liquid viscosity exhibit very similar temperature dependencies over large temperature intervals, despite various chemical short-range orders in different alloys. We attribute this to the relatively high packing of these glass-forming alloy melts, where the dynamic properties of the melt are governed by a single structural relaxation timescale. In addition, for several Zr-based glass-forming alloys, a mismatch in the melt kinetics can be found in the undercooled liquid region, indicating the presence of a strong-fragile transition. With the knowledge of the liquid dynamics, we are able to estimate the timescale of the transition, which is on the order of tens of seconds. This indicates that long range mass transport is required, which points to an underlying transition mechanism incompatible with local structural changes only. Such a transition mechanism is distinct from that reported in the oxides, water or other liquids. Nevertheless, the relation between structural relaxation time and melt viscosity seems to still hold, even in undercooled liquid region and across the strong-fragile transition.

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*Speaker

Oral Presentations

Abstracts

O 1

On crystal nucleation- and crystal growth-controlled type bulk metallic glasses and the nature of incubation period before crystallization of a supercooled liquid

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Abstract

Two general types of bulk (massive, volumetric) metallic glasses are formed by suppressing either nucleation or growth process of a competing crystalline phase(s). Most of Ti-, Zr- and Cu-based bulk metallic glasses to be presented here are of the former type. Moreover, nanocrystallization of a Ti50Ni23Cu22Sn5 bulk metallic glass, which formation is crystal nucleation-controlled, was studied within the supercooled liquid region by using a state-of-the-art experimental technique with elemental mapping at near-atomic resolution. A special focus was made on the nature of incubation period at constant temperature and pressure which is still poorly understood from both theoretical and experimental viewpoints. Molecular dynamics simulation performed for the Ti55Ni45 liquid acting as a simplified model system of the (Ti,Sn)55(Ni,Cu)45 alloy illustrated the solute partitioning process in the liquid state. Both experimental and simulation data indicate formation of nanometer-range chemical rearrangements which are supposed to reduce the energy barrier in the complex energy landscape[1]. This process leads to a high density of homogeneously nucleating crystallites after the completion of a macroscopically observed incubation period. On the contrary, the Fe48Cr15Mo14C15B6RE2 bulk glass forming alloys (RE stands for rare earth) and a Zr65Al7.5Ni10Pd17.5 one represent the latter glass family. The reasons for significantly enhanced glass-forming ability of the Fe-based alloys are connected with low growth rate of the c-Fe36Cr12Mo10 phase which nuclei exist in the glassy phase. The low growth rate is connected with large inhomogeneous strain in the growing nanoparticles, while nucleation of eutectic colonies is hampered by slow diffusion of a rare-earth alloying element. Phase separation in Zr-based bulk metallic glasses will also be reported together with its strong effect on their properties. -[1]. Z. Wang, C.L. Chen, S. V. Ketov, K. Akagi, A. A. Tsarkov, Y. Ikuhara and D. V. Louzguine-Luzgin, Materials & Design, 156, (2018), 504-513.

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*Speaker

O 2

Reduced glass transition in amorphous Cu64Zr36/Cu64Hf36 metallic nanolayers

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Abstract

Amorphous metallic coatings have recently emerged as promising thin film materials – thin film metallic glasses - due to their excellent chemical stability, good wear resistance and exceptionally high strength. Many reports exist on the influence of confinement in thin film organic glasses. Little data exists, however, on the influence of confinement on the glass transition in bulk metallic glasses. In order to study the influence of a confined glassy structure, we prepared purely amorphous/amorphous layered thin films of CuHf and CuZr with layer thicknesses ranging from several nanometers to 1 μm by unbalanced dc magnetron co-sputtering from elemental targets. Systematic thermal analysis has been performed using conventional and modulated scanning calorimetry in order to study the specific glass transitions of the constituting components as a function of the layer thickness. The results are backed with experiments characterizing the structural properties by transmission electron microscopy and X-ray diffraction. Hardness and elastic properties were studied using nanoindentation. Theoretical assessment by molecular dynamics simulations indicate a significant mobility in the interface regions and confirm a shift of the glass transition temperature to lower temperatures even approaching theoretically limiting Kauzmann temperature for Cu64Zr36 glass.

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[*] Speaker

O 3

Morphological aspect of crystal nucleation and glass transition in supercooled metallic melt

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Abstract

We investigate the nucleation and growth of a crystalline nucleus in a supercooled molybdenum and tantalum using the molecular dynamics method [1]. We consider the nucleation as a multi-dimensional process [2-4] and study the probability density function of the largest crystal formation. We show that nuclei of complex shapes form during the simulations [4], so the size of the largest nucleus and the parameter measuring the shape deviation from spherical (asphericity) are considered as the reaction coordinates. Simulations reveal 3 paths for crystal nucleus shape and size evolution. The first path is the formation of a crystal that does not grow any further. We found the stability regions on the probability density surface. If the cluster falls into them, then the probability of crystallization of the system is small. The second path is the crystal nucleation through low values of the asphericity parameter. Crystal growth occurs by the attachment of atoms one by one, as in the classical nucleation theory. The third path is nucleation due to the merging with small crystals (coalescence). We also show that the cooling rate significantly affects the nucleation mechanism. The report was prepared within the framework of the Basic Research Program at the National Research University Higher School of Economics (HSE) and supported within the framework of a subsidy by the Russian Academic Excellence Project '5–100'.

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*Speaker

O 4

Peculiarities in crystallization of Al- and Co-based amorphous alloys.

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Abstract

Co-based alloys are considered to be the promising materials for BMG production. However, their physical properties at high temperature are practically unknown. In this work we investigated the temperature dependences of density (by gamma-penetration method), electrical resistivity (by contactless method in rotating magnetic field) and magnetic susceptibility (by Faraday's method) in crystalline and liquid states and DTA of Co48Fe25Si4B19Nb4 alloy and with additions of neodymium (1 and 2 at.%). The alloy of nominal composition was obtained by remelting the pure components (purity > 99.8%) in an induction furnace in argon atmosphere for 1 hour at 1400 C. X-ray analysis showed that the main phases of the crystalline sample (obtained at low cooling rate) are: pure Co, Co2Si and (Fe,Co)23(B,Nb)6. Bulk amorphous metal rods with a diameter of 2 mm and a height of 17-20 mm were obtained by a cast suction method into a water-cooled copper mold. Amorphous ribbons (width 4 mm, thickness 55 mcm) were prepared by a standard planar flow method. It was found that in liquid state neodymium additions lower density of the alloy nonmonotonously, increase its resistivity and have little effect on its magnetic susceptibility. The crystallization kinetics of amorphous alloys was studied using differential thermal analysis on a Pelker Elmer installation with a heating and cooling rate of 10 K / min. It was stated that crystallization of the initial amorphous alloy proceeds in one stage (a metastable intermetallic compound (Fe,Co)23(B,Nb)6 appears), and of the alloys containing neodymium - in two stages. The formation of Nd2B borides is highly probable at the second stage of crystallization. Nd additions were found to positively affect the glass forming ability of Co48Fe25Si4B19Nb4 alloy, increasing the range of amorphous state existence by more than 30 K.

The reported study was funded by RFBR according to the research project 18-03-00433.

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*Speaker

O 5

Microscopic and macroscopic characterization of the relaxation processes in metallic glasses

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Abstract

Aging and relaxation of bulk metallic glasses (BMG) are important phenomena from the point of view of applications, e.g., aging determines and alters the long-time stability of their mechanical properties and the temperature dependence of viscosity in the supercooled liquid region (SCL) which is crucial for thermoplastic forming. All these processes are linked to structural relaxation. A comparison of relaxation time (
tau) of various experimental techniques gives insight into relaxation mechanisms across the different dynamical regimes.In this investigation, relaxation processes and aging dynamics of BMGs of Vit4 are probed in both the microscopic and macroscopic scales using X-ray photon correlation spectroscopy (XPCS) and dynamic mechanical analysis (DMA). The former technique probes the relaxation dynamics from local to mesoscopic length scales within a time window of 101-104 seconds. The latter technique applies a stress in the tension mode of deformation, characterizing relaxation times from _˜ 100 to 104 seconds on the macroscopic scale. The corresponding relaxation times have been measured as a function of temperature from 450 K to 628 K, covering both SCL and the glassy regions. In the SCL region, the absolute value of
tau is very similar for XPCS and DMA, which indicates that the structural relaxation exhibits no length scale dependence. In addition, the temperature dependence of relaxation time is well consistent with that of the viscosity. In contrast, the glassy region presents a more complex relaxation depending on the thermal protocols and survey methods. In the microscopic scale, physical aging and temperature leads to different dynamic regimes, while in the macroscopic scale aging and temperature changes the relative contribution of viscoelastic and anelastic processes.

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[*]Speaker

O 6

Study of dynamic mechanical behavior of Cu64Zr36 metallic glass investigated by atomistic simulations

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Abstract

In this work, the dynamic mechanical behavior of Cu64Zr36 metallic glass is systematically analyzed by Molecular Dynamic simulations. The storage modulus and loss modulus are obtained by applying an oscillating strain under different loading conditions. Since the elastic constants of isotropic materials are uniquely determined by any two moduli, we establish a relationship between the complex moduli of the Cu64Zr36 metallic glass under different constraints that can be used to predict the storage modulus and loss modulus under various loading conditions. The storage modulus and loss modulus evolve with temperature, and the main relaxation appears around the glass transition temperature Tg. Numerical results show that the dynamic mechanical behavior is highly frequency dependent: the main relaxation peak is shifted to low temperature domain as the loading frequency decreases, which is consistent with experimental observations of typical metallic glasses. In order to establish the atomic mechanisms of energy dissipation, we have analyzed the atomic displacements as a function of temperature. At low temperatures, the atomic displacements after each loading cycle are almost zero. Around the glass transition temperature Tg, the displacements of most atoms get larger and larger after each cycle, which contribute to the energy dissipated during each cycle. On the contrary, the icosahedra clusters in Cu64Zr36 metallic glass are stable and almost in their original positions after each cycle, thus contributing to the stored energy representing the elastic component during each cycle. Finally, we investigate the influence of a B2-CuZr crystalline nanoprecipitate on the dynamic mechanical behavior and the structural evolution during the deformation and heating. Our work provides insightful information for better understanding the dynamic mechanical behavior of metallic glasses and nanocomposites at the atomic scale.

Keywords: Metallic glass; Dynamic mechanical analysis; Molecular dynamics simulations; nanocomposites

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*Speaker

O 7

local viscoelastic spectrum in a supercooled liquid near the glass transition by molecular dynamics

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Abstract

Amorphous materials usually show non-Debye relaxation behaviour, and the origin of the stretch exponent has aroused lots of interests, which is come to down to the local relaxation behaviour . Here, we investigate the local dynamic modulus spectra directly in a model glass just above the glass transition temperature by performing a mechanical spectroscopy analysis with molecular dynamics simulations. We find that the spectra, at the local as well as on the global scale, can be well described by the Cole-Davidson formula in the frequency range explored with simulations. Surprisingly, the Cole-Davidson stretching exponent does not change with the size of the local region that is probed. The local relaxation time displays a broad distribution, as expected based on dynamic heterogeneity concepts, but the stretching is obtained independently of this distribution. We find that the size dependence of the local relaxation time and moduli can be well explained by the elastic shoving model.

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*Speaker

O 8

Liquid Ga-In alloys: Thermo-physical measurements, liquid transformations and pressure dependent phase diagram

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Abstract

Ga-In alloys are materials with potential to be used in numerous applications e.g., liquid metal electronic circuits, stretchable/flexible electronics-based pressure sensors and as heat transfer agents in accelerators. Despite these promising applications, only few studies of its high temperature properties of these alloys have been made. We review the unique properties of Ga-In binary system and present high accuracy sound velocity and density measurements over a large range of temperature. The results are introduced into a thermodynamic model from which the pressure dependent phase diagram is constructed. Following recent indications of a liquid crossover at the eutectic composition (86%at Ga), in the temperature range of about 400-500K, we report on sound velocity and electrical resistivity measurements that provide additional confirmation of a temperature-driven structural transformation at the eutectic composition as well as in Ga and two other compositions at ambient pressure. To further investigate this transformation, we performed differential scanning calorimetry measurements to investigate thermal aspects of structural changes.

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*Speaker

O 9

Molecular Dynamics Simulation of Low-Energy Deposition of Amorphous Nickel Phosphide

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Abstract

Amorphous Ni100-xPx (typically 15< x< 22) can be prepared by rapid quenching of the melt, or as coatings by electroless (chemical) deposition. In the latter process the nickel is reduced chemically with electron transfer on the plating surface. We report the results of a molecular dynamics (MD) simulation of atom-by-atom deposition as a function of the kinetic energy of the incoming atoms and the temperature of the substrate. MD deposition with atom speeds corresponding to thermal motion are expected to reproduce important aspect of either chemical or electrochemical deposition, whereas high atom speeds correspond to the regime of sputtering deposition. The substrate temperature controls the rate of surface diffusion relative to the deposition rate. The structure and properties of the MD-generated deposits are compared to those of MD simulated quenching of the bulk liquid.

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*Speaker

O 10

Impact of hybridization on metallic-glass formation and design

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Abstract

Designing glass and controlling its formation at the atomic scale have been desired over decades. As a novel glassy material, metallic glasses are considered to exhibit a random atomic packing. Generally, the atomic-level packing efficiency is believed to be closely related to the mechanism of their formation. However, in this work, we show that the hybridization of bonds indicated by Mott's pseudogap can affect the bond length and the atomic packing, which effectively tailors the formation metallic glasses. A *p*-*d* hybridization between the post-transition metal Al and the transition metal was shown by the 27Al isotropic shifts and the spin-lattice relaxation time of Zr-Co-Al alloys using nuclear magnetic resonance. These bonds favor the formation of metallic glasses by introducing a string-like structure and further stabilize glassy systems via a reduction of the density of states at the Fermi level. Our work has implications for understanding the glass formation mechanism and might open up new possibilities on the design of metallic glasses from the perspective of atomic interactions.

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*Speaker

O 11

Relationships between glass structure and properties in single and mixed thallium and/or silver thiogermanate glasses

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Abstract

Glasses properties in the Ag(Tl)-Ge-S system were studied using thermal analysis, conductivity and tracer diffusion measurements. The structural investigations were performed by Raman spectroscopy, high-energy x-ray and neutron diffraction completed by RMC/DFT modelling.
Raman spectroscopy reveals that structural motifs in (Tl2S)x(GeS2)1-x ($0 \leq x \leq 0.5$) and (Ag2S)x(GeS2)1-x ($0.3 \leq x \leq 0.5$) glasses are reminiscent of respective crystalline counterparts. Thermodynamic instability of Ag-poor crystals explains a wide composition range of phase-separated glasses consisting of silver-poor (1-2 at.% Ag) and silver-rich ($\geq$ 20 mol. % Ag) glassy phases.

Diffraction studies indicate the continuous Ge-S backbone fragmentation with metal addition. Vitreous thallium thiogermanates are composed of large clusters ($x \leq 0.3$) and small oligomers ($x >$ 0.3) connected by thallium, and do not have extended structural motifs. On the contrary, in silver thiogermanates, a significant part of Ge and S species are connected, forming long chains. The observed structural differences explain markedly higher glass transition temperatures in Ag-Ge-S glasses compared to their thallium counterparts.

Conductivity behaviour is also different for thallium and silver thiogermanates. The (Tl2S)x(GeS2)1-x glasses can be divided into two groups: (1) semiconducting glasses at $x \leq 0.3$, and (2) ion-conducting vitreous alloys at $x >$ 0.3. (Ag2S)x(GeS2)1-x glasses show high Ag+ ionic conductivity over the large composition range due to the Ag-S(iso) preferential conduction pathways formed by the isolated sulphur connected to silver.
Mixed Ag2S-Tl2S-(GeS)-GeS2 glasses exhibit a non-monotonic change of ionic conductivity and a diffusivity crossover measured using 204Tl and 108mAg tracers, i.e., they show the mixed cation effect centred at r = Ag/(Tl+Ag) = 0.2. Raman spectroscopy measurements reveal that the structure of the mixed glasses is not a simple mixture of the end-members and the both cations are not separated spatially in the glass network but rather located in close proximity to each other.

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*Speaker

O 12

Structural signature of beta-relaxation in La-based metallic glasses

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Abstract

The secondary beta-relaxation is an intrinsic feature in glassy materials. However, its structural origin is still not well understood. Here we report that the beta-relaxations in La50Al15Ni35 and La50Al15Cu35 metallic glasses mainly depend on the vibration of small Ni and Cu atoms in local cages. By using advanced synchrotron x-ray techniques and theoretical calculations, we elucidate that the tricapped-trigonal-prism-like polyhedra with more large La atoms in shells favor the local vibration of center Ni atoms, leading to the pronounced beta-relaxation event. In contrast, Cu atoms are relatively close-packed with some Cu in the nearest neighbors while they could easily diffuse out of the cages compared to Ni, somehow triggering the onset of alpha-relaxation. This work provides a pathway to understand the different structural relaxation behaviors in metallic glasses and other glassy materials from their local atomic packing and dynamics.

