

*3<sup>rd</sup> International Workshop*  
*on*  
*Challenges of Molecular Dynamics Simulations*  
*of*  
*Glass and Amorphous Materials*

*São Carlos, SP – Brazil*

*09-10-11-12 / July / 2017*

## WELCOME

*The International Workshop on Challenges of Atomistic Simulation of Glasses* is an initiative of the TC27 – Technical Committee 27 – “Atomistic Modeling and Simulation of Glass” approved by the International Commission of Glass – ICG, in 2009.

After the 1<sup>st</sup> workshop held in France (2012), the 2<sup>nd</sup> one in China (2015), the 3<sup>rd</sup> workshop is held in São Carlos, Brazil.

The aim of this workshop is bringing together the world leading experts to discuss the most challenging issues of atomistic simulations, such as, the best procedure of glass formation using computer simulation; influence of the system size of the simulation;

How to address the mixed glass former and mixed modifier effect in oxide glass simulations; how to simulated diffusion in glasses; the challenge in simulate chalcogenide glasses, among other.

## Organizing Committee

**Jincheng Du**

*Department of Materials Science and Engineering, University of North Texas, Denton, Texas, U.S.A*

**Carlo Massobrio**

*Univer. de Strasbourg, CNRS, Institut de Phys. et Chim. des Matér. de Strasbourg, Strasbourg, France*

**Alastair Cormack**

*School of Engineering, Alfred University, USA*

**Edgar Zanotto**

*Departamento de Engenharia de Materiais, Universidade Federal de São Carlos, Brazil*

**José Pedro Rino**

*Departamento de Física, Universidade Federal de São Carlos, Brazil*

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July, 08, transfer from São Paulo to São Carlos at ~10:00 am. Reception at 7 pm

**Program**

	<b>09/July</b>	<b>10/July</b>	<b>11/July</b>	<b>12/July</b>
<b>9:00 – 9:50</b>	<b>Opening: Du, Rino, Zanotto</b>	<b>E. Furet</b>	<b>G. Ori</b>	<b>A. Tandia</b>
<b>9:50 – 10:30</b>	<b>A. Takada</b>	<b>J. Habasaki</b>	<b>E. Lampin</b>	<b>A. Zeidler</b>
<b>10:30 – 11:00</b>	<b>Coffee break</b>	<b>Coffee break</b>	<b>Coffee break</b>	<b>Coffee break</b>
<b>11:00 – 11:40</b>	<b>M. Bauchy</b>	<b>L. Huang</b>	<b>J.P. Rino</b>	<b>S. Sen</b>
<b>11:40 – 12:20</b>	<b>A. Cormack</b>	<b>H. Inoue</b>	<b>P. Salmon</b>	<b>Closing Remarks</b>
<b>12:20 – 14:30</b>	<b>Lunch</b>	<b>Lunch</b>	<b>Lunch</b>	<b>Departure to São Paulo</b>
<b>14:30 – 15:10</b>	<b>M.V. Coulet</b>	<b>S. Ispas</b>	<b>Excursion to Brotas</b>	
<b>15:10 – 15:50</b>	<b>J-M Delaye</b>	<b>W. Kob</b>	<b>Excursion</b>	
<b>15:50 – 16:30</b>	<b>Coffee</b>	<b>Coffee</b>	<b>Excursion</b>	
<b>16:30 – 17:10</b>	<b>J. Du</b>	<b>M.C. Ribeiro</b>	<b>Excursion</b>	
<b>17:10 – 17:40</b>	<b>G. Ferlat</b>	<b>C. Massobrio</b>		
		<b>Happy hour + dinner</b>		

## Geometrical modelling of SiO<sub>2</sub> and B<sub>2</sub>O<sub>3</sub> systems

Akira Takada<sup>a,b</sup>

<sup>a</sup>Asahi Glass Company, 1150 Hazawa-cho, Kanagawa, Yokohama 2218755, Japan

<sup>b</sup>University College London, Gower Street, London W1E6BT, UK

### Abstract

Since Bernal proposed liquid structures could be understood by the concept of random close-packed model, many theoretical studies have been carried out for modelling monatomic liquids and amorphous metals with the increase of the power of computers. However, oxide glasses like silicate glass are comprised of species with different atomic radius and they do not have close-packed structure. In this study, the author investigated the structural features of SiO<sub>2</sub> and B<sub>2</sub>O<sub>3</sub> systems in terms of Voronoi tessellation. It is found that the difference in coordination numbers, local volume and geometrical symmetry between crystals and glass can be distinguished in terms of Voronoi tessellation.