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*Speaker

O 13

A microscopic look at the Johari-Goldstein relaxation in a hydrogen-bonded liquid.

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Abstract

Understanding the glass transition requires getting the picture of the dynamical processes that intervene in it. Glass-forming liquids show a characteristic decoupling of relaxation processes when they are cooled down towards the glassy state. Two main relaxations can indeed be distinguished: the well known α-relaxation, directly related to the process of dynamic arrest, and the faster Johari-Goldstein or β-relaxation. This last one is still under scrutiny as it is strictly related to and act as a precursor of the α-relaxation [1]. Its full explanation is therefore crucial for a complete theory of the glass transition, and necessitates information at the microscopic scale. However, probing the molecular dynamics of this process when its timescale is well separated from that of the α-one ($>$ 1 ns) is extremely challenging both using simulations [2-3] and experimentally. To this aim, nuclear γ-resonance time domain interferometry (TDI) has been utilized to investigate 5-methyl2-hexanol, a hydrogen-bonded liquid with a pronounced process as probed by dielectric spectroscopy [4]. TDI, indeed is one of the few techniques able to probe dynamics with characteristic times in the range 10 ns-10 μs, that is in the time-range where the βrelaxation decouples from the α, at the Ångstrom length-scale [5-6]. Our measurements [7], spanning both inter- and intra-molecular distances, demonstrate that the β-relaxation consists of cooperative and spatially restricted rearrangements, and allow us to estimate its characteristic length-scale.

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*Speaker

O 14

Microscopic and macroscopic characterization of the relaxation processes in metallic glasses

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Abstract

Aging and relaxation of bulk metallic glasses (BMG) are important phenomena from the point of view of applications, e.g., aging determines and alters the long-time stability of their mechanical properties and the temperature dependence of viscosity in the supercooled liquid region (SCL) which is crucial for thermoplastic forming. All these processes are linked to structural relaxation. A comparison of relaxation time (*tau*) of various experimental techniques gives insight into relaxation mechanisms across the different dynamical regimes.In this investigation, relaxation processes and aging dynamics of BMGs of Vit4 are probed in both the microscopic and macroscopic scales using X-ray photon correlation spectroscopy (XPCS) and dynamic mechanical analysis (DMA). The former technique probes the relaxation dynamics from local to mesoscopic length scales within a time window of 101-104 seconds. The latter technique applies a stress in the tension mode of deformation, characterizing relaxation times from _˜ 100 to 104 seconds on the macroscopic scale. The corresponding relaxation times have been measured as a function of temperature from 450 K to 628 K, covering both SCL and the glassy regions. In the SCL region, the absolute value of *tau* is very similar for XPCS and DMA, which indicates that the structural relaxation exhibits no length scale dependence. In addition, the temperature dependence of relaxation time is well consistent with that of the viscosity. In contrast, the glassy region presents a more complex relaxation depending on the thermal protocols and survey methods. In the microscopic scale, physical aging and temperature leads to different dynamic regimes, while in the macroscopic scale aging and temperature changes the relative contribution of viscoelastic and anelastic processes.

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[*]Speaker

O 15

Entropy-driven docosahedral short-range order in simple liquids and glasses

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Abstract

The energetically favored icosahedral structure has been seen as the central figure for describing the local structure of simple liquids and glasses. Although regular icosahedral structures are rarely found, it is accepted that distorted icosahedral structures occur in simple liquids and glasses. However, which local structure dominates and why it is more frequent than the others remain unanswered questions. In this study, by using a recently developed structure descriptor, we show that docosahedral structures are the most favored not only in models of simple liquids and glasses but also in an experimental colloid glass (Phys. Rev. E 99, 022121 (2019)). We also show that the the predominance of docosahedral structures is entropy-driven. Our findings represent a significant milestone towards comprehending mysterious phenomena such as supercooling, glass transition, and crystallization, where local structures play a key role.

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*Speaker

O 16

Cluster-plus-glue-atom model for metallic glasses and solid solutions

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Abstract

Metallic glasses and solid solutions always exhibit special properties at specific compositions. There is an urgent need to understand the structural origin behind the stable solutions, so that the composition design theory can be established to effectively guide alloy development. Metallic glasses and solid solutions are both characterized by short-range order, and our group has previously proposed the cluster-plus-glue-atom model based on Friedel oscillations to describe the short-range ordered structures. In this model, any structure can be dissociated into a nearest-neighbor cluster plus a few glue atoms situated between the clusters, formulated as [cluster](glue atom)x, with x meaning the number of glue atoms. For metallic glasses, based on a large number of experimental results, the number of glue atoms is determined to be 1 or 3. In constructing the composition formulas of metallic glasses, the detailed procedures using the cluster-plus-glue-atom approach have already been established, among which the key step is to select the proper principal clusters from the corresponding devitrification phases according to the structural homology of amorphous and crystalline states. For solid solutions, the cluster parts can be easily defined in the corresponding crystalline phases, and the key problem is to determine the glue atoms. By introducing the spherical-periodic resonance theory, the number of glue atoms in the cluster formulas of solid solutions can be determined from the physical nature of structural stability. The calculated compositions agree well with the most commonly used alloy specifications, thus explaining the commercial industrial alloys successfully. Based on the cluster-plus-glue-atom model, chemical structural units in stable solutions are proposed, which mimic the molecules in chemical substances. The composition origin of short-range ordered materials is then unveiled in terms of chemical structural units, and the composition design theory for metallic glasses and solid solutions is developed.

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*Speaker

O 17

Short range order in liquids – quasi-crystalline model

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Abstract

The short range order in selected liquid metals and water 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 underlying liquid-liquid phase transitions in the supercooled regime which are not directly accessible and which lead to changes in the liquid structure. We demonstrate that the quasi-crystalline model allows quantitative characterization of the short range order in liquids as well as its classification in terms of the short range order in reference structures. It is found that simple metals, rare gases and Lennard-Jones liquids all exhibit similar short range order. Upon rapid cooling rapidly into an amorphous, glassy state the short range order is transformed - leading to a clear signature in the radial distribution function. In contrast, 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. Finally, the quasi-crystalline model was applied to determine the short range order in water and amorphous ice identifying transitions in the short range order as the thermodynamic conditions are varied.

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[*] Speaker

O 18

Liquid-liquid transitions in bulk metallic glass forming liquids

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Abstract

Polymorphic transitions are very common in crystalline materials and can be first order transitions like e.g. from austenite to ferrite or second order like in the case of the ordering transition from BCC to B2. Recently polymorphic transitions within the liquid state termed polyamorphisms have been observed or proposed. In this contribution experiments on kinetics, thermodynamics and structure of molten Zr, Cu, Au and Fe-based alloys in the equilibrium state as well as in the undercooled state are presented. In particular the two alloys Zr41.2Ti13.8Cu12.5Ni10.0Be22.5 (Vit1) and Zr58.5Cu15.6Ni12.8Al10.3Nb2.8 (Vit106a) can be investigated in the entire supercooled liquid region. The results suggest that the liquid alloys undergo a weak first order phase transformation likely from a short range ordered fragile state at high to a medium range ordered strong state at low temperatures. The results are discussed in a bigger picture that emerges when comparing fragile-strong transitions in different material classes. For glass forming metallic liquids it appears that these liquid-liquid transitions are rather the norm than the exception.

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*Speaker

O 19

Caught in the act: The glass transition in undercooled metallic liquids observed in-situ by synchrotron X-ray diffraction

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Abstract

Molten metallic alloys can form amorphous solids when cooled fast enough to temperatures below their glass transition avoiding crystallisation. During the glass transition, the viscosity increases by more than 12 orders of magnitude within a narrow temperature interval. However, the changes in the atomic structure accompanying this vitrification are only very subtle. Here we discuss structural changes observed in-situ by ultrafast high-energy X-ray diffraction in glass-forming liquids from temperatures above the liquidus temperature to well below the glass transition temperature. This enables a detailed investigation of the miniscule changes of the atomic arrangements leading to the significant slowdown of the kinetics during the glass transition. Analysis of the short and medium range order indicates temperature dependent structural changes along the liquid alloy's pathway to vitrification that may be related to liquid-liquid or fragile-to-strong crossovers [1,2] as well as to the influence of global resonances on structure formation[3].

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*Speaker

O 20

Viscosity of supercooled water under pressure and two-state interpretation of water anomalies

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Abstract

Among the numerous anomalies of water, the effect of pressure on its transport coefficients is particularly striking. Around room temperature, an increase in pressure from ambient results in a decrease of viscosity and rotational correlation time, while the translational diffusion coefficient increases. At high enough pressure, the pressure dependence is reversed and water behaves as a normal liquid. The pressure anomalies for translational and rotational diffusion have been followed deep in the supercooled region. However, up to now, viscosity data for supercooled water under pressure was not available. We report for the first time such data, obtained with a Poiseuille flow experiment performed up to 300 MPa and down to 20◦C below the melting line, and by the observation of Brownian colloids up to 100MPa and down to 25◦C supercooling. Our data reveal a large intensification of the viscosity anomaly upon cooling: pressurization at 244 K reduces the viscosity of water by nearly a factor of 2. The location of the viscosity minimum follows that of the translational diffusion coefficient maximum. We discuss experimental data on dynamic properties in the framework of two-state models for water. Combining a modified version of a previous dynamic model with an existing, quantitative model for thermodynamics, we obtain an accurate description of dynamic properties of stable and supercooled water under pressure. We discuss the possible connection with a putative phase transition between two distinct liquid forms of supercooled water. Motivated by analogies between solutes and pressure and recent experiments on water-glycerol mixtures we also present measurements of the viscosity of supercooled water-glycerol mixtures rich in water.

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*Speaker

O 21

Collective plasticity in a model binary glass spanning five orders of magnitude strain rate.

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Abstract

Atomistic simulations of a Lennard Jones binary glass system are performed to investigate collective plasticity under simple shear stress conditions. Strain rates spanning five orders of magnitude are considered. It is found that as the strain rate reduces significant mobility of atoms mediate the plasticity. System spanning slip at the higher strain rates is found to become less localized. Structural relaxation during such events now plays an important role, producing a rich spectrum of atomic-scale activity in terms of spatial and temporal correlation. At the slowest strain rate considered, the emergence of serration-like behaviour is seen in the stress-strain curve.

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*Speaker

O 22

Influence of the presence of crystalline defects in bulk metallic glasses on cracking and plasticity

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Abstract

Dating back to over thirty years, bulk metallic glasses (BMGs) are relatively new materials that exhibit exceptional mechanical properties (strength, hardness, toughness, stored elastic energy ...), compared to those of most crystalline metallic alloys. Their apparent brittleness under uniaxial loading, however, is still a major obstacle to their industrialization. BMGs often contain crystalline defects developed, intentionally or not, during their complex and delicate elaboration. These flaws are known to affect their fracture toughness and their plastic behaviour. This paper reviews more than ten years of work about this subject on Zr-based and Fe-based bulk metallic glasses that may contain a low volume fraction of crystalline defects of different natures, e.g. dendrites or spherulites, depending on the synthesis method. Dedicated experimental set-ups, mainly bending tests on notched beam, were developed to create in the specimen a proper pre-crack by fatigue and then load it monotonically up to fracture. Indentation tests were also used to introduce cracks in the sample. The measured fracture toughness and the fractographic observations allow to conclude that these crystalline defects facilitate pre-cracking, but result in an embrittlement that is more or less significant depending on their type. The influence of the loading mode of the crack - mode I, II or mixed - was also investigated. It was shown that this parameter plays a key role in the ways cracks initiate and propagate, whether steadily or catastrophically, in the BMG. Finally, by means of finite element computations analyzing the mechanical interaction between a defect and a crack, explanation on how the crystalline flaws presence can affect fracture toughness and how they can perturbate crack growth, under mode I and mode II, was proposed.

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*Speaker

O 23

A new long-term nanoindentation relaxation method to characterize the time-dependent behavior of thin ZrNi metallic glass films

Guillaume Kermouche*[1], Paul Baral[1], Jean-Luc Loubet[2], Matteo Ghidelli[3], Hosni Idrissi[3], Jean-Pierre Raskin[3], and Thomas Pardoen[3]

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Abstract

The characterization of the time-dependent behavior of thin metallic glass films is one of the key-issue for surface engineering. nanomechanical testing such as nanoindentation testing, micropillar compression, or lab-on-chip experiments have already been used for that purpose. Such a measurement requires to load a constant material volume located in the thin film. Unfortunately, this condition is not fulfilled in the commonly used creep nanoindentation testing, contrary to micro tensile lab-on-chip experiments or micropillar compression testing. Therefore we propose to use a new indentation relaxation test. The method consists in maintaining a constant contact area during the test by playing on the contact stiffness between the tip and the material that leads to very stable experiments. Relaxation tests are performed up to 10h with excellent reproducibility. Very low viscoplastic strain rates can be extracted from the measurements – typically between 10^{-7} and 10^{-4} s^{-1}. An extensive study of ZrNi metallic glasses viscoplastic behavior is performed using several experimental set-up (lab on chips, nanoindentation relaxation, ...) . It is shown that apparent activation volume and thus strain rate sensitivity remain constant on a wide range of strain rates – from 10^{-9} and 10^{-1} s^{-1}. We evidence, thanks to the long-term indentation relaxation test that the underlying deformation mechanism remain unchanged on the entire tested strain rate range.

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*Speaker

O 24

Ab initio study of the properties of liquid uranium for temperatures up to 2050 K.

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Abstract

Uranium compounds are used as fissile materials in nuclear reactors. In present day reactors the most used nuclear fuel is uranium dioxide, but other compounds, such as uranium carbide and uranium mononotride, are also being considered for generation-IV reactors [1,2]. Upon possible accidents where the coolant would not circulate or be lost, the core of the reactor would get heated to very high temperatures, and it is essential to understand the behaviour of the nuclear fuel under such conditions for proper risk assessment. UO2 and UC would eventually melt, but UN would not reach a melting process since at temperatures around 2000K it decomposes into gaseous nitrogen and liquid U. It should be noted that the experimental study of liquid U is difficult and scarce. For instance, there is no experimental information about its static structure factor. In this contribution we analyze the properties of liquid U, studied through ab initio methods, for three temperatures ranging from its melting point to the dissociation temperature of UN. We show results for the static structure and also for several dynamic properties, including atomic diffusion and viscosity.

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[*] Speaker

O 25

Metallic glasses and melt under high pressure conditions

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Abstract

After the discovery of power-law and fractal nature in metallic glasses at ambient conditions [1], Zeng et al revealed "universal" fractional non-cubic power law for density of metallic glasses, and corresponding constant fractal dimensionality [2-4]. Here we will present the updated result on this topic, based on the experimental data for several metallic glasses at broader pressure range using synchrotron x-ray scattering and micro-tomography techniques. [5, 6] To further check the validity of non-cubic power law in non-crystalline systems under compression environment, one melting sample, i. e. Ga under pressure was investigated as well, and the multiple fractal dimensionality based on various peaks analysis in real space and reciprocal space was found. [7] Pressure induced meting mechanism in Ga was proposed based on the results of local structural PDF analysis [8]. Furthermore, preliminary results for XPCS studies of selected metallic glasses under high pressure conditions will be presented.

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*Speaker

O 26

Structure of the glass-forming Al-Y-Ni alloys formed from liquid upon high pressure solidification

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Abstract

The synthesis of amorphous materials based on aluminum, alloyed with REM, is carried out mainly by high-speed quenching of melt with cooling rates of more than 100000 deg/s. We studied mechanisms of effect of pressure (from 0.8 to 2.5 GPa) on solidification processes of Al95Y5, Al87Y5Ni8 melts with the aim of obtaining an amorphous-crystalline state at cooling rates less than 1000 deg/s. The evolution of morphological features of structural components of the alloys (rod-shaped Al3Y primary crystals, (a-Al+Al3Y) eutectic in Al95Y5; as well as Al23Ni6Y4 primary crystals of similar type, (a-Al+Al23Ni6Y4) eutectic in Al87Y5Ni8), from thermophysical conditions of solidification of the melt (pressure, cooling rate, temperature and time of exposure in the liquid). At 0.8 GPa, _˜ 5 deg/s, 1323 K, an increase in the exposure time to 3 min was found to lead to the fragmentation of primary crystals and modification of eutectic in both alloys. With an increase in pressure up to 2.5 GPa and a cooling rate of up to _˜ 1000 deg/s under the same solidification conditions, disperse (2-3 μm) primary yttrium aluminides of cuboid form are formed in Al95Y5 alloy (the maximum linear size of the primary crystals in the original sample is _˜ 100 μm). The alloying of the alloy with nickel (Al87Y5Ni8) leads to a noticeable increase in volume fraction of primary aluminides and replacement of their cuboid form by plates of ternary phase. It is shown that a simultaneous increase in pressure and cooling rate leads to milling of the matrix of alloys, as well as its eutectic component, which is accompanied by an increase in microhardness of latter several times (2-4) compared to initial state. No supposed amorphous phases were found in the studied alloys.

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*Speaker

O 27

The singularity of four-point correlation functions at the phase transition point of copper/nickel melt

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Abstract

The phase transition point of the substance, in spite of its exclusive effect on the behavior of a substance, is not special for its thermodynamic functions. It is shown that certain four-point motion correlators have singularities in the neighbourhood of the phase transition point. Four-point correlation functions by the definition relate the states of two particles at two different moments of time. Correlation coefficient CC(T, t) was chosen as the main characterizing function, which analyzes the evolution of collective movements in a liquid. Its physical meaning is the value of the average cosine of the angle between the particle displacement vectors in the diagnostic cluster with a certain size in a characteristic time of observation. This function do not explicitly depend on the value of the system temperature due to the normalization on the length of the displacement vectors in its definition. This property of the function allows us to observe changes in the properties of the spatial structure of the system under isochoric cooling. The temperature behavior of such correlators is different in the liquid stable and supercooled metastable liquid phase of a copper and nickel (results for copper on fig.1). These correlators were calculated for systems of pure metal melts with EAM interaction potential, modelled by the molecular dynamics method. The effect appears at different cooling rates, showing little dependence on the type of material and the size of the system. The physical meaning of the effect is also given.

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*Speaker

O 28

Thermodynamic properties of heavy alkali liquid metals measured by picoseconds acoustics

Simon Ayrinhac[*†1], Michel Gauthier[1], Daniele Antonangeli[1], Marc Morand[1], Yiuri Garino[1], Philippe Rosier[1], Paraskevas Parisiades[1], and Frédéric Decremps[1]

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Abstract

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. Alkali liquid metals present complicated phase diagram with occurrence of many maxima in the melting line which can underlie possibly a LLPT. Picosecond acoustics technique 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. Improvements of the set-up are being made currently, adding laser heating to reach T in the range 1300-4000 K, ongoing monitoring of P/T combined with acoustics measurements, and also enhancing the speed and efficiency of data acquisition. This technique have been applied firstly to 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]. We also studied heavy 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]. In addition, l-Cs present anomalies in the equation of state of liquid around 5 GPa [8], but this is controversial [9]. We will present sound velocity measurements in l-Cs [10] and in l-Rb which can bring new informations on these two issues.

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[*] Speaker

O 29

Thermophysical properties of undercooled liquid Zr-Cu-x alloys under microgravity

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Abstract

Zr-Cu-Al and Zr-Cu-Ni are ternary alloy systems with a high glass forming ability. Additions of Al to binary Cu50Zr50 enhance the glass forming ability up to a concentration of 8 at.% Al. The Zr-Cu-Ni system is a base model system to study the glass forming ability of bulk metallic glasses. Because Cu50Zr50 as a congruently melting phase does not exhibit chemical segregation and constitutional effects, Zr-Cu-Ni represents a highly interesting material for investigations from both theoretical and experimental viewpoints, with possible applications in industry. Measurements of growth velocity as a function of undercooling in the environment of reduced gravity will be compared with the ones measured on ground. It is pertinent to note that the alloys of higher Cu content ($\geq$20 at.%) show abnormal behavior, i.e. an abrupt decrease in growth velocity, at high undercoolings. Another important aspect is the transport of heat that is released during crystallization at the solidification front into the undercooled melt. The temperature-dependent electrical resistivity of metallic liquids is important for casting processes. The thermal conductivity plays a crucial role for the solidification dynamics. The TEMPUS facility (electromagnetic levitation during parabolic flight) allows measuring the electrical conductivity s of a sample. Via the Wiedemann-Franz-law, the thermal conductivity l can be calculated from the electrical conductivity. In the past, the dendrite and eutectic growth kinetics of glass-forming Cu-Zr alloys are experimentally investigated. For modelling the crystallization kinetics from the undercooled melt, the thermal conductivity is one of the most important parameters. It controls the heat flow in front of liquid/solid interface. For the Zr-Cu-Al and Zr-Cu-Ni systems, we present results from Parabolic Flights and ground-based electromagnetic levitation furnace.

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*Speaker

O 30

Alloy order revisited: Calculation of the radii and order parameter of the layers for binary alloys with spherical symmetry

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Abstract

We investigate the mathematical basis of the calculation of the order parameter in a binary alloy with spherical symmetry, including the case of alloys made up of atoms of very different sizes. This approach, relying on the eigenstates of the exchange operator of the alloy components, reveals different spherical layers, with inner and outer radii that are solutions of a certain equation. These layers have variable thickness but always contain numbers of atoms of each species that are exactly in the ratio of the concentrations of these two species in the alloy. Thus the order parameter is correctly formalized. This method allows retrieving the Bhatia-Thornton formalism used for the description of binary alloys. Their formalism is retrieved by a different physical and mathematical approach from the original one. The present approach is used to investigate the order in the Bi0.3Ga0.7 liquid alloy. It is possible to determine eight layers and their order parameter on the interatomic distance-range [0, 15]. Our method opens the possibility to study long-range effect of the truncation of the interatomic potentials in numerical simulations. This approach, free of any arbitrary choice, improves the accuracy in the determination of the layers and of their order in liquid and amorphous binary alloys.

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*Speaker

O 31

Spherical-periodic order as structural homology of liquid, amorphous, and crystalline states

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Abstract

It has been widely accepted that there exists short-range ordered behavior in disordered states, and the root cause of short-range order is just Friedel oscillations. Due to Friedel oscillations, the spherical-periodic order occurs and dominates liquid as well as amorphous structure formation. Since crystals grow from liquid and amorphous states, liquid structure features may also exist in crystalline phases, including the three simple crystals (face-centered cubic, hexagonal close-packed, and body-centered cubic structures) and the complex crystals related to metallic glasses. For a specific crystal, the lattice planes corresponding to the highest peak in reciprocal space are set as the principal resonance lattice planes, and their inter-planar spacing is considered to be the Friedel wavelength. After scaled with the thus-obtained Friedel wavelengths, the spherical-periodic features in crystalline phases are revealed. Spherical-periodic order in crystals will shine new light on the structural origin of completely ordered crystals, and will also represent the common structural homology of liquid, amorphous, and crystalline states. For the complex crystals related to bulk metallic glasses, among the multiple nearest-neighbor clusters developed from all the non-equivalent atomic sites in a given phase, there always exists a principal cluster, centered by which the spherical periodicity, both topologically and chemically, is the most distinct. Then the principal clusters plus specific glue atoms just constitute the short-range-order structural units shared by liquid, amorphous, and the corresponding crystalline phases. This is the so-called cluster-plus-glue-atom model, formulated as [cluster](glue atom)x, where the cluster is a nearest-neighbor coordination polyhedron and x means the number of glue atoms situated between the clusters. In constructing the composition formulas of metallic glasses, the detailed procedures using the cluster-plus-glue-atom approach have already been established, among which the key step is to select the proper principal clusters from the corresponding devitrification phases.

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*Speaker

O 32

The three-dimensional fractals of stars with icosahedral symmetry

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Abstract

Penrose tiling [1] is often considered as the initial lattice of decagonal quasicrystals [2]. This tiling can be represented as set of clusters of five-pointed stars [3]. It is shown that the Penrose tiling can be obtained using fractals of regular five-pointed stars [4]. The fractals are constructed by arranging the stars of each step so, that their centres are located at the vertices of the polygons of the previous step. The points of the previous step are deleted. The stars can have one of two orientations. Relative size of the stars at each step is set by the integer degree of the "golden mean" t = (1 + 5 ˆ 0.5) / 2 * 1.618. These stars can touch and cross each other. We propose to apply this technique to the building of the three-dimensional fractal of stars. A great stellated dodecahedron (SI) and a small stellated dodecahedron (SD) [5] were chosen as building elements of the fractals. SI can be obtained by extending the edges of an icosahedron to the intersection; SD can be drawn by extending the edges of a dodecahedron to their intersection. All faces of these polyhedra have the form of regular five-pointed stars. To construct the fractals, the ratio of the initial sizes of SI and SD are chosen in such a way that the faces of these polyhedra are equal. Both polyhedra have an icosahedral symmetry, and their orientations are chosen so that the directions of its symmetry axes coincide.

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*Speaker

O 33

Structural relaxations in metallic glass membranes stimulated by in-situ hydrogenation

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Abstract

Amorphous membranes for H2/CO2 separation are emerging as an alternative to the more expensive Pd-based, but to date their lifetime during application is severely limited by aging, due to the combined effects of temperature and hydrogen absorption. Here, we used X-ray photon correlation spectroscopy to follow the evolution of the structural relaxations in Ni-based metallic glasses membranes (Ni-MGM) during in-situ hydrogenation. We find that the hydrogen leads to an instantaneous and reversible rejuvenation of the glass characterized by an increase of the atomic mobility of almost two orders of magnitude and a concomitant decrease of the medium range order. However, while the acceleration persists in Ni-MGMs containing Zr independently of the thermal history, in pure Ni-MGMs it is strongly reduced by pre-annealing the membrane. We ascribe the relaxation mechanism in Zr Ni-MGMs to a chemisorption effect altering the local structure while in pure Ni-MGMs the observed rejuvenation is likely connected to the physisorption of hydrogen releasing the free volume. These results highlight the importance of drawing a microscopic picture of the complexity of metallic glasses for a proper exploitation of their unique properties [1].

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*Speaker

O 34

Hydrogen storage in Pd-based metallic glass nanofilms via electrochemical methods

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Abstract

In this study, the hydrogen electrosorption and evolution mechanisms in _˜50 nm thick Pd-Cu-Si based metallic glass nanofilms and Pd polycrystal nanofilm deposited by dc magnetron sputtering were investigated. The findings highlight the strong influence of Pd substitution with Cu atoms on the films' hydrogen electrosorption efficiency. Electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) of the mentioned nanofilms was performed in full spectrum including ad/absorption, desorption and evolution of hydrogen in a conventional three-electrode configuration. To the best of our knowledge, this is the first time thin film metallic glasses in general are investigated using EIS and CV to assess the frequency- and potential-dependent electrosorption mechanism of hydrogen over a broad potential range. Electrochemical circuit modeling (ECM) of the EIS provided the relationship between the composition-dependent hydrogen evolution and hydrogen absorption/adsorption processes. The adsorption capacitance parameter involving the a- and ß-hydride formation of the MG2 (5 at. % Cu) and MG5 (20 at. % Cu) nanofilms is 4.7 and 3.9 times higher than that of the crystalline Pd nanofilm, respectively. In terms of the volumetric hydrogen adsorption capacity, the value for MG5 is 4 times (_˜231 C/cm3) higher than for Pd films of several microns in thickness (calculated as _˜57 C/cm3). Furthermore, Aberration-corrected HRTEM and STEM-HAADF/-EELS techniques as well as the hydrogen to metal storage ratio obtained from the combinatorial chronoamperometry and CV confirms the higher hydrogen sorption kinetics of Pd metallic glasses compared to crystalline Pd and other Pd

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[*] Speaker

O 35

Mechanical behaviors of metallic glassy thin films

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Abstract

In this talk, recent progress in mechanical behaviors of metallic glassy thin films (MGTFs) in Zhejiang University will be briefly summarized. Superb elastic strain limit in Ni-Nb MGTF and the underlying mechanisms will be introduced. The key factors that control the plastic deformation mode of MGTFs are outlined. The availability of two-dimensional MGTFs stimulates comprehensive studies in those fields, which will enhance the understanding of the correlation of structure and properties, and develop the new designing strategy for engineers.

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*Speaker

O 36

VULKAM

Sébastien Gravier*†[1]

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Abstract

Vulkam presentation

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[*] Speaker

O 37

The influence of minor additions of sulfur in Zr- and Cu-based bulk metallic glass forming liquids

Benedikt Bochtler[*†1], Alexander Kuball[1], Oliver Gross[1], and Ralf Busch[1]

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Abstract

Bulk metallic glasses (BMGs) combine extraordinary strength with a large elastic limit, making them desirable structural materials, especially as they can be shaped by thermoplastic forming, unlike any other metallic material. Just recently, a new group of sulfur-containing BMGs was discovered [1], opening a wide range of possibilities for the modification of known alloys. In this context it was shown, that minor additions of sulfur significantly increase the supercooled liquid region of Zr52.5Cu17.9Ni14.6Al10Ti5 (Vit105) and Cu47Ti34Zr11Ni8 (Vit101). In this study, the influence of minor sulfur additions to these two alloy compositions is thoroughly investigated. The thermophysical properties of the alloys are assessed using differential scanning calorimetry (DSC), thermo-mechanical analysis (TMA), and high-temperature Couette rheometry. The results are discussed regarding the glass-forming ability and the thermal stability upon heating of the sulfur-bearing alloys in comparison to their unmodified base alloys. In-situ high energy synchrotron X-ray diffraction experiments are conducted, resolving the temperature dependence of the structure of the glassy and the liquid phase, and furthermore revealing the crystallization behavior. Regarding the influence of minor additions of sulfur on the thermal stability of the alloys, special focus is laid on the connection of this property to the thermoplastic formability of the alloys. Thermoplastic deformation experiments are conducted in a custom-built thermoplastic forming machine in order to evaluate the formability. In summary, the general influence of minor sulfur additions in Vit105 and Vit101 is discussed in the context of thermophysical properties, crystallization behavior, and the connection of these properties to the thermoplastic formability of the alloys.

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[*] Speaker

O 38

Study of surface crystallization during the elaboration of a ZrCoAl bulk metallic glass.

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[2]Vulkam (Vulkam) – add new organisation – Batiment Ampère 101 rue de la physique 38402 Saint Martin d'hères Cédex France, France

Abstract

Casting of metallic glasses sometimes induces surface crystallization despite the fact that the surface is expected to be the region where the cooling rate is the highest. This phenomenon has been observed on various metallic glasses, even for those with large critical diameters (Abrosimova et al., 2001; Koster, 1988; Wang, 2014). Such surface crystallization can be detrimental when the target applications are focused on surface properties, such as corrosion resistance for biomedical applications. It is thus important to identify the origin of this phenomenon for suppressing it in order to cast small net shaped parts. For this study, a ZrCoAl amorphous alloy with a large critical diameter was used. It has been shown that samples processed using copper-mould suction casting present crystallization only at the surface, while the bulk was totally amorphous. Using in-house highly reproducible suction casting and micro-casting processes, the influence of the casting techniques, as well as the moulding parameters were investigated (mould material and temperature, working atmosphere, applied pressure, interface temperature...). For each condition, the extent of surface crystallization was characterized. The origin of surface crystallization using conventional copper-mould suction casting is explained and we show that the alternative injection casting method can completely suppress this effect.

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*Speaker

O 39

Short- and medium-range order in Cu-Zr metallic glasses analyzed using the p3 code

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Abstract

Metallic glasses are materials that lack the long-range order of crystals but behave mechanically like solids. Their excellent mechanical properties, such as extreme strength, high elasticity and low internal friction, make them promising candidates for numerous applications that span from electronic devices to structural materials. However, while the relation between the structure and properties of crystals have been largely studied, the mechanisms that come into play in metallic glasses remain poorly understood. It remains a challenge to explain phenomena such as the glass transition and how the atomic structure of these materials is related to their outstanding mechanical properties. Using molecular dynamics simulations, we study the structural evolution of $Cu50Zr50$ and $Cu64.5Zr35.5$ metallic glasses during the cooling of the sample. To study the generated atomic configurations, we use a recently developed method to characterize local structures obtained by a Voronoi tessellation, called p3 code [1] This technique alleviates the limits of the conventional Voronoi indices by better distinguishing different types of local structures [2], and hence allows a better identification the key local structures at the short-range order. Then, to develop the knowledge of the atomic structure beyond the short-range order, we study how different local structures are arranged and how they form networks, depending on the atomic composition and the cooling rate of the quenching. Our study reveals which types of arrangements of local structures are or are not favored during the formation of a glass. These results represent an important stepping towards the understanding of the relationship between the structure and properties of metallic glasses.