### Brief Biographical Notes

*After graduating from Tokyo University at which I studied applied mathematics, I joined Asahi Glass Company. I have been performing a variety of computer simulations of macroscopic and microscopic phenomena on glass. My recent major concern is to construct a bridge between microscopic (glass structure) and microscopic phenomena (glass properties) on glass. I am joining the activities of TC-3 (Glass Structure) and TC-27 (Atomistic modelling and Simulation) under ICG. In addition, I have a research project at University College London as a visiting professor.*

*I have recently finished my presidency at the Japan Society of Industrial and Applied Mathematics (JSAM; a number of member is about 1,700). I am a member of Science Council of Japan.*

*He is Fellow of JSIAM and Fellow of SGT (Society of Glass Technology).*

## Stretched Exponential Relaxation of Glasses: Origin of the Mixed Alkali Effect

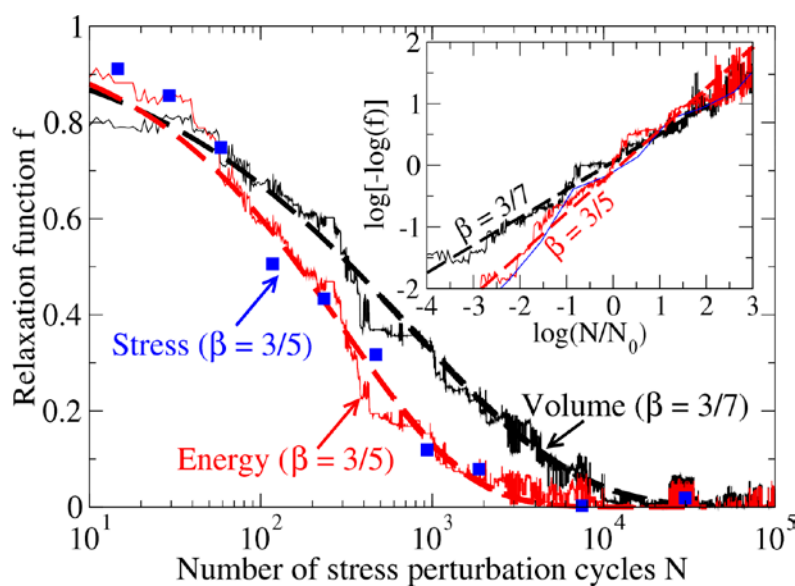
Yingtian Yu<sup>1</sup>, John C. Mauro<sup>2</sup> & Mathieu Bauchy<sup>1\*</sup>

<sup>1</sup> University of California, Los Angeles, CA, USA

<sup>2</sup> Science and Technology Division, Corning Incorporated, Corning, NY, USA

### Abstract

Although it is indeed commonly believed that, as frozen supercooled liquids, glasses should continue to flow over the years (e.g., in the case of the stained-glass windows of medieval cathedrals), the dramatic increase of their viscosity below the glass transition temperature suggests, on the contrary, that their relaxation time is on the order of  $10^{32}$  years at room temperature. However, a recent study conducted by Mauro *et al.* reported the intriguing dynamics of the relaxation of a commercial Corning® Gorilla Glass® at room temperature, over 1.5 years. Here, we report a novel atomistic simulation method allowing us to directly access the long-term (years) dynamics of glass relaxation at room temperature. Based on the simulation of a series of mixed alkali silicate glasses, we demonstrate that room-temperature relaxation is a direct consequence of the mixed alkali effect. Although both volume and energy feature a stretched exponential relaxation, our results reveal a bifurcation of the stretching exponents, with  $\beta = 3/5$  and  $3/7$  for energy and volume relaxation, respectively. Relaxation is found to occur through the diffusion of local stressed structural instabilities inside the atomic network, which anneal each other when a compressed atomic unit meets one that is under tension. The driving force for such diffusion-trap relaxation mechanism is found to be at a maximum when the concentrations of each alkali atom equals each other, which arises from a balance between the concentration of each alkali atom and the magnitude of the local stress that they undergo.