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*Speaker

O 40

Signatures of structural differences in Pt-P- and Pd-P-based bulk glass-forming liquids

Oliver Gross*†[1], Nico Neuber[1], Alexander Kuball[1], Benedikt Bochtler[1], Simon Hechler[1], Maximilian Frey[1], and Ralf Busch[1]

[1]Saarland University - Chair of Metallic Materials (LMW) – Saarland University, 66123 Saarbrücken, Germany

Abstract

The thermophysical properties of Pt-P-based bulk glass-forming liquids are determined using calorimetric and thermomechanical experiments. The comparison of the data to that of the Pd-P-based liquids indicate the existence of structural differences between the two congeneric alloy families. Therefore, the structure of the Pt-P- and Pd-P-based bulk glass-forming liquids is investigated by synchrotron X-ray scattering experiments. Although Pt and Pd are considered to be topologically equivalent in structural models [1], drastic changes in the total structure factor and in the reduced pair distribution function are observed upon gradual substitution. These variations indicate the existence of significant structural differences on various length scales. A pronounced pre-peak at low Q-values in the total structure factor of Pt42.5Cu27Ni9.5P21 implies the existence of a pronounced medium range order (MRO) that is vanishing when Pt is replaced by Pd. Instead a shoulder in the second peak appears that is most pronounced in the Pd-P-based liquids revealing a mostly icosahedral short-range order (SRO). The structural data indicate that the dominant polyhedra and the distribution of their connection schemes from Pt-P- to Pd-P-based alloys gradually change, which is likely to be connected to the different sensitivities to annealing or cooling rate induced embrittlement [2,3]. The structural evolution of the total structure factor and the reduced pair distribution function with increasing temperature suggest the (partial) dissolution of both the MRO and the SRO which reflects the thermodynamic properties of the liquids.

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*Speaker

O 41

Structural Properties of Expanded Liquid Carbon C60

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Abstract

Abstract:
We present analytical calculations as well as canonical ensemble Monte Carlo computer simulations (NVT-MC) for the structure factor and the radial distribution function for liquid C60 at high temperatures up to the Liquid-Vapor critical point. We employed the sticky hard-sphere (SHS) model potential for C60 fluid to obtain analytical expressions for and via the analytical solution of the OZ equation. The temperature dependence of the sticky parameter is obtained via the second Virial coefficient of C60. The SHS equation of state is also used to calculate the Liquid-Vapour coexistent curve and the critical parameters, TC=2007 K, ρC=0.48 nm-3 and PC= 54.4 bars.

In order to validate our analytical results, we have compared S(q) and g(r) with those from NVT-MC simulation on C60 fullerene fluid at different phase points on temperature-density plane of the phase diagram. In our simulation the C60 fullerene molecules have been modeled as highly coarse-grained spheres, using an inter-molecular potential proposed by Girifalco (J. Phys. Chem., 96, 858 (1992)). The structure factors S(q) have been calculated from NVT-MC trajectories at all the phase points studied here. The comparison shows some agreement at low temperature range. The results of and at different temperatures could explain the expansion mechanism of C60 at extreme conditions of temperatures and pressures. 2.5.0.0

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*Speaker

O 42

Thermophysical properties of undercooled liquid Zr-Cu-x alloys under microgravity

Stefanie Koch*[1], Peter Galenko[1], Georg Lohöfer[2], and Markus Rettenmayr[1]

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[2]German Aerospace Center (DLR) – 51170 Cologne, Germany

Abstract

Zr-Cu-Al and Zr-Cu-Ni are ternary alloy systems with a high glass forming ability. Additions of Al to binary Cu50Zr50 enhance the glass forming ability up to a concentration of 8 at.% Al. The Zr-Cu-Ni system is a base model system to study the glass forming ability of bulk metallic glasses. Because Cu50Zr50 as a congruently melting phase does not exhibit chemical segregation and constitutional effects, Zr-Cu-Ni represents a highly interesting material for investigations from both theoretical and experimental viewpoints, with possible applications in industry. Measurements of growth velocity as a function of undercooling in the environment of reduced gravity will be compared with the ones measured on ground. It is pertinent to note that the alloys of higher Cu content (≥20 at.%) show abnormal behavior, i.e. an abrupt decrease in growth velocity, at high undercoolings. Another important aspect is the transport of heat that is released during crystallization at the solidification front into the undercooled melt. The temperature-dependent electrical resistivity of metallic liquids is important for casting processes. The thermal conductivity plays a crucial role for the solidification dynamics. The TEMPUS facility (electromagnetic levitation during parabolic flight) allows measuring the electrical conductivity s of a sample. Via the Wiedemann-Franz-law, the thermal conductivity l can be calculated from the electrical conductivity. In the past, the dendrite and eutectic growth kinetics of glass-forming Cu-Zr alloys are experimentally investigated. For modelling the crystallization kinetics from the undercooled melt, the thermal conductivity is one of the most important parameters. It controls the heat flow in front of liquid/solid interface. For the Zr-Cu-Al and Zr-Cu-Ni systems, we present results from Parabolic Flights and ground-based electromagnetic levitation furnace.

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*Speaker

O 43

The role of Ga addition on the thermodynamics, kinetics, and tarnishing properties of the Au-Ag-Pd-Cu-Si bulk metallic glass forming system

Nico Neuber*[1], Oliver Gross[1], James P. Best[2], Mikhail Polyakov[2], Johann Michler[2], Miriam Eisenbart[3], Alexander Heiss[3], Ulrich E. Klotz[3], Ralf Busch[1], and Isabella Gallino[1]

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Abstract

Effective strategies to increase the tarnishing resistance of the 18 K (karat) gold-based bulk metallic glass-forming composition Au49Ag5.5Pd2.3Cu26.9Si16.3 were recently found through the addition of Ga at the expense of Cu combined with a sufficient reduction of Si [1]. However, the modification of the alloy is accompanied by a reduction of the glass-forming ability (GFA) from 5 to 2 mm in terms of the critical casting thickness and eventually collapses for Ga contents higher than _˜9 at%. Thermodynamic and kinetic studies of the newly discovered 18 K Au-Ag-Pd-Cu-Ga-Si system shed light on the reason for the loss in GFA with increasing Ga content. Investigations of the liquid kinetics in terms of viscosity and transition time, assessed by three-point beam bending and the Tg-shift method, reveal an unexpected change of the fragility to stronger liquid kinetics with increasing Ga concentration, usually attributed to an increase in the GFA. In contrast, thermodynamic considerations based on specific heat capacity measurements reveal an ascending driving force for crystallization with increasing Ga-content, being accountable for the drop in the GFA. Due to this, a Ga-rich melt beyond the threshold concentration of 9 at% is not desirable for the production of BMGs from the liquid state. With the intention to outrun this barrier, while preserving the amorphous structure, Ga-ion implantation with a liquid metal focused ion beam (FIB) source is used as a post-processing routine for a cast Ga-containing Au-BMG. This low temperature method allows to successfully cross the thermodynamic borderline concentration, validated by Monte-Carlo (TRIM) simulations, and to achieve an additional improvement of the tarnishing resistance in the Ga-enriched areas [2].

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-[2] N. Neuber et al., Acta Mater. 165 (2018) 315–326. doi:10.1016/j.actamat.2018.11.052.

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[*] Speaker

O 44

Metallic glasses micro-parts molding and determination of the alloy properties by an experimental inverse analysis.

Bruno Lavisse*[1], Xavier Cerutti[2], Alexis Lenain[2], Georges Kapelski[1], Sébastien Gravier[2], and Rémi Daudin[1]

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[2]Vulkam (Vulkam) – add new organisation – Batiment Ampère 101 rue de la physique 38402 Saint Martin d'hères Cédex France, France

Abstract

Remarkable properties of amorphous metallic alloys in terms of corrosion, biocompatibility wear resistance and elastic strain (in the order of 1.8%) are of greater interest. The quasi-lack of shrinkage after alloy solidification provides very tight tolerance geometries (about 1 μm).

Amorphous metallic glasses micro-parts can be shaped through thermoplastic forming above the glass transition temperature. This process is however restricted to very few stable compositions and therefore limits the range of properties for micro-parts. To overtake those restrictions, a highly reproducible micro-casting process has recently been developed to specifically produce metallic glasses micro-parts. This technique enables very small and net-shaped parts to be obtained directly from the melt while using metallic glasses presenting reduced thermal stability above Tg and low critical diameters. Therefore, it highly expands the choice of the micro-part compositions and consequently the range of final properties.

In this work it has been shown that such micro-parts may be directly molded into Silicon molds without any damages. Small cylinders with diameters close to just a few tens of micrometer in size can be casted. This demonstrate the huge potential of this process in terms of micro-mold filling. Moreover, by assuming laminar flow characteristics in this simple geometries during the alloy injection, by controlling molding parameters (pressure and injection velocity) and by measuring the filling length of the cylinder, physical properties and "castability" of the amorphous alloys can be determined.

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*Speaker

O 45

Convective effects in undercooled liquids during dendritic crystallization

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Abstract

Solidification of metastable undercooled liquid metals provides an insight into the fundamentals of phase change. Purely diffusion driven solidification has been described by analytic models such as the LKT theory. However, in practice achieving such conditions is very difficult with fluid flow almost always present. Techniques to achieve high undercoolings, such as electromagnetic levitation must provide a force to counter gravity, but this in turn is also a driver of flow [1]. Even the addition of a high magnetic field to supress fluid flow can inadvertently drive secondary thermoelectric magneto-hydrodynamic flows in the vicinity of solidification. Consequently, it has been necessary to extend the analytic models to include the influence of fluid flow [2]. The present work is devoted to analytical and numerical investigation of the fluid flow effect of dendritic crystallization in undercooled liquids. Crystallization kinetics is analysed in detail by a model of non-equilibrium dendritic growth with fluid flow [3]. The model for convection transport of heat and mass are tested against a combined enthalpy based lattice Boltzmann method describing solidification and fluid flow. Different criteria of the dendrite tip stability [4] is tested against data of numerical simulations of crystallization of undercooled liquids.

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-[3] P.K. Galenko, D.A. Danilov, K. Reuther, D.V. Alexandrov, M. Rettenmayr, D.M. Herlach, J. Crystal Growth 457 (2017) 349-355.
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*Speaker

O 46

The fragility of bulk metallic glass forming liquids studied via modulated DSC

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Abstract

Fragility describes the susceptibility of a liquid's relaxation time or equilibrium viscosity to temperature changes. Liquids are termed 'strong' if these properties show a rather Arrhenius-like dependency and are termed 'fragile' if distinct deviations from Arrhenius behavior are observed. In case of metallic glass formers, fragility plays a decisive role for the glass forming ability, since it directly influences the crystallization kinetics, and is therefore subject of vital research. In the present study, fragility of various bulk metallic glass formers is studied using modulated dynamic scanning calorimetry. Thereby, heating and cooling scans through the thermal glass transition are performed with a small underlying rate, which is amplified by a sinusoidal thermal oscillation with small amplitude and distinct period length. The dynamic glass transition is analyzed by splitting the total heat flow in a reversing and a non-reversing component [1]. The dynamic glass transition shifts with the applied period length of modulation, thereby allowing to connect the (mean) relaxation time of the liquid with a respective temperature value. By applying various scans with different periods, the fragility of the measured alloys can be quantified by fitting the obtained data points using the VFT equation. The results are compared with existing fragility studies of these alloys and good agreement is found. Especially systems with high thermal stability and wide supercooled liquid regions allow to obtain numerous data points by using only one sample, thereby facilitating and accelerating data acquisition in comparison to other calorimetric or thermomechanical methods.

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*Speaker

O 47

Electronic transport in solid Ni64-Zr36. alloy (amorphous and recrystallized). Effect of temperature and time.

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Abstract

In present work, we characterize structural changes of Ni64-Zr36 alloys, particularly the recrystallization of amorphous alloys by resistivity and by Absolute Thermoelectric Power (ATP). The Ni64Zr36 master alloy was prepared by arc melting using pure Ni (99.97%) and Zr (99.8%). Glassy ribbons were produced by single-roller melt spinning on a Cu wheel under an argon atmosphere. We discuss the value of resistivity and ATP in the framework of the extended Faber- Ziman formalism. We focus especially on the change of sign of the ATP between the amorphous alloy (positive ATP) and the recrystallized one (negative ATP). We also discuss the value of the resistivity, lower in the crystallized phase than in the amorphous phase at room temperature and that is classic, but surprisingly higher between 200 and 550∘C.

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*Speaker

O 48

Yttria precipitates formation in a Cu-based amorphous alloy to improve mechanical properties.

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Abstract

For the past decades, intense efforts have been done to produce new metallic glasses with increased ductility. Several means are used to reach this purpose : rejuvenation, in-situ or ex-situ composites processing, or microalloying with different elements. Recently, it has been shown that the yttrium addition can help to increase the ductility. For example, ductility increases over 2 points with 1 at. % of yttrium. However, the cause responsible for this improvement remained to be define. In this work, we highlighted the presence of Y2O3 precipitates, investigating at nanoscale the distribution of these features. Two kinds of precipitates exist in Cu-based amorphous alloys : small solid ones and large hollow ones. The results of this work suggest that nano and micro crystallized areas are induced by the precipitates, leading to a composite structure and a better ductility. 2D (TEM experiments) and 3D microscopy (FIB reconstruction) experiments allowed us to obtain the volume fraction of these features. We also propose an explanation concerning the hollow precipitaes formation based on Kirkendall hypothesis. Our model is in accordance with the experimental parameters used during the BMs processing.

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*Speaker

O 49

On the existence of two contributions from collective excitations to the transverse dynamics of liquid metals

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Abstract

It was found recently that transverse spectral functions in several liquid metals (Li, Zn, Ni, Fe, Tl, Pb) contain additional smeared-out high-frequency peak for wave numbers in the second pseudo-Brillouin zone. In order to rationalize the pressure dependence of the contributions from different propagating processes to transverse spectral functions in liquid metals we performed ab-initio molecular dynamics simulations for liquid Na and Al in a wide range of pressures. We report spectra of longitudinal and transverse collective excitations, as well as compare them with the peak positions of the Fourier-spectra of velocity autocorrelation functions (vibrational density of states). In the case of Na, the influence of density/pressure is investigated by considering four pressures ranging from 15 to 147 GPa. In the case of Al, the temperature influence is considered between 600 K in the supercooled liquid up to 1700 K well above the melting point. Both temperature and density dependences of the spectra of collective excitations are analyzed with a focus on the appearance of a second, high-frequency, modes in the transverse spectra.

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*Speaker

O 50

Phonon excitations in liquid Au

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Abstract

In 2009, we found an indication of transverse acoustic (TA) phonon modes in liquid Ga in addition to the usual longitudinal acoustic (LA) modes by inelastic x-ray scattering (IXS) [1]. We also detected the TA signals in liquid Sn [2], Zn [3], and transition metals of Fe and Cu [3]. We analyzed the IXS data using current correlation functions, which are in good agreement with results of an ab initio molecular dynamics simulation [2]. Thereby, the theoretical LA and TA data show a mixing effect, i.e., mixtures of two excitation branches of quasi-LA and -TA contribuutions, and the experimental data are always very similar to the theoretical LA result. Based on these experimental and theoretical results, we have investigated particle dynamics of liquid Au, which has attracted much attention as a functional metal of catalysis. However, the inelastic neutron experiment has not yet been carried out so far owing to a very high absorption of neutrons and a relatively high melting temperature of 1063 degreeC. We measured IXS at BL35XU of SPring-8 uing a high-resolution IXS spectrometer with an energy resolution of about 1.5 meV. We observed the S(Q,omega) spectra at 1100 degreeC and the LA modes are clearly seen exhibiting a positive dispersion relation as the other liquid metals. In addition, the TA-like shoulders are observed. The obtained data will be analyzed using a modified version of generalized Langevin formalism, from which microscopic dynamic parameters, such as relaxation rates, viscosity, and moduli of both the LA and TA excitations, will be evaluated, and shown in the presentation.

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*Speaker

O 51

Phonons attenuation in a 2D nanocomposite

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Abstract

Thermal transport in nanostructured glass is interesting for recently proposed new applications. The propagation properties of thermal waves in composite material made of an elastic matrix with regularly spaced elastic inclusions are studied by combining complete analysis of the energy transport and vibration modes. With the help of a large number of finite element calculations, we have performed a parametric study of the apparent attenuation of a wave packet in a 2D solid with circular inclusions. Different materials are studied that differ by the stiffness of the components and the radius of the inclusions. The sensitivity to the frequency of the travelling wave is also studied in details. These three parameters can be used as control parameters, to tune sound velocity together with phonon scattering. It shows a non-monotonous dependence on the frequency, for specific values of the stiffness ratio between inclusions and matrix, thus revealing an optimum structure for apparent energy attenuation. These results are compared to the modal analysis and the calculation of the vibrational density of states for the different ranges of parameters. In this works, the viscoelastic properties is taken into count to represent the amorphous dissipation, which has been verified by comparing to compare with the Dynamic Molecular Simulation.

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*Speaker

O 52

Characterization of a novel titanium based bulk metallic glass in the quaternary

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Abstract

In this work, recently discovered titanium-based metallic glasses containing sulfur as a key element for glass formation are characterized in detail. While general characteristics of this new family of bulk metallic glasses have been reported [1,2], this work is set to provide detailed information about the specific

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*Speaker

O 53

Development of novel bulk glass-forming alloy compositions in the Ti(Zr)-Ni-Cu-S system

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Abstract

Amorphous metals possess a disordered atomic structure which is responsible for their high strength and elasticity in comparison to their crystalline counterparts. Recently, we reported on the bulk glass formation in the Ti-Ni-S system [1]. The alloy compositions feature an extremely high titanium content of up to 70 at% and a specific strength that exceeds that of conventional Ti-alloys by far. In this work, glass-forming alloy compositions are developed by adding small amounts of S to the ternary eutectic (Ti65.5Ni22.5Cu12), improving the glass-forming ability significantly. The compositions were cast into water-cooled copper molds with varying diameter using a suction casting device. The amorphous character of the samples is confirmed, and the crystallization sequence is investigated for samples exceeding the critical casting thickness by X-ray diffraction experiments. The substitution of Ti by Zr further improves the glass-forming ability and a critical diameter of 1 mm is reached. Thermal analysis reveals that the new glass-forming compositions do not exhibit a stable supercooled liquid region upon heating and show multiple crystallization events. This study shows that the glass-forming region in the Ti(Zr)-Cu-Ni-S extends over a larger compositional range than previously expected, providing new approaches for the development of Ti-based bulk glass-forming alloys.

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*Speaker

O 54

On the relationship between short-range structure and atomic dynamics in melts of glass-forming metallic alloys

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Abstract

We investigated the short-range order and the atomic dynamics in different stable and undercooled glass-forming metallic melts. In order to undercool the melts below the melting temperature and to avoid chemical reactions with crucible materials, the samples are containerlessly processed by electromagnetic or the electrostatic levitation. For glass-forming melts of Zr-Ni and Hf-Ni alloys full sets of partial structure factors were determined by neutron diffraction combined with an isotopic substitution technique [1,2], while Ni and Hf self-diffusion coefficients were measured as a function of temperature by quasielastic neutron scattering [2,3]. Similar as recently reported for Zr36Ni64 [4], a decoupling of the diffusion coefficients of the alloy components is observed for Hf35Ni65, showing that Ni diffuses faster than Hf. The relationship between short-range structure and atomic dynamics is discussed within the mode-coupling theory. For ternary Hf10Zr25Ni65 melts pronounced deviations of the temperature dependence of the atomic dynamics from an Arrhenius behavior are observed, while it can be accurately described by the scaling law of mode-coupling theory [5]. Although the measured overall packing fraction remains almost unchanged, the dynamics in Hf10Zr25Ni65 are slower compared to Zr36Ni64. This corresponds also to a higher critical temperature and might be induced by different chemical interactions in the melts.

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*Speaker

O 55

Glass structure and characteristic connectivity of mobile ions in fast ion-conducting chalcogenide glasses

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Abstract

AgI-doped As2Se3 glasses show fast ionic conduction at room temperature. Their ionic conductivity increases exponentially with increasing AgI content. High-energy X-ray diffraction, neutron diffraction and extended X-ray absorption fine structure experiments have been carried out for (AgI)x(As2Se3)1-x glasses and the local atomic arrangement was determined. However, detailed structure information is still inadequate at intermediate- and long-range scales. In this study, the relations between the glass structure and the ionic conduction will be discussed.Structure modelling of (AgI)x(As2Se3)1-x(x= 0, 0.4 and 0.6) glasses have been performed by the reverse Monte Carlo (RMC) technique using data sets of neutron diffraction (ND) and high energy X-ray diffraction (HEXRD) experiments in order to construct the detailed three-dimensional structure of the system. For the case of (AgI)0.6(As2Se3)0.4 glass, the differential structure factors obtained by the anomalous X-ray scattering (AXS) experiments were additionally applied in the present RMC modelling.It was demonstrated that the addition of a large amount of AgI does not significantly affect the short-range ordering of the host glass network matrix constructed by AsSe3/2 pyramidal units. It is also predicted that the structure model for the present (AgI)x(As2Se3)1-x glasses is microscopically phase-separated into a pseudo-binary mixture of the AsSe3/2 host network matrix and conduction pathways of mobileAg ions. The structure models obtained by the RMC modeling with AXS data sets shows that the mobile Ag ions are correlated each other within a short length scale, indicating the cooperative motion of mobile ions in the conduction pathways. Three-dimensional development of these cooperative correlation of mobile Ag ions would be strongly related to the improvement of the ionic migration in the present glass systems.

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[*] Speaker

O 56

Structure and properties of Al-Cu-Fe and Al-Cu-Ni melts

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Abstract

In this study, a comparative analysis of the structural parameters and concentration dependences of the viscosity and crystallization ability of quasicrystal-forming Al-Cu-Fe melts and liquid Al-Cu-Ni alloys was carried out. The functions of the radial distribution of atoms (rdf) of Al-Cu-Fe and Al-Cu-Ni melts from various concentration regions were determined by X-ray structural analysis and ab initio molecular dynamics. The main feature of the experimental rdf of the Al-Cu-Fe system is the presence of a shoulder at the first peak at small r. Viscosity and crystallization ability of Al-Cu-Fe and Al-Cu-Ni melts in a wide concentration range were determined by viscometry and differential thermal analysis. The concentration behavior of the viscosity of Al-Cu-Fe liquid alloys is similar to concentration changes of their melting temperatures. The coefficient of kinematic viscosity of the melts most of the investigated compounds near the melting point has a value of _˜ 7.5 10-7 m2/s. The value of viscosity of Al-Cu-Ni melts at the melting point is lower than viscosity of molten Al-Cu-Fe alloys and depends on the concentration.

This work was supported by the Russian Science Foundation (Grant No. RNF 18-12-00438)

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*Speaker

O 57

The factors affecting the carbide formation in ternary iron-chromium-carbon system close to the melting point

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Abstract

The ternary iron-chromium-carbon alloy system is the foundation stone of the large class of industrially important materials – stainless steels and white cast irons. It is known that iron-chromium-carbon melt forms upon crystallization a series of carbidic and mixed carbidic phases, moreover, their relative stability experiences significant changes near the concentration point of 13 at.% of chromium. This fact is very important for practical metallurgy, but the cause of the phenomenon is poorly understood. Recently, with ab initio simulations, it was found that magnetic frustration caused by competing ferromagnetic Fe-Fe and antiferromagnetic Cr-Cr interactions tends to either strongly reduce local magnetic moments on atoms of transition elements while maintaining collinearity, or leads to non-collinear magnetic structures. This effect is responsible for the short-range inversion in Fe-Cr alloys at a Cr concentration of 11 at.%. This suggests that one of the factors determining the stability of various carbide phases may be the change in magnetic moments on iron atoms introduced by chromium impurities. The report presents the result for ab initio molecular dynamics studies of Fe-Cr-C melts at temperatures near the melting point in the vicinity of the γ-(Fe, Cr)C eutectic in the concentration range of 12-18 at.% of chromium. The purpose of this study is to assess the influence of local frustration of magnetic interactions between chromium and iron atoms on the structure of the short-range order of the melt, the magnitude of the magnetic moments and the total energy of the melt.

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*Speaker

O 58

Transition from high-entropy to conventional alloys in amorphous and crystalline systems

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Abstract

The study of transition from conventional concentrated alloys (CA) to high-entropy ones (HEA) composed from the same elements is apparently very important, both for understanding the formation of HEAs and for proper evaluation of their potential with respect to that of corresponding CAs. However,this transition has so far been studied in only two alloy systems: crystalline (CrMnFeCo)1-xNix alloys [Mat.Sci.Eng.A 696(2017)228] and amorphous (a-) (TiZrNbCu)1-xNix alloys [J.Mat.Res.33(2018)3170]. In spite of very different atomic structure and chemical make-up both alloy systems showed pronounced change in properties on crossing from the HEA to CA concentration range. We present new results for both types of alloys and compare the effects of HEA-CA transition on selected properties of these systems. For the amorphous alloys, combining early and late transition metals, we present results for electronic structure (ES , studied with UPS), atomic structure (studied with XRD and SXPD) and physical properties for a new a-(TiZrNbNi)1-xCux alloy system (x< =0.52) which inspite of large atomic size mismatch and negative mixing enthalpy shows ideal solution behaviour, thus no change in properties when crossing from a-HEA to a-CA concentration range. In particular, its atomic structure and physical parameters show linear variations with x which extrapolate to parameters of a pure Cu as was the case in binary a-Ti,Zr,Hf-Cu alloys [J.Alloys Comp.621(2015)136]. In (CrMnFeCo)1-xNix alloys we show the evolution of the ES, studied with UPS, and of magnetism (magnetic moments and critical temperatures) with x which provide better insight into the nature of the transition from CA to HEA. The transition to HEAs is accompanied by the rapid supression and the change of type of magnetism . We also compare our results with theoretical and experimental results for equiatomic CrMnFeCoNi alloy and its low and medium entropy derivatives.Our results show strong influence of chemical short-range order on transition from CA to HEA.

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*Speaker

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Partial pair correlation functions of liquid VZrNbHfTa high-entropy alloy

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Abstract

High entropy alloy (HEA) consists of five or more components, and atomic fraction for every component should not be less than 5% and more than 35% and at the same time. Such alloy possesses high configurational entropy. In the most cases it is important that such an alloy should be single phase fully disordered solid solution or amorphous. One of the known phase formation rules for HEAs is based on a study of partial pair correlation functions in liquid state [1]. If all partial pair correlation functions are similar to each other than probability of formation of HEA is high. At present work partial pair correlation functions for liquid equiatomic VZrNbHfTa alloy were calculated via ab initio molecular dynamics using SIESTA [2]. Temperature was chosen to be 10% higher than mean melting temperature of pure components. Density was chosen to correspond minimum of energy-volume dependence of supercell. Time step was typical for molecular dynamics simulation, i.e. 1 fs, number of steps was set to 1500. Number of atoms in supercell was 250. Figure 1 demonstrates some of partial pair correlation functions for this system. According to figure 1 positions and heights the 1st peak of pair correlation functions are almost the same. It should be noted, that for other 10 partial pair correlation functions positions of the 1st peak and heights of it are close to demonstrated, which allows to conclude that probability of formation of single phase solid solution is high for VZrNbHfTa system.

Acknowledgments:the work was carried out according to the state assignment for IMET UB RAS. Calculations were performed using recourses of IMM UB RAS URAN cluster.

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*Speaker

O 60

Novel 'transrotational' solid state order: exotic nanostructures discovered by TEM for crystal growth in thin amorphous films

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Abstract

Novel 'transrotational' solid state order: exotic nanostructures discovered by TEM for crystal growth in thin amorphous films

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*Speaker

O 61

High resolution inductive electrical resistivity measurement of electromagnetically levitated liquid metal droplets

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Abstract

For investigations of highly reacting metallic melts, metallic melts at high temperatures, or undercooled metallic melts, containerless handling methods of the liquid as well as contactless measurement methods are beneficial or even mandatory. For the undisturbed containerless processing of metallic melts the well-established electromagnetic levitation technique is used in microgravity, which applies high frequency alternating magnetic fields for the contactless handling and heating of the specimen. The μg environment enables the use of the high frequency magnetic levitation fields also for a simultaneous inductive and thus noncontact measurement of the electrical resistivity of the levitated liquid metal droplet. In the present talk we explain the measurement technique and report on measurements of this quantity on several liquid metals and semiconductors which have been processed in the electromagnetic levitation facility "TEMPUS" during its 20sec lasting parabolic flights on board of aircrafts and in the "ISS/EML" facility on board of the "International Space Station" ISS.

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*Speaker

O 62

X-ray photon correlation spectroscopy for probing slow atomic scale relaxations in glasses and supercooled liquids.

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Abstract

X-ray photon correlation spectroscopy is a well established scattering technique for studying dynamics in a wide variety of systems. It is analogue to dynamic light scattering but due to high penetrating power and short wavelength of the X-rays, it allows the investigation of opaque samples and the access to atomic length scale. Microscopic dynamics at the atomic level is of great interest in particular for glass community. However its exploration with XPCS has not been possible until recently, due to the low scattering signal. Increase in coherent flux and advance in the data treatment of sparse signal opened unique capabilities of probing slow diffusion in crystals and atomic relaxations in glasses. Forthcoming upgrades of the synchrotron sources promise up to 100 fold improvement in a signal to noise ratio hence 10000 times faster processes can be probed. This opens possibilities for extending XPCS application to the dynamical studies in deep supercooled liquids, disordered materials under pressure etc. Here we review the XPCS studies applied to glasses and discuss the future prospects with new upgraded synchrotron sources.

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*Speaker

O 63

Unraveling non-equilibrium thermal relaxation in semiconductors using ultrafast x-ray diffuse scattering measurement at PAL-XFEL

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Abstract

Understanding transient dynamics of phonons via generation of hot charge carriers in solids at relevant length- and time-scale is of fundamental interest and is a necessity to take full benefit of recent technological advancements in microelectronic and optoelectronic devices. Typically, ultrafast laser excitation of semiconductors results in the generation of free electron-hole pairs and their subsequent relaxation is mediated by electron-phonon coupling process, of which distributions are known to be far away from equilibrium defined by Bose-Einstein distribution. In our recent work, we demonstrate capturing ultrafast lattice thermalization processes by means of momentum- and time-resolved X-ray diffuse scattering measurement performed at a hard x-ray free electron laser facility at Pohang Light Source. Based on our measurement, initial non-equilibrium population and subsequent relaxation dynamics prior to complete lattice thermalization (within 50 ps) are elucidated.

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*Speaker

O 64

Pressure-induced structural change of liquid sulfur from polymeric liquid to simple liquid

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Abstract

Liquid sulfur near the melting temperature of 388 K consists of S8 ring molecules. With increasing temperature, a structural transition from molecular liquid to chain polymeric liquid occurs. For high pressure conditions, some experimental and theoretical studies have been reported[Brazhkin, 1991; Zhao, 2014; Liu, 2014; Plašienka, 2015] for structural changes in liquid sulfur from long-chain to short-chain structures under high pressure up to 15.8 GPa. However, structural properties under further high pressure (i.e., structures that reach beyond a chain structure) have not been discussed. For this reason, in this study, we have investigated the structural properties of liquid sulfur under high pressures up to approximately 500 GPa by means of ab initio molecular dynamics simulations[5]. From our simulations, it is found that the liquid sulfur has a covalent-like interactions even in metallic state, and liquid sulfur has a simple liquid structure at 320 GPa and higher pressures. In this study, we will also discuss the similarities of pressure-induced structural change in other liquid chalcogens[Shimojo, 2003; Ohmura, 2011].

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*Speaker

O 65

Behaviors of disordered alloys under various thermodynamic conditions

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Abstract

In this talk, I will mention behaviors of disordered alloys under various thermodynamic conditions: 1. Development of bulk metallic glasses at ambient condition by varying thermodynamic parameter of composition, 2. Atomic structure of liquid metals at high temperature by varying thermodynamic parameter of temperature, 3. Phase transformation of metallic glasses at high hydrostatic pressure by varying thermodynamic parameter of pressure.

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*Speaker

O 66

Comparative estimation of the properties of liquid metals at high temperatures and pressures using the methods of classical and first-principle molecular dynamics

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Abstract

One of the foreground tasks of computer simulation is the prediction of metal properties at high temperatures and pressures, for example, under shock compression conditions. Most of the works on the shock compression of metals were published in the 50s – 80s of the 20th century, however, the data processing of the shock compression was carried out using approximate methods, and only recently the embedded atom model (EAM) was applied to describe highly compressed states, as a result were calculated multiparticle interatomic potentials of metals. According to the shock compression data, one of the authors, the parameters of the EAM potential were found and then the properties of the metal models at high temperature and pressure were determined [1]. Another method for calculating properties under shock compression is the ab initio quantum mechanical method. It allows the properties calculation without attracting any model approximations but it requires a lot of power and is really time consumable. This method has its limitations, for example, the error of the energy calculation using the ab initio method is (5-10) meV / atom [2]. To estimate the forecasting power of both methods, we compared the data obtained for the same states under conditions of shock compression for four liquid metals Na (4,000 K), Bi (10,000 K), Ni (4,450 K) and Fe (6,000 K). EAM potentials [1] and ab initio SIESTA package [3,4] were used. Both methods gave similar results for the coefficient of self-diffusion and the functions of the pair distribution of atoms but the pressure difference can reach up to 30%.