### **Brief Biographical Notes**

*Mathieu Bauchy is a computational material scientist with a strong interest in glassy and cementitious materials. Mathieu is presently an Assistant Professor in the Civil and Environmental Engineering Department at University of California, Los Angeles (UCLA). His research group focuses on reducing the carbon footprint of materials and enhancing their engineering properties, including the resistance to fracture, aging, and irradiation. Prior to joining UCLA, Mathieu was a Postdoctoral Assistant at the Massachusetts Institute of Technology (MIT). He received his Ph.D. at Université Pierre et Marie Curie (Paris). His thesis was dedicated to the development of high-performance silicate and chalcogenide glasses by means of atomic-scale simulations.*



## Reactivity of CAS Glasses

A. N. Cormack<sup>1</sup>, L. Wang<sup>1</sup>, G. Agnello<sup>2</sup>, R. Manley<sup>2</sup> and N. Smith<sup>2</sup>

<sup>1</sup>School of Engineering, Alfred University; <sup>2</sup>Corning, Incorporated

Probing the reactivity of glasses and their surfaces is, in many ways, an ideal task for molecular dynamics, since time evolution is inherently included. The major drawbacks are, of course, well-known. The length of an MD simulation, or trajectory, is generally many orders of magnitude shorter than corresponding real-time experiments, and the sample sizes are usually also similarly disparate. Notwithstanding, it is now possible to contemplate the investigation of surface reactivity using classical MD simulations, which can be run for long enough to observe, for example, the chemisorption, or dissociation, of water molecules, as well as their physisorption.

The challenge concerns the analysis and interpretation of the data. Once a reaction – the formation of a silanol group, for example – has been observed, one wants to wind the clock back to investigate the structural circumstances behind its formation. This involves the visualization of many MD timesteps, and the ability to label species of interest.

In this presentation, we will discuss our efforts in this direction, with respect to the interaction of water on a series of calcium aluminosilicate glass surfaces.

### Brief Biographical Notes



*Alastair N. Cormack is the Interim Dean and Van Derck Fréchet Professor of Ceramic Science in the Inamori School of Engineering at Alfred University. He earned his MA from the University of Cambridge and MSc and PhD degrees, in solid state chemistry, from the University of Wales, Aberystwyth. After a post-doctoral stint in the Department of Chemistry, University College London, he joined the New York State College of Ceramics at Alfred University in 1985, as an assistant professor, being promoted to full professor in 1992. In 2003 he was asked to be the interim dean of the School of Engineering and in 2004 he was appointed as the founding dean of the Kazuo Inamori School of Engineering, in which position he served until 2009.*

*He is a Chartered Chemist and Chartered Scientist in the UK, a Fellow of the Royal Society of Chemistry, a Fellow of the American Ceramic Society, a Fellow of the Society of Glass Technology and a Fellow of the Mineralogical Society. He served as Editor, North America, for Solid State Ionics from 2004 to 2009, is currently a member of the Commission on Journals of the International Union of Crystallography and a co-editor of IUCrJ, and an Editorial Board Member for Biomedical Glasses.*

*He has published over 170 peer reviewed scientific papers and given numerous invited presentations at international conferences and institutions. He was conference chair and organizer of the 14<sup>th</sup> International Conference on the Physics of Non-crystalline Solids, held in Niagara Falls, NY in September 2015, the co-chair and organizer of SSI-17, the 17<sup>th</sup> International Conference on Solid State Ionics, in Toronto, Canada, in 2009, and conference chair and organizer of NCM9, the 9<sup>th</sup> International Conference on the Structure of Non-Crystalline Materials, in Corning, NY, in 2004.*

## Liquids and amorphous GeSbTe alloys: an experimentalist's view.

M.-Vanessa Coulet

MADIREL – UMR 7246- CNRS and Aix-Marseille Univ. – Campus de St Jérôme –  
13397 MARSEILLE CEDEX 20 – FRANCE

### Abstract

GeSbTe ternary phase diagram is probably the richer in term of interesting compounds or alloys for applications in the field of phase change materials (PCM). Those materials are particularly interesting because they involve in their process of operation three different states of a defined alloy which are the crystalline, amorphous and liquid states. This presentation focuses on the disordered phases of PCM for different alloys with a special emphasis on the experimental results and the inherent difficulties in obtaining reliable and high quality datasets.