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*Speaker

O 67

plasticity of amorphous materials: from atomic to mesoscopic scale

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Abstract

The plastic behavior of glasses and disordered solids displays a rich and complex phenomenology, from scale free avalanches to localization of the strain field in shear bands. The recent years have seen an increasing effort of modeling of these phenomena at different length and time scales. In complement of numerous numerical simulations at atomistic scale of model or more realistic glasses, a new class of lattice models has emerged at mesoscopic scale that rely on the coupling between a local threshold dynamics and elastic interactions. The latter "Eshelby" interaction is associated to the internal stress induced by local rearrangeùment taking place in the surrounding elastic matrix and is characterized by a quadrupolar symmetry. While these lattice models reproduce most of the phenomenology observed in amorphous plasticity, a quantitative link remains to be done with atomistic sipmulations. Here we use a technique recently developed to characterize local yield stress in atomistic simulations to propose and study the quantitative connection between simulations operationg at atomistic and mesocopic scales.

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*Speaker

O 68

Full decomposition of plasticity in terms of Eshelby inclusions in amorphous solids studied with molecular dynamics

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Abstract

In 1979 [1] Ali Argon introduced the concept of local shear transformation which underlies the modern approaches to describe plasticity in amorphous systems. Under mechanical sollicitation, some local structural reorganisations occur, mostly of shear character and typically involving few dozens of particles. Such local rearrangements, also called Shear Transformation Zones (STZs), induce a characteristic elastic response in the material. An appropriate continuum mechanics description of this behaviour is given by the Eshelby inclusion problem where the rearrangement is characterized by a strain transformation matrix. These STZs and their elastic consequences have been extensively observed in molecular dynamics calculations(MD)[2], they have been observed in model colloidal glasses [3] and they represent the basic bricks of several mesocopic models for plasticity [2]. Eventhough the Eshelby inclusion play a central role for the description and the understanding of amorphous plasticity, only few works have been dedicated to a systematic representation of the MD results in terms of STZs and Eshelby inclusions. In this talk I will present an original technique designed for that purpose using three dimensional samples of amorphous silicon submitted to simple shear deformation [4]. First, the localization of the relevant STZs are identified and in a second step the STZs are represented in terms of Eshelby inclusions. In this way the full stress-strain relation can be reconstructed with a good accuracy while the analysis of the transformation strain tensors give information at the mesoscopic scale consistently with the underlying interaction model.

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*Speaker

O 69

Self-diffusion in Mercury investigated with quasi-elastic neutron scattering

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Abstract

Diffusion is a fundamental property of liquid with a high importance to many aspects in physics and material science. Despite the technical relevance it's still not very well understood how atomic diffusion depends on melt properties. Pure metals serve in this respect as a simple model system, due to the absent of internal degrees of freedom and short-range orders. We studied here Mercury which is especially interesting, since it has a rather high density and is the only the liquid metal at ambient temperatures ($Tl = 234$ K). It is therefore an ideal candidate to investigate diffusion mechanisms over a wide temperature range for liquid metals and alloys. Classically, self-diffusion coefficients are determined by ex-situ capillary techniques. However, these methods come with some disadvantages, like density- and/or temperature gradient-driven convection, which may lead to measurement artifacts up to several 100 % on absolute scales. We utilize here quasi-elastic neutron scattering (QENS) to determine the self-diffusion coefficients in liquid Mercury. QENS allows reliable and precise in-situ observation of atomic transport processes on microscopic scales, unaffected by any convection. The measurements were carried out in the temperature range between 240 and 350 K at the multi-disc chopper time-of-flight spectrometer TOFTOF at the research neutron source Heinz Maier-Leibnitz (FRM II). The obtained diffusion coefficient and its temperature dependence are compared with other pure metallic melts and discussed in the context of the influence of the atomic mass, molar volume, and the melting point on the atomic diffusion in liquid metals.

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*Speaker

O 70

From supercooled to glass: opposite effects of weak self-propulsion on relaxation

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Abstract

We study experimentally a sediment of self-propelled Brownian particles with densities ranging from dilute to ergodic supercooled to nonergodic glass. We observe a dramatic slow-down of relaxation of nonergodic states when particles become weakly self-propelled. By contrast, ergodic supercooled states always relax faster with self-propulsion. Our system is a monolayer of micron-size gold-platinum Janus particles, which become active/self-propelled upon adding a solution of hydrogen peroxide due to self-phoretic mechanisms. We characterise the activity level in our system with an effective temperature defined from the density profile. Standard glassy physics describes well the ergodic regime provided the replacement of the ambient temperature by this effective temperature: higher temperature implies faster relaxation. However beyond the glass transition, the relaxation of the nonergodic system abruptly slows down at low but nonzero activities. As we increase further activity, the relaxation speeds up until it exceeds the passive situation. This nonmonotonic behaviour cannot be described by a simple increase in temperature. To explain this phenomenon, we correlated particle displacement orientation and calculated the average length of correlated domains. It shows first a decrease and then an increase with the effective temperature. In particular, the minimum correlated domain length corresponds to the effective temperature where we detected the slowest relaxation. This suggests that relaxation in sufficiently active glass follows collective motion mechanisms, while cooperative motion dominates at zero and low activities. We propose that directed motion makes cage exploration less efficient and thus slows down cooperative relaxation with respect to a passive glass.

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*Speaker

O 71

Specific features of dynamics in expanded liquid mercury in the region of metal-nonmetal transition: Ab initio study

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Abstract

Static and dynamic properties of expanded liquid mercury were studied by scattering experiments [1], classical [2] and ab initio [3] simulations in order to reveal changes in atomistic structure and dynamics across the metal-nonmetal (M-NM) transition, which takes place close to the density 9 g/cm3. One of the features of collective dynamics was reported a plateau in density dependence of the speed of sound in the M-NM transition region. However a question arises whether some other features in dynamics can be observed close to the M-NM transition. We performed ab initio molecular dynamics simulations of liquid Hg along the isothermal line 1750K and 7 densities in the range 7-13.5 g/cm3 using a system of 200 particles. Electron-ion interaction was represented by PAW potentials with 12 valence electrons/atom, and PBE-GGA was taken in exchange-correlation functional. We observed the emergence of gap in the electronic density of states at the density 9.25 g/cm3. Various time correlation functions, relaxation times and elastic moduli were calculated for different densities of expanded mercury. We report non-monotonic behavior of the Maxwell relaxation time, as well as non-monotonic change in the density dependence of the shear-stress autocorrelation functions right in the M-NM transition region.

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*Speaker

The Stokes-Einstein relation of a simple liquid metal and its relationship to changes in the microscopic dynamics with increasing temperature

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Abstract

The Stokes-Einstein relation is well fulfilled for many liquids near the melting point. Deviations have been reported in the supercooled state, which have been related to dynamic heterogeneity. Here we report a study on violations of the SE-relation on a simple monatomic liquid metal, based on experimental data with increasing temperature [1]. The violation can be related to changes in the microscopic dynamics and point to a change in the dynamics of the equilibrium state of the liquid metal distinctly above the melting point. Those changes in dynamics originate from changes in the correlated movement of particles and might suggest a crossover of the liquid state from a high temperature more fluid-like state to a more viscous-like liquid state deep in the equilibrium liquid state. Similar observations in other liquid metals [2,3] and alloys indicate a universal character for such a crossover.

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*Speaker

O 73

To understanding of slow and non-monotonic relaxation processes in liquid eutectics

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Abstract

Some well known physical phenomena, observed in metallurgical processes, raise questions to physicists so far. The reason of these questions is the absence of a reliable description of these phenomena in terms of a generally accepted theory. One of these phenomena is the slow non-monotonic relaxation processes in glass-forming metal melts after melting [1], which relaxation time reaches few hours. In metallurgy these effects are explained as the result of slow dissolution of refractory solid phase fragments in liquid. However, the kinetics of these relaxation processes cannot be explained in terms of the linear diffusion model.Our theoretical description is based on the Cahn-Hilliard theory and functional methods of non-equilibrium dynamics [2]. For binary systems with eutectic equilibrium, the existence of liquid e liquid critical point in the solid-liquid two-phase area is established. The width of corresponding fluctuation region is estimated by Ginsburg-Levanyuk criterion, and constitutes up to several hundred degrees [3]. In this region, the system can be described in terms of non-equilibrium dynamics, and the homogenization process of the melt can be presented as an inverse one to spinodal decomposition. We show that in a binary solution in the presence of liquid phase of non-homogeneous composition, and a stoichiometric phase, for local solute concentration exceeding some critical value, the dynamical instability takes place that explains the relaxation processes slowing [4].

The work was supported by Russian Foundation for Basic Research, Grant 18-02-00643.

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*Speaker

O 74

Investigations on the annealing-induced structural changes in the Zr48Cu36Al8Ag8 bulk metallic glass and their effects on the kinetic and mechanical properties

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Abstract

The kinetic properties in vicinity of the glass transition temperature of the Zr48Cu36Al8Ag8 bulk glass-forming liquid are investigated by thermomechanical and calorimetric experiments. It is observed that the equilibrium viscosity in the deeply supercooled liquid (SCL) does not exhibit the typical Vogel-Fulcher-Tammann temperature dependence. Within the SCL, the viscosity increases and remains at high values until crystallization intervenes, indicating significant structural changes. The structural changes occurring in the SCL are investigated by synchrotron X-ray scattering experiments revealing the formation of nano-crystals that cannot be detected in differential scanning calorimetry or conventional X-ray diffractometry. Nano-crystals embedded in the glassy matrix were shown to have a positive effect on the plasticity of BMGs [1]. Thus, flexural three-point beam bending experiments are performed on as-cast and heat-treated samples. The heat treatment in the supercooled liquid is conducted in a custom-built device, allowing for fast cooling of the samples. The enthalpic states of as-cast and heat-treated samples are compared by determination of their fictive temperature and the fracture surface of the tested beams is investigated by scanning electron microscopy, revealing different morphologies.

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*Speaker

O 75

Control of microstructural evolution of bimetallic Janus particles

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Abstract

Nowadays, the coalescence of nanoclusters continues to be a subject of active theoretical and experimental research of basic and technological interest owing to its importance in understanding the structure of cluster-assembled materials. The term "Janus particles" is referred to a class of particles presenting two (or more) surface regions exhibiting different properties and disposed in an asymmetric fashion. It is this asymmetric structure what makes Janus particles very interesting for a wide range of applications in different fields, such as sensors, surfactants, coatings, drug-delivery, self-propelled carriers, or probes. In this talk our experimental and theoretical work on bimetallic Janus particles (JPs) will be presented. Experimentally, we examined the variables and methods able to produce a controllable and large yield of JPs, allowing rational design of scalable methods. At the same time, we conducted a series of classical Molecular Dynamics simulations to gain a deeper understanding of the different processes taking place during the formation of JPs and to provide further guidance for the experiment. Special attention was paid to the coalescence collision of two drops, the effect of Weber number, impact velocity and drop size ratio.

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*Speaker

O 76

Critical Casimir Effect as a Complex Response of Near-Critical Binary Liquid Mixture Analyzed with Atomic Force Microscopy

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Abstract

A characteristic force arises between two surfaces placed in near-critical binary liquid mixture due to increase in correlation length [1]. This phenomena is called critical Casimir effect as an analogy with Casimir effect of vacuum field. Direct detection of critical Casimir force has been implemented by using optical tweezer technique [2]. In the present study the measurement is extended to its detection as a complex response by using a modulation technique of atomic force microscopy (AFM). Interaction between a glass sphere with a diameter of 15 micron and a mica substrate was analyzed in binary mixture of lutidine and water close to the phase separation temperature. By applying sinusoidal modulation to the AFM force sensor, both the gradient of in-phase interaction force and the viscous drag coefficient, i.e., a viscoelasticity, were detected simultaneously. A characteristic gradient of attractive force was observed to increase as the temperature approached up to the critical condition in a range of 0.6 ◦C, which is attributed to the critical Casimir effect. Temperature-dependent potential energy of critical Casimir effect at the smallest sphere-substrate distance reached -1.8E-17 J, a value 3 orders of magnitude larger than that reported by Hertlein et al. [2] because of the larger interaction area and the smaller distance. A characteristic increase was also observed in the drag coefficient. This is attributed to an increase in interaction between like molecules with the correlation length.

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*Speaker

O 77

Density fluctuations of supercooled liquid Te

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Abstract

Liquid Te is known to exhibit many thermodynamic anomalies similar to liquid water [1]; density shows maximum slightly above melting temperature (Tm=450C), positive temperature coefficient of sound velocity and "fast sound" phenomena [2]. Thus, a unifying concept is now being constructed to understand these anomalous liquids: The key is liquid-liquid transition (LLT) or corresponding 'second critical point' [3]. The experimental work to prove the concept is still halfway, because the real, which means 1st-order, LLT is located in deep supercooled and high pressure region, where no one can reach to. Recent small-angle x-ray scattering (SAXS) experiment using free electron laser for liquid water indicates that the density fluctuation shows maximum in deep supercooled 'no-man's land' [4], which should be a strong supporting information of the real LLT. About liquid Te system, we already proved that density fluctuation shows maximum in the middle of LLT for liquid Se-Te mixtures [5] in the previous SAXS experiment at SPring-8/BL04B2, by using imaging plate (scan speed: over 20min / spectrum) as a detector. But we could not get any evidence for pure liquid Te above Tm at that time. Recently a new detector (Perkin Elmer, XRD1621AN3) with much faster scan speed (1min) was introduced to the beamline and we carried out the measurement again by using it. We succeeded to obtain about 20 spectra during supercooling (down to about 310 C) and to observe that density fluctuation shows maximum in the region.

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*Speaker

O 78

Thermodynamic perturbation theory: Mon's correction in terms of pair potentials

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Abstract

Thermodynamic perturbation theory (TPT) [1] is one of the best instruments for quantitative studies of fluids including liquid metals and their alloys (see, for example, review [2]). Nevertheless, in the work of Mon [3] it was shown that the high temperature approximation [1] of the TPT with the hard-sphere (HS) reference system (realized mostly by the variational method [4]) is incorrect when applied to substances described by interatomic pair interactions with a soft repulsive part. This inaccuracy is caused by the difference between the configuration space of the non-singular model system chosen for description of a real system and the configuration space of the HS reference system. An importance of the work [3] cannot be challenged, however, the made by Mon overthrow of fundamentals did not create a due furore. Moreover, this work remains practically unnoticed or ignored in scientific literature almost 20 years (only 10 citations on the "Web of Science" since the publishing in 2000 up to now). In this presentation I am going to focus an attention of the LAM community on the Mon outstanding work; show what compensatory operation allows to apply the TPT with hard-core reference potential to non-singular pair potentials in spite of the drawback of this theory found by Mon; and discuss in this context the necessity of a reconsideration of our outlooks on TPT applications to metal liquids. The work was supported by Act 211 Government of the Russian Federation (contract ? 02.A03.21.0006) and by the Fundamental Research Program of UB RAS (project 18-10-3-28).

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*Speaker

O 79

Thermo-physical characterization of sulfur-bearing bulk metallic glasses

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Abstract

Bulk metallic glasses (BMGs) can be produced in many metallic systems when quenching the equilibrium liquid at sufficiently high cooling rates. Recently, we reported on several novel multicomponent systems containing sulfur, in which bulk glass formation is observed by copper mold casting. In comparison to well-known BMG forming systems, in particular the Pd-, Zr- and Ti-based alloys are of special scientific interest due to different conspicuities in their thermo-physical properties. These thermo-physical properties play a key role in the process of glass formation and the resulting glass forming ability (GFA) and glass forming range (GFR). In this study, Pd- and Ti-based alloys are characterized using different techniques such as differential scanning calorimetry (DSC), thermo-mechanical analysis (TMA) and electromagnetic levitation (EML). The temperature sensitivity of the thermodynamic and kinetic contributions is discussed with respect to the process of glass formation in each alloy system. Additionally, in-situ high energy synchrotron X-ray experiments are conducted in order to investigate the temperature dependence of the liquid and glassy structure and to identify the crystalline phases, competing with glass formation and restricting the GFA. Finally, the effect of sulfur on the process of glass formation is investigated. In general, the results of this work facilitate an extended understanding about the process of glass formation, yielding new approaches for the development of novel BMG forming alloys.

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*Speaker

Poster Presentations

Abstracts

P 1

Transition from HEA to conventional alloys: insight from UPS and magnetism

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Abstract

In metallic systems electronic structure (ES) determines almost all their properties. Therefore, a change in properties of multicomponent alloys on crossing from HEA to conventional alloy(CA) concentration range in the same alloy system reflects the corresponding change in ES. Here we provide main results of the ongoing study of the evolution of ES and magnetism accompanying a transition from HEA to CA in ploycrystalline (CrMnFeCo)1-xNix alloys [Mat.Sci.Eng.A 696(2017)228] and amorphous (TiZrNbTL1)1-x(TL2)x (TL1=Cu or Ni, TL2=Ni [J.Mat.Res. 33(2018)3170], Cu or Co) alloys. For all amorphous alloys, Ultraviolet Photoemission Spectroscopy (UPS) showed split-band shape of the valence band with the electronic density of states (DOS) around the Fermi level dominated with d-states of Ti, Zr and Nb, whereas the 3d-states of late transition metals Co, Ni and Cu were at higher binding energies. However the amount of splitting depends strongly on particular metal and to lesser amount on its content x. Spliting of DOS affects strongly all properties (atomic parameters, magnetism and electronic transport) of these alloys and the change in properties on transition from HEA to CA depends on amount of splitting. In polycrystalline (CrMnFeCo)1-xNix alloys all constituents form common band [npjcompumats 5(2019)1]. Our non spin resolved UPS study of polycrystalline samples cannot provide full information about the band structure and magnetic state of these alloys. However, a comparison of the measured spectra for selected alloys with these of constituent metals and with the results of a-i calculations of the band stucture for some alloys provides a qualitative insight into the evolution of electronic structure with x. This insight is strenghtened by the results of the simultaneous study of the evolution of magnetism with x in the same alloy system.rder on transition from CA to HEA.

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[*] Speaker

P 2

Features of collective dynamics in liquid In along the melting line up to 10 GPa

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Abstract

Collective dynamics of liquid metals under high pressure is of great interest because of possible emergence of coupling between short-wavelength longitudinal (L) and transverse (T) collective excitations, which however is absent on macroscopic scales. Furthermore, S. Hosokawa et al. [1] reported observation of a signal from transverse excitations in dynamic structure factor of liquid Ga from inelastic x-ray scattering experiments. Also, T. Bryk et al. [2,3] studied collective excitations in liquid polyvalent Tl via ab initio molecular dynamics and observed emergence of unusually high-frequency second branch of T-modes in liquid Tl. Therefore there is considerable interest to study collective excitations in another liquid metal of the same group, liquid In. We performed ab initio molecular dynamics simulations of liquid In at three pressures up to 10 GPa along the melting line using a system of 300 particles with electron-ion interaction represented by PAW potentials. Static structure, velocity autocorrelation functions, mean square displacements and various collective time correlation functions were calculated and analyzed. The dispersion curves of longitudinal and transverse collective excitations are reported. We discuss the location of the observed two branches of T-modes for the studied pressures and their correlation with the peaks of the Fourier-spectrum of velocity autocorrelation functions.

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*Speaker

P 3

Effect of Local Structure of Glassy GeCuTe Alloys on the Crystallization Temperature

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Abstract

GeCuTe alloys on the pseudo binary line between GeTe and CuTe are phase change materials exhibiting a higher thermal stability than the usually used GeSbTe alloys.[1] When deposited as a thin film, the crystallization temperature of the amorphous state of the GeCuTe alloys shows an unusual behavior in dependence on the Cu content.[2] Starting with GeTe the crystallization temperature increases upon increasing the CuTe content and reaches a maximum at around 15at% Cu. It is reasonable to assume the amorphous structure to be responsible for this behavior. Therefore, we have measured EXAFS spectra of amorphous GeCuTe samples with 5at%, 15at% and 25at% Cu at the Ge-, Cu- and Te-K edge at SPring-8. In this way the evolution of the local structure of each atomic species around the maximum of crystallization temperature can be investigated and the structural origin of the crystallization temperature maximum can be identified.

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*Speaker

P 4

First principles study of the structural and dynamical properties of some liquid 3d transition metals near melting

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Abstract

Several static and dynamic properties of some bulk liquid 3d transition metals (Sc, V and Cr) at thermodynamic conditions near their respective melting points, have been evaluated by ab-initio molecular dynamics simulations. The calculated static structure is compared with the available experimental data [1]. For all systems, we obtain an asymmetric second peak in the structure factor, which underlines a notable local icosahedral short-range order in the liquid. The calculated dynamic structure factors show side peaks which point to the existence of collective density excitations. Several transport coefficients have also been evaluated and compared with the available experimental data.

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[*] Speaker

P 5

Intermediate range order of amorphous Cu2GeTe3 based on ab initio molecular dynamics simulations

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Abstract

Phase transition materials, e.g., GeSbTe (GST), attracts many scientific interests because of applications for electronic storage devices. Cu2GeSe3 (CGT) is also one of the phase transition materials, which changes rapidly between crystal and amorphous states. In order to clarify the phase change mechanism, several experimental and theoretical studies on the crystalline and amorphous phases were carried out so far [1-4]. In these studies, it is suggested that GeTe4 and CuTe4 tetrahedral units exist in both amorphous and crystalline states, and these local structures enhance the fast phase transition. It would however be necessary to confirm the intermediate range structure, such as the distribution of the ring size, while the local structure of amorphous state is well established. We have investigated the static structure of amorphous Cu2GeTe3 based on ab initio molecular dynamics simulations. We used 144 atom system in a cubic supercell under periodic boundary conditions. In this study, we focused on the intermediate range structure. We have performed ring analysis using the cutoff distance rc = 3.2 Å. The ring size with the highest population is 3. This size of ring corresponds to triangle structure mainly consisting of Cu atoms. We found that the ring size with the next highest population is about 6, which may correspond to the local structure of the crystalline phase.

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*Speaker

P 6

Surface tension measurement of the molten ZrO2

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Abstract

To predict a progress of a core meltdown accident, it is essential to know the physical properties of molten corium, of which important components are UO2 and ZrO2. Surface tension is one of such properties; however, there are almost no data because of their high melting temperature, high reactivity, and high volatility. In order to avoid these problems, the measurement should be done in a very short time. To this end, we developed a new technique, droplet impingement method. In this method, the surface tension is evaluated from the deformation of the droplet during the impingement, which means that the measurement is done in a very short time. In this study, we first check the accuracy of this method using molten Al2O3. Then, we show the surface tension of molten ZrO2 measured by this method. A sample with 2mm in diameter was levitated by an aerodynamic levitation technique. A separable nozzle was used so that the sample could be dropped onto an Al2O3 plate placed under the nozzle. The sample was melted by a CO2 laser, and immediately dropped onto the plate by opening the nozzle. The impingement behavior of the sample was recorded by a high-speed camera. From the recorded data, we evaluated the kinetic energy of the droplet just before the impingement and the increase of the surface area by the deformation of the droplet during the impingement. By assuming that the kinetic energy is equal to the increase of the surface energy and lost energy by viscos deformation, the surface tension was calculated. The surface tension was about 0.65 N/m at 2500 K for Al2O3 and about 0.8 N/m at 3000 K for ZrO2. The measured value of Al2O3 is in good agreement with the literature value, suggesting that we successfully measured ZrO2.

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*Speaker

P 7

Inter-diffusion measurements of Ge-Ni alloys with low absorption contrast difference by time-resolved X-ray radiography

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Abstract

The diffusion processes in liquid Al-Ni and Zr-Ni have been investigated effectually. Based on reference self- and inter-diffusion coefficients of these systems, we suggest replacing the non-Ni component of the binary alloy with Ge, as it has an in-between atomic number but is a semi-conductor at solid state. We strive to determine, whether there are differences in the diffusion behavior caused by a semi-conductor alloy component. We present self- and inter-diffusion coefficients of liquid Ge-Ni alloys with focus on the inter-diffusion measurement. While self-diffusion coefficients can be measured very accurately by quasi-elastic neutron scattering, the determination of accurate inter-diffusion coefficients is more challenging. We obtain inter-diffusion coefficients by a combination of in-situ X-ray absorption contrast radiography with a shear cell furnace. In contrast to the long-capillary method, a shear cell furnace has the advantage, that the sample can be fully melted until thermal equilibrium, before it is brought into physical contact with another sample of different composition. In that way, we control the exact start of the diffusion process, guarantee thermal stability and observe in-situ changes of concentration via X-ray radiography. However, the challenge about the Ge-Ni system is, that even for large composition differences of $\geq$10at% Ge, the Ge-Ni samples show a low X-ray absorption contrast among each other. Therefore we introduce a background correction approach in combination with the Sauer-Freise method, which makes it possible to get meaningful inter-diffusion coefficients even for binary systems with low absorption contrast difference.

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*Speaker

P 8

Structure Determination of a new Molecular White-Light Source

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Abstract

Recently, molecules of the general composition [(SnR)4S6] have been found to exhibit interesting non-linear optical properties. Depending on the organic group R, these amorphous materials either show a highly brilliant and directional white light emission or second-harmonics generation (SHG) when targeted with infrared radiation.[1,2] The determination of the cluster geometry as well as the general amorphous structure of these compounds via experimental methods are difficult tasks. Here, we want to present the latest work regarding structure determination of [(SnPh)4S6] using X-ray Diffraction (XRD) coupled with molecular Reverse-Monte-Carlo (RMC) modelling [3].

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*Speaker

P 9

Structural and Dynamic Properties of Aluminosilicate (Al2O3)x-(SiO2)1-x Melts: A Molecular Dynamics Study

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Abstract

The aim of this work is to study the structural and dynamic properties for aluminosilicates (Al2O3)x-(SiO2)1-x (AS) as a function of the aluminates Al2O3 concentration x by means of molecular dynamics simulation. The first part of this work is devoted to the test of the parameter of the Born-Mayer-Huggins type potential developed recently for the CaO-Al2O3-SiO2 system [1,2]. For this purpose, we compared the X-ray structure factor, the radial function distribution (RDF), the viscosity and the self-diffusion coefficient to experimental data and other molecular dynamics simulation found in the literature. This potential gives a good description of the atomic structural and dynamics properties for all compositions than other potential existed in literature. The evolution of the viscosity was discussed in the second part it decreases with show the transition of fragility around 50% aluminates from strong behavior fragile behavior. We show that the evolution of the fragility is correlated to the evolution of structural entities like the triply bonded oxygen (TBO), AlO5 and AlO6, which increase with the fragility.

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*Speaker

P 10

The short range order in liquid water and amorphous ice

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Abstract

The Quasi Crystalline Model (QCM) was applied to analyze experimentally determined partial radial distribution functions (RDFs) of water at different temperatures and pressures in order to determine the Short Range Order (SRO) of this unique liquid. The same analysis was also conducted on the partials RDFs of crystalline ice at 220K at ambient pressure and of the three known phases of amorphous ice: the Low Density, High Density, and Very High Density. It was found that at low temperature and pressure the SRO of water is similar to ice Ih structure. At higher pressures and low temperatures the SRO is similar to tetragonal ice III structures with c/a ratio of 0.8. At higher temperatures of 423K and 573K the SRO obtained was similar to cubic ice VII and rhombohedral ice II respectively. As for the amorphous ices, we conclude from the QCM analysis that these three forms are structurally distinct with SRO of ice Ih, ice III and ice II for the LDA, HDA, and VHDA respectively.

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*Speaker

P 11

Ga-In alloys – pressure dependence of phase diagram and thermo-physical measurements

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Abstract

The Ga-In binary system consists of low melting alloys with a eutectic point at 86%at Ga and 288 K, i.e. below room temperature. Consequently, Ga-In alloys are rapidly evolving as a highly promising class of alloys in multiple novel applications including, printing of electronic circuits, stretchable/flexible electronics and liquid metal based pressure sensors and as heat transfer agents in accelerators. Despite all these novel applications only few studies of the thermo-physical properties of these alloys have been made. We present high accuracy measurements across large range of temperature, of two physical properties which are sensitive to structural changes- sound velocity and electrical resistivity. These results are incorporated into thermodynamic model of the free energy from which the pressure dependent phase diagram of Ga-In is constructed. We predict that the eutectic point will shift non-monotonously with temperature to higher In content as the pressure is increased.

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*Speaker

P 12

Indications of liquid transition in Ga and Ga-In alloys

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Abstract

Recently there have been reports on a liquid crossover in eutectic Ga-In alloy in the temperature range of about 400-500K. We report on experimental observations that provide additional evidence for a temperature-driven structural transformation in the eutectic Ga-In alloy as well as in Ga and two other compositions at ambient pressure. We employ several methods including sound velocity, electrical resistivity and differential scanning calorimetry measurements that investigate different aspects of structural changes. In the sound velocity measurements there is a shift in the slope of the temperature dependence. In measurements of the electrical resistivity there are non-monotonous trend changes with temperature that create extremums. For differential scanning calorimeter (DSC) measurements there were deviations from linearity. All these phenomena are observed in the same temperature range beyond melting which supports the hypothesis of a possible novel transition in the melt.

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*Speaker

P 13

Density, electroresistivity and magnetic susceptibility of CoFeSiBNb alloy in crystalline, liquid and amorphous states

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Abstract

Co-based alloys are considered to be the promising materials for BMG production. However, their physical properties at high temperature are practically unknown. In this work we investigated the temperature dependences of density (by gamma-penetration method), electrical resistivity (by contactless method in rotating magnetic field) and magnetic susceptibility (by Faraday's method) in crystalline and liquid states and DTA of Co48Fe25Si4B19Nb4 alloy and with additions of neodymium (1 and 2 at.%). The alloy of nominal composition was obtained by remelting the pure components (purity > 99.8%) in an induction furnace in argon atmosphere for 1 hour at 1400 C. X-ray analysis showed that the main phases of the crystalline sample (obtained at low cooling rate) are: pure Co, Co2Si and (Fe,Co)23(B,Nb)6. Bulk amorphous metal rods with a diameter of 2 mm and a height of 17-20 mm were obtained by a cast suction method into a water-cooled copper mold. Amorphous ribbons (width 4 mm, thickness 55 mcm) were prepared by a standard planar flow method. It was found that in liquid state neodymium additions lower density of the alloy nonmonotonously, increase its resistivity and have little effect on its magnetic susceptibility. The crystallization kinetics of amorphous alloys was studied using differential thermal analysis on a Pelker Elmer installation with a heating and cooling rate of 10 K / min. It was stated that crystallization of the initial amorphous alloy proceeds in one stage (a metastable intermetallic compound (Fe,Co)23(B,Nb)6 appears), and of the alloys containing neodymium - in two stages. The formation of Nd2B borides is highly probable at the second stage of crystallization. Nd additions were found to positively affect the glass forming ability of Co48Fe25Si4B19Nb4 alloy, increasing the range of amorphous state existence by more than 30 K.

The reported study was funded by RFBR according to the research project 18-03-00433.

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*Speaker

P 14

Density and electrical resistivity of Al-Ni-Co-REM alloys in liquid state

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Abstract

Aluminum-based metallic glasses (Al > 80 at.%) with 3d-transition metals (TM) and rare earth metals (REM) have unique physical properties, combining high strength and plasticity together with high corrosion resistance. Nowadays these alloys are used as protecting materials in the devices working in corrosive medium. However, their physical properties in liquid state are practically unknown. In this work we investigated density and electrical resistivity of Al-Ni-Co-REM alloys in solid and liquid states.The master alloys (MA) of Al86Ni4Co4REM6 and Al86Ni6Co2REM6 (REM = Nd, Sm, Gd, Tb, Yb) compositions were prepared by remelting of pure initial components in the resistance furnace during half an hour at 1923 K in argon atmosphere. Their chemical compositions were analyzed using atom adsorption spectroscopy. Density was measured using the absolute variant of gamma absorption method on an automated experimental set-up in helium atmosphere. The accuracy of density values determination was ± 0.5%. Electroresistivity was investigated by contactless method in rotating magnetic field on automated experimental set-up in helium atmosphere. The accuracy of resistivity values determination is estimated to be ± 3%. It was found that heat treatment of the investigated melts can influence greatly on their structure before crystallization/solidification. The optimal combinations of Ni-Co ratio and rare earth elements providing high glass forming ability of the alloys are established.

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*Speaker

P 15

Small-scale plasticity of CuZr metallic glass studied by Molecular Dynamics simulations

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Abstract

The microscopic origin of plasticity of metallic glasses (MG) is a very crucial issue since the possibility to improve the poor ductility of MG relies on the understanding of their mechanisms of plasticity at the atomic scale. We investigate the mechanical behavior of CuxZr100-x MG by atomistic Molecular Dynamics simulations to assess their plastic response for different compositions (different values of x) and for different relaxation states of the system, and by varying external parameters such as strain rate and temperature. We perform quasi-static and dynamic shear and tensile tests under different conditions. The stress-strain curves exhibit strain softening and a serrated flow in the quasi-static case, indicating numerous plastic events, while the behavior is smoother in the dynamic case. By increasing the strain rate the amplitude of overshoot on stress-strain curves is higher, and a map of the local atomic strains reveals a transition from a localized deformation with shear bands to a more homogenous deformation. We have also found that the shear modulus and Young modulus both slightly decrease by increasing temperature. Moreover, the effect of preparation of glass on the mechanical response has been investigated, specifically by changing the quenching rate and by performing an annealing treatment on the relaxed glassy state. By comparing the tensile tests with and without annealing treatment we observe that slower quenching rate induces a higher fraction of Cu-centered icosahedra structure in the glass and meanwhile the stress overshoot is lower compared to MG without annealing. In addition, the evolutions on both maximum stress and fraction of the Cu-centered icosahedra clusters in MG is consistent during the annealing process, thus the variations of the stress-strain curves caused by different quenching rates can be understood from a structural point of view.