The first part is devoted to the liquid state. Neutron diffraction and inelastic scattering as well as x-ray absorption measurements performed on a wide range of Te-based alloys are presented. It is shown that the liquid structure, in addition to be a good starting point to describe the amorphous phase, provides useful information on the suitability of an alloy to be a good phase change material. Moreover, it serves as an important input for first-principles molecular dynamics calculations.

The amorphous state of some PCM is at the centre of second part of this presentation. More precisely various experimental strategies are proposed to follow the structure and other physical properties from the amorphous phase up to the crystallization. In spite of being far from working conditions, it is shown that such measurements, close to the thermodynamic equilibrium, are clear indicators of the cycling ability of a given composition.

### Brief Biographical Notes



*Marie-Vanessa Coulet is researcher at the French National Research Council (CNRS). She obtained her PhD in Material Science from the University of Provence in Marseille, France. She is working in material science and her main activities are in structure determination using large scale facilities and thermodynamics using calorimetry. She is interested in (i) disordered systems such as liquid and amorphous chalcogenides and (ii) materials with high specific surface area such as metallic nanopowders and metal-organic frameworks.*



## Classical potentials for Molecular Dynamics Simulations of SiO<sub>2</sub>-B<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>O glasses

Le-Hai Kieu<sup>1</sup>, Fabien Pacaud<sup>1,2</sup>, Mathieu Salanne<sup>2</sup>, Jean-Marc Delaye<sup>1\*</sup>

<sup>1</sup>CEA Marcoule, DEN/DE2D, Service d'Etudes de Vitrification et procédés hautes Températures, BP17171, F-30207 Bagnols-sur-Cèze CEDEX, France

<sup>2</sup>Sorbonne Universités, UPMC Univ. Paris 06, PHENIX, F-75005 Paris, France

### Abstract

French nuclear glasses, used for the storage of high level – long lived radioelements, have complex compositions with more than 30 oxides. To better understand the basic mechanisms about structure, radiation effects, leaching or mechanical properties, many studies have been performed using simplified compositions [1]. In particular, it has been shown that SiO<sub>2</sub>-B<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>O glasses in the same relative proportions as in the real glass have the same qualitative behaviour under irradiation by heavy ions: the glass swells, the hardness decreases, the fracture toughness increases ... Hence the interest of studying this glass to investigate the structural and mechanical properties of nuclear glasses.

Classical molecular dynamics is a powerful tool for representing a glassy structure at the atomistic scale and for investigating its behaviour under different external solicitations: radiation effects, fracture, nanoindentation ... But to perform calculations scientifically sounded, precise classical interatomic potentials are required. It is why for several years, different works have been undertaken to fit classical potentials to represent SiO<sub>2</sub>-B<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>O ternary glasses.

In a first step, classical potentials of the Buckingham form have been fitted on experimental data [2] to study the behaviour under fracturing of three SiO<sub>2</sub>-B<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>O glasses. The qualities and limits of these potentials will be presented.

After this, a new approach has been adopted to fit PIM (Polarizable Ion Model) potentials [3] completely on ab initio data. In this case, the objective was to simulate the dynamical properties of several SiO<sub>2</sub>-B<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>O glasses in the liquid state. Again, the qualities and the limits of these potentials will be presented.

[1] D.A. Kilymis, J.-M. Delaye, S. Ispas, *J. Chem. Phys.* 145 (2016) 044505

[2] L.-H. Kieu, J.-M. Delaye, L. Cormier, C. Stolz, *J. Non-Cryst. Solids*, 357 (2011) 3313

[3] Y. Ishii, M. Salanne, T. Charpentier, K. Shiraki, K. Kasahara, N. Ohtori, *J. Phys. Chem. C*, 120 (2016) 24370

### Brief Biographical Notes

*Jean-Marc Delaye has been graduated from the "Ecole Supérieure d'Electricité", (Gif/Yvette, France) in 1987. He pursued his studies with a PhD at CEA Saclay dedicated to the study of diffusion mechanisms in amorphous materials using atomistic simulations. In 1995, he was engaged at CEA Saclay to work on radiation effects in nuclear glasses using computational methods. He moved to CEA Marcoule in 1997. He was appointed Expert Senior then Research Director in the field of nuclear glass simulation in 2012.*

## Structure and structural evolution of oxyfluoride glasses from molecular dynamics simulations: insights into phase separation and crystal nucleation

Jincheng Du

Department of Materials Science and Engineering, University of North Texas, Denton, Texas, U.S.A.

### Abstract

Oxyfluoride glasses are an intriguing type of glass system due to their structural complexity and functional applications as luminescent glass-ceramics that combine the superior emission properties of fluoride crystals and stable oxide glass matrix, and as fast ion conductors. In both cases, it is critical to understand the structures of these glasses and the impact of structure heterogeneity and phase separation on the properties. In this talk, I will present study of oxyfluoride glasses using large scale molecular dynamics simulations with effective partial charge potentials to understand the glass structures of several fluoro-silicate and fluoro-aluminosilicate glasses. From these simulations, for the first time, we observe initial stages of phase separation and the evolution of structures with and evolution with glass composition and temperature. Very importantly, it was found that aluminium ions serves as a linkage between the fluoride rich regions and silicate rich regions. These results were correlated with experimental structural characterization and optical photoluminescence measurements. The results show that atomistic computer simulations can provide insights to phase separation and the initial stage of crystallization of inorganic glasses, hence contribute to the understanding of the structure-property relationships in these glasses and design of glass-ceramics for various applications.

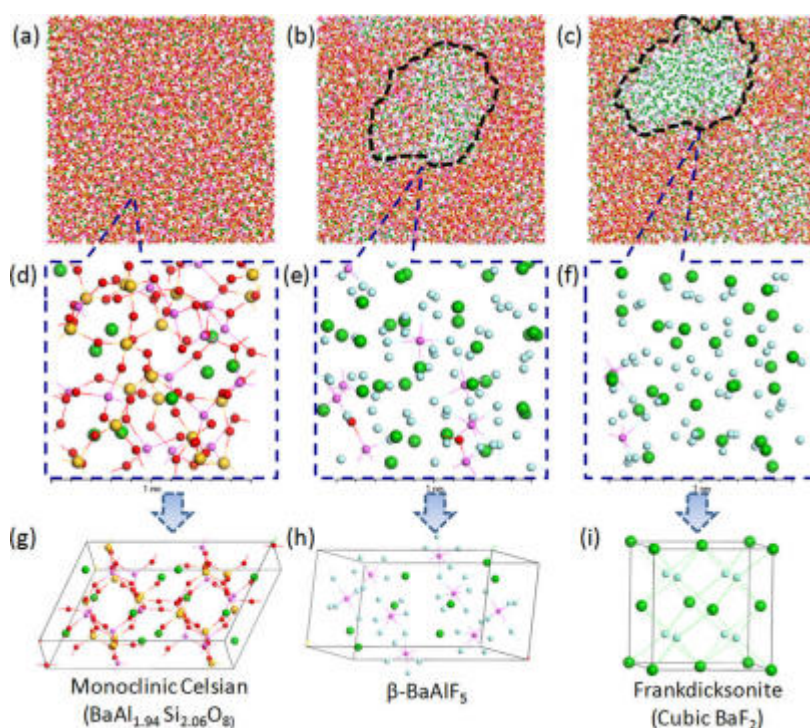
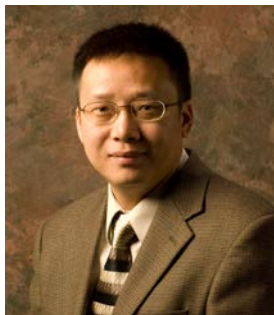


Fig. 1 Snapshots of oxyfluoride glass from MD simulations and their correlation to different crystalline phases. (Zhao et al. *J. Phys. Chem. C.*, 120 (2016)17726)

### **Brief Biographical Notes**



*Dr. Jincheng Du is an Associate Professor in Material Science and Engineering at the University of North Texas, Denton, Texas, USA. He received his Ph.D. in Ceramics from Alfred University and postdoctoral training at Pacific Northwest National Laboratory and University of Virginia. His current research focuses on applying classical and first principles atomistic computer simulations of glasses, ceramic and nanostructured materials, defects and interfaces in materials, with an aim to understand the structural origin of properties for materials with biomedical, environmental, energy and microelectronic applications. Dr. Du has over 100 peer reviewed journal publications and given over 50 invited talks and seminars in international conferences and at institutions around world. Dr. Du is the technical committee Chair of TC27 Atomistic simulations of glass of International Commission on Glass (ICG). He also serves as a member of the leadership team of the Glass and Optical Materials Division (GOMD) of American Ceramic Society.*

## Navigating at will on a system's phase-diagram: crystallisation versus vitrification, amorphous-amorphous transitions and other challenging topics

Silvio Pipolo<sup>1</sup>, Mathieu Salanne<sup>2</sup>, Guillaume Ferlat\*<sup>1</sup>,  
A. Marco Saitta<sup>1</sup> & Fabio Pietrucci<sup>1</sup>

*1 Sorbonne Universités - UPMC Univ. Paris 6, Institut de Minéralogie, de Physique  
des Matériaux et de Cosmochimie, 75005 Paris, France*

*2 Sorbonne Universités - UPMC Univ. Paris 6, Lab. PHENIX, 75005 Paris, France*

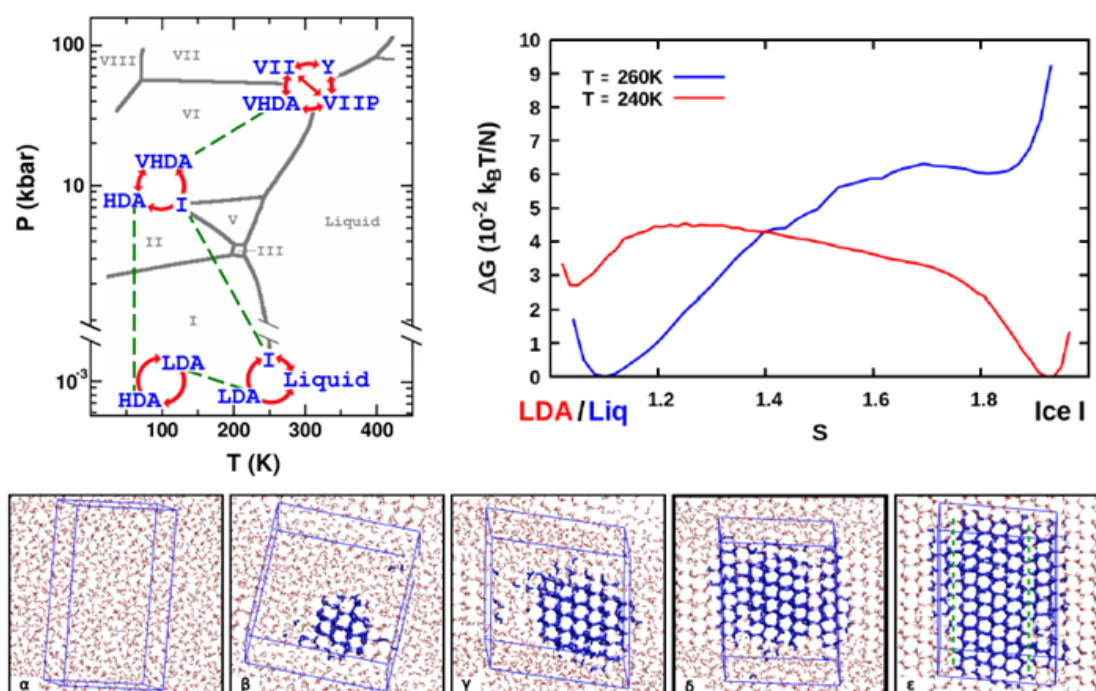
### Abstract

A major challenge of materials science is the synthesis of new predicted polymorphic structures with desired properties. Atomistic simulations combined with enhanced sampling techniques provide a powerful computational tool for investigating the mechanism and the energetics of transformations in materials but the standard approaches for phase transitions lack of transferability.

Water is a challenging system in this context because of its uniquely rich polymorphism and predicted but yet unconfirmed features (e.g. liquid-liquid transitions).

Here we show that using a novel set of coordinates, capturing changes in the topology of the interatomic network, we are able to systematically track transitions among liquid, amorphous and crystalline forms throughout the whole phase diagram of water, including the nucleation of crystals above and below the melting point.

Our general approach is not specific to water and can be applied to any structural phase transition, including those occurring in oxides and metals. On-going projects in B<sub>2</sub>O<sub>3</sub> will be briefly addressed.



Ref.: Navigating at will on the water phase-diagram, arXiv:1703.00753



## Brief Biographical Notes

**Guillaume Ferlat**, Associate professor

Institut de Minéralogie, Physique des Matériaux et Cosmochimie  
Université P. & M. Curie, 4 place Jussieu, 75005 Paris, France.

e-mail : [ferlat@impmc.upmc.fr](mailto:ferlat@impmc.upmc.fr) web : <http://www.impmc.upmc.fr/~ferlat>

- [2016] *Habilitation à Diriger des Recherches – Univ. P. & M. Curie, Paris VI*  
*Structural order in disordered systems: from glasses to supercritical solutions.*  
*Contributions from atomistic simulations*
- [2003-] Associate professor, IMPMC, University P. & M. Curie, Paris, France
- [2003] Postdoctoral Researcher, University of Cambridge, UK (Pr. E. Artacho).
- [2002] PhD in Condensed Matter Physics - University of Lyon I (Pr A. San Miguel)

**Research:** Structural transformations in liquids and glasses, poly(a)morphism

**Tools:** First-principles molecular dynamics, DFT calculations

**30 publications** in peer-reviewed international journals (including 1 Nature Materials, 1 PNAS and 2 PRL), 1 book chapter.

### Selection of publications:

- 1) H. Hay, **G. Ferlat**, M. Casula, A. P. Seitsonen, F. Mauri, Dispersion effects in SiO<sub>2</sub> polymorphs: an ab initio study, *Physical Review B* **92**, 144111 (2015).
- 2) O. L. Alderman, **G. Ferlat**, A. Baroni, M. Salanne et al., Liquid B<sub>2</sub>O<sub>3</sub> up to 1700K: x-ray diffraction and boroxol ring dissolution, *Journal of Physics: Condensed Matter*, **27** 455104 (2015).
- 3) **G. Ferlat**, A.P. Seitsonen, M. Lazzeri, F. Mauri, Hidden polymorphs drive vitrification in B<sub>2</sub>O<sub>3</sub>, *Nature Materials* **11**, 925 (2012).
- 4) R. Jonchiere, A.P. Seitsonen, **G. Ferlat**, A.M. Saitta, R. Vuilleumier, Van der Waals effects in ab-initio water at ambient and supercritical conditions, *Journal of Chemical Physics*, **135**, 154503 (2011).
- 5) **G. Ferlat**, T. Charpentier, A.P. Seitsonen, A. Takada et al., Boroxol rings in liquid and vitreous B<sub>2</sub>O<sub>3</sub> from first-principles, *Physical Review Letters* **101**, 065504 (2008).

## Characterization of Telluride Glasses by Means of First-Principles Molecular Dynamics Simulations

Eric Furet\*<sup>a</sup>, Lila Bouëssel du Bourg<sup>a</sup>, Claire Roiland<sup>a</sup>, Laurent Le Pollès<sup>a</sup>, Bruno Bureau<sup>a</sup>, Michaël Deschamps<sup>b</sup>, C. J. Pickard<sup>c</sup>

<sup>a</sup> ISCR - UMR