Keywords: metallic glasses; Molecular Dynamics; mechanical behavior; plasticity

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*Speaker

P 16

Surface texturing of metallic glasses by ultrashort laser pulses

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Abstract

Metallic glasses attract substantial research efforts due to their unique mechanical and chemical properties leading to a high corrosion and wear resistance in the context of surface engineering. These better aptitudes compared to other metals and alloys are allowed by the absence of grain boundaries and related crystalline defects. Whether in bulk or thin films, their manufacturing remains complex and expensive, and their use is thus limited to niche markets with higher production value such as watchmaking, micromechanics or biomedical implants. However, due to the exposition to extreme environmental aggressions, surface treatments techniques have emerged as a promising way to improve material resistance. In particular, surface processing by laser irradiation has been proposed over the past decade to modify the physico-chemistry of the amorphous metal. Upon multi-shot irradiation, a laser pulse can trigger a modulated arrangement of topography with a contrast of hundreds of nanometers and a large variety of periodicities. By rippling the surface, ultrafast lasers are able to structure a surface at the nanoscale with an unprecedented degree of accuracy. Our work aims at investigating the interaction between a femtosecond laser and a metallic glass sample in different dose regimes of irradiation. Several compositions of bulk or thin film metallic glass (Zr-Al-Cu-Ni-Ti and Zr-Ti-Cu-Ni-Be) have been irradiated to self-organize the amorphous surfaces. Microstructural analysis by SEM and AFM performed on the untreated and irradiated samples reveal the formation of hierarchical submicronic structures controllable by the laser polarization. These results provide new routes to achieve surface functionalization improving metal glass features such as wettability behaviour or corrosion and erosion resistance.

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[*] Speaker

P 17

Metal-Nonmetal Phase Separation in Expanding Liquid Alkali Metals

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Abstract

Liquid Rubidium has been thoroughly explored by inelastic neutron scattering over the past two decades [1,2]. The full set of dynamic data now available offers a completely new view onto the conversion of the dense liquid metal into an insulating expanded fluid. This transition sets in considerably earlier than believed so far and extends over a relatively wide range of the average liquid density. The measured data suggest, that the metallic fluid decomposes into a nanoemulsion of metallic and non-metallic domains where the metallic domains constantly disappear with ongoing expansion. The observed collective modes of the fluid appear as an unambiguous signature of the metallic phase which allows to directly observe the disappearance of metallicity. The density related variations of the dynamic scattering law S(Q,w) agree well with observations obtained from other S(Q)-studies [3] which were carried out along the same density range. A similar behaviour is found in expanded liquid mercury [4] and it is tempting to speculate that this kind of transition is characteristic for any density related metal to non-metal transition in a fluid metallic system.

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*Speaker

P 18

New approach of lubricant behavior in high loaded contact

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Abstract

Friction is related to the loss of energy due to the relative motion of two solid bodies in contact. To reduce friction and wear, contacts are commonly lubricated by thin films where the shear deformation concentrates. In the elastohydrodynamic lubrication regime, highly loaded contacts make these very thin films (_˜100nm) endure extreme conditions of pressure and shear velocity. At high sliding, friction curves exhibit a plateau regime related to the limiting shear stress (LSS) of the lubricant [1]. The main hypothesis from literature to explain this plateau is the lubricant glass transition occurring under such high pressure (> GPa). Yet, lubricants behavior remain physically weakly understood. It is still predicted by empirical, non predicted models. Generally, friction tests leads to a contact thickness about 100 nm, that makes any physical probe experiment very difficult to manage. However, the measured quantities are macroscopic, and averaged over a whole contact exhibiting a complex distribution of pressures and thicknesses. In this work, two model lubricants (an ester and a linear alkane) have been experimentally probed in a tribometer and by Brillouin light scattering (BSL) spectroscopy. A diamond anvil cell was used to investigate a wide range of temperatures and pressures. The BLS technique revealed to be an effective tool to bring out the lubricant glass transition [2]. Moreover, by fitting the BLS spectra with appropriate models, visco-elastic properties such as elastic modulus, sound velocity and time relaxation could be extracted from the spectra post-processing. These physical properties have then been analyzed in regards to the macroscopic friction measured in a contact under the same conditions.

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*Speaker

P 19

Structure and proton conduction of inorganic acid Cs2(HSO4)(H2PO4) melt and glass - A molecular dynamics study -

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Abstract

The inorganic solid acids, e.g. CsH2PO4 and CsHSO4 are known as solid electrolytes with high proton conduction, i.e. "superprotonic conductors". They exhibit protonic conductivity about 10-2 S/cm in their superprotonic phase, which is comparable to those of liquid electrolytes. The inorganic solid acids are promising candidates of solid electrolytes for the fuel cells operating at 400-500K. The high protonic conductivity is also observed in the complex system Cs2(HSO4)(H2PO4) above the transition temperature about 370K. The structure change occurs from a monoclinic structure to a cubic structure at this temperature. The important characteristic is that the high temperature structure remains by cooling from the superprotonic phase. Moreover, the glass state is formed by rapid quench from the molten phase, which also exhibits high proton conduction at room temperature. Although several molecular dynamics (MD) simulation studies including the ab initio MD studies have been performed on CsH2PO4 and CsHSO4, no MD study has been reported on Cs2(HSO4)(H2PO4), as far as we know. These facts prompt us to perform MD simulation in the molten and glass state of Cs2(HSO4)(H2PO4) to investigate the structure, and the proton conduction. The glass transition will also be discussed. The screened BM type inter-ionic potentials are used for the interaction between constituent ions, which includes the environmental effect of surrounding ions and the polarizations of ions.

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*Speaker

P 20

Pressure-induced effects in the dispersion of collective exitations in polyvalent liquid metals

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Abstract

Collective dynamics of metallic melts at high pressures is one of the open issues of condensed matter physics. By means of ab initio molecular dynamics simulation we examine features of longitudinal and transverse current spectral functions and corresponding dispersions of collective excitations in typical polivalent liquid metals Al and Pb [1] as a function of pressure along the melting line, which are not always present at ambient pressure [2]. We firmly establish the emergence of a second branch of high-frequency transverse modes with pressure in these metals, that we correlate with the pronounced high-frequency shoulder in the vibrational density of states. The structural and thermodynamic origin of the pressure-induced evolution of longitudinal and transverse exitations in polyvalent liquid metals is discussed.

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*Speaker

P 21

Viscosity of liquid Na-K alloys from molecular dynamics simulations

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Abstract

The shear viscosity of liquid Na-K alloys is computed from molecular dynamics simulations using the Green-Kubo formalism. Interatomic interactions are described using effective pair potentials computed from Fiolhais pseudo-potential and self-consistent screening. The composition dependence of the viscosity is first investigated at 373 K, then its temperature dependence at three different compositions, namely Na_10-K_90, Na_50-K_50, and Na_90-K_10. Simulation results are first compared with available experimental data. The evolution of the viscosity of the alloys versus temperature is similar to that of a pure one component fluid. This is discussed in connection with the weak chemical order of the mixtures.

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[*] Speaker

P 22

Multicomponent Melt of Nanocrystalline Soft Magnetic Alloy

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Abstract

The temperature dependence of the viscosity and density of Fe73.5Cu1Mo3Si13.5B9 melt was studied. At the heating stage, the activation energy of the viscous flow *Ea* decreases from 47 to 41 kJ/mol when passing through temperature $Tk = 1770$ K, and remains unchanged upon cooling. In the cooling stage after overheating above the Tk, the melt has a larger relative free volume than in the heating stage at the same temperature. The size of the microparticles participating in the viscous flow and the diffusion coefficient were calculated for the transport mechanisms in terms of the statistical theory of the absolute reaction rates. At a temperature of 1600 K, after the melt is overheated above the temperature $Tk = 1770$ K, the size of the microparticles decreases by a factor of two, to 0.4 nm, and the diffusion coefficient increases from 2.4·10-10 to 4.5·10-10 m2/s.

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*Speaker

P 23

Thermodynamic properties and stability of the supercooled liquids of Nb-based solid solutions using electrostatic levitation

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Abstract

Refractory alloys have been highlighted from their superior properties as well as potential applications. High entropy alloy forming isomorphous solution with equivalent compositions of three to five elements keeps good strength even higher than 1000 K, in where conventional heat-resisting alloys cannot be used anymore. However it is not clearly understood why and how does the alloy form isomorphous solution and reveal such stable solid solution even high temperatures. In order to study formation and stability of the refractory alloy liquids, we select Nb-based isomorphous alloy systems; a few elements such as W, Mo, and Zr surrounding niobium on the periodic table may reveal interesting mixing behaviors with niobium because they have similar atomic radii but different mixing enthalpy with those of niobium. Binary alloy beads are made with an arc melter and fully melted with a heating laser-combined electrostatic levitator. The molten alloys are cooled below their liquids temperatures, but still exist in undercooled, metastable state due to suppressed nucleation in the containerless melting method. From melting-cooling curves of the alloys, we can obtain undercoolability data as well as solidus and liquidus temperatures. Furthermore, density variation during undercooling and solidification is also recorded for the levitated samples. Based on experimental data such as density, melting temperatures and undercoolability, we have estimated excess free volume and interfacial free energy related to solid nucleation. In addition, fusion enthalpy of the binary alloys has estimated based on CalPhad calculations. Finally, we have tried to discuss about the stability of the supercooled liquids from viewpoints of volume and energy changes described above.

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*Speaker

P 24

Tuning ab-initio molecular dynamics simulations for Cu-based glass forming alloys

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Abstract

The efficiency of ab-initio molecular dynamics simulations of metallic systems relies on the quality of the pseudopotentials used to treat the electronic structure. For plane-wave based density functionals, the length of the electronic cycles depends largely on the choice of parameters such as the energy cutoff, which in turn affects the accuracy of the simulation. On the basis of modern pseudopotentials, this influence is investigated on the pair structure and the pressure for representative Cu-based glass forming liquid alloys.

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[*] Speaker

P 25

Spicing up: The influence of Fe, Co or Ni additions on the structure of Zr-Cu-Al-based bulk metallic glasses

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Abstract

Bulk metallic glasses (BMGs) are among the most widely studied metallic materials. Their amorphous structure leads to extraordinary properties from both the basic-research as well as the engineering point of view. Understanding the formation and the nature of the amorphous structure in metallic solids and uncovering the relations between structure, processing and properties remain among the most intriguing open questions in the field. As one of the most important families of bulk glass-forming alloys discovered so far Zr-Cu-Al-based alloys play a major role in deciphering the structure-property-relationships of BMGs [1,2]. Here we explore the influence of the addition of Fe, Co or Ni on structural features of Zr-Cu-Al BMGs using high-energy synchrotron X-ray diffraction measurements and pair distribution function (PDF) analysis. It is found that "spicing" Zr-Cu-Al with these elements increases the "level of disorder" of the amorphous structure, in line with the "confusion design principle" [3] and promote chemical ordering in the short range region. Furthermore, the effects of the additions on global resonances on structure formation is scrutinized [4]. The structural investigations are complemented by the investigation of thermo-physical and mechanical properties providing also valuable insights necessary for future applications of BMGs as engineering materials.

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*Speaker

P 26

Theoretical and experimental investigations of the magnetic properties of amorphous alloys

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Abstract

Examination of the main terms of the amorphous ferromagnetic model (Biryukov's theory) is realized in this work. It has been shown that the hypothesis about the low correlation between the spin and the electrostatic components is correct for the spin-system of amorphous magnetic that permits to interpret collectively the different magnetometer measurements.

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*Speaker

P 27

Plastic Flow and Fracture in Fe-based Amorphous Nanocrystalline Alloy

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Abstract

Fe-based amorphous nanocrystalline alloys have been attracting tremendous research interest because of their excellent soft magnetic properties. However, their applications are hindered because of their room-temperature brittleness and the underlying mechanisms are yet to be fully understood. In this work, we successfully fabricated a series of Fe-based amorphous nanocrystalline alloys through the controlled nanocrystallization in Fe-based amorphous ribbons, which resulted in rather thin amorphous inter-granular films with an average thickness reducing from 10 nm to less than 0.5 nm as the volume fraction (Vf) of the nanocrystals increased from 16% to 95%. According to the extensive microcompression experiments, we demonstrated that the yielding strain of the amorphous nanocrystalline alloys decreases progressively with the increasing Vf and identified three types of distinctive deformation behaviors, including (I) shear banding for $Vf < 70\%$, (II) shear banding induced cavitation and cracking for $70\% < Vf < 90\%$ and (III) distributed plasticity for $Vf > 90\%$. Through transmission electron microscopy and strain rate sensitivity analyses, we revealed that plasticity in our Fe-based amorphous-nanocrystalline alloys is mainly accommodated by the soft amorphous inter-granular films rather than the hard nanocrystals. Based on these results, we developed a micromechanical and thermodynamic model which quantitatively explains the yielding behavior of the amorphous nanocrystalline alloys and their unusual phenomenon of ductile-brittle-ductile transition, as manifested by the three deformation behaviors. Our current findings provide important insights into the design of strong-yet-ductile soft magnetic amorphous nanocrystalline alloys.

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*Speaker

P 28

Unconventional anti-aging dynamics in ultra-stable metallic glasses

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Abstract

Conventional (rapidly quenched) metallic glasses (MG) usually manifest aging dynamics, the metastable glassy state trying to relax towards the equilibrium configuration with time [1]. Aging usually tends to impair the mechanical properties of MGs. Ultra-stable metallic glasses (UMGs) are promising candidates to address the stability issues of conventional MG. By means of X-ray photon correlation spectroscopy, we find a clear signature of ultrastability at the atomic level, which results in slower relaxation dynamics of UMGs with respect to conventional MGs. Moreover, we also evidence a peculiar acceleration of the dynamics by annealing at temperatures near Tg. This surprising phenomenon, called Anti-Aging, can be interpreted in the framework of the potential energy landscape [2].

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*Speaker

P 29

Boson-peak-like anomaly in the low temperature heat capacity of strain glasses

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Abstract

Boson peak has been found in various structural glasses, such as metallic glasses and oxide glasses, and is treated as the fingerprint of glassy state. The origin of boson peak, however, is still under debate until now. Here we report a boson-peak-like anomaly found in strain glasses, a new glassy state with frozen strain short-range ordering. Strain glass transition is a conjugate glass transition of a ferroelastic/martensitic transformation, in which strain is the order parameter. In comparison with the martensitic phase (a strain long-range ordered state), the strain glass exhibits an abnormal increase in the heat capacity at low temperature, and a peak around 10 K. Through the molecular dynamics simulation, we find there are excess excitations at the low frequency range in the phonon density of states (PDOS) of strain glass, which is closely related to the Von Hove Singularity in the PDOS of martensite. Our work indicates glassy states share common dynamic properties, and may help to deepen the understanding on the origin of boson peak.

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*Speaker

P 30

Refining localized dynamic modes in glasses

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Abstract

The dynamic modes in glasses are complicated and abundant due to their nonequilibrium nature. After prolonged isothermal annealing below the glass transition temperature, an endothermic prepeak appears on the DSC traces for different kinds of glasses, making these dynamic modes with intermediate time scale observable. Here, we study the prepeak in metallic glasses by thermodynamics analysis and dynamical mechanical spectroscopy. Estimated activation energy of the prepeak is similar to the empirical value of 26RTg for β-relaxation in MGs, suggesting the close connection between prepeak and β-relaxation. The prepeak shifts to higher temperature and merges with the glass transition overshoot by increasing annealing temperature or extending annealing time, which implies the underlying correlation between the prepeak and glass transition. Our results provide a route for manifesting the localized dynamic modes in glasses.

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*Speaker

P 31

Multiple Pathways of Nucleation on Extremely Supersaturated Bulk Aqueous Solutions

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Abstract

Measuring solution structure and its evolution in supersaturated aqueous solutions has been highly desired, since it provide a key clue for multiple pathways of nucleation (MPN) in microscopic viewpoint. Here, we measure the structural evolution of solute molecules in extremely supersaturated solutions (KH2PO4 (KDP) and NH4H2PO4 (ADP)) beyond MZWL using the combination of ESL and synchrotron X-ray diffraction. The results reveals a symmetry change of H2PO4 molecular structure from C2v to C1 in the highly supersaturated KDP solution indicating a solution-solution transition which is absent in the ADP solution. In addition, the two solutions show different structural evolution in medium range ordering with supersaturation. Our result suggests that changes in short range and medium range order structures in solutions ultimately determines the route of nucleation and phase selection. This work provides an important milestone for atomic- and molecular-scale understanding of various nucleation phenomena that occurs through self-organization of solutes in molecule-level and will impact a wide range of research area from biology to the material science.

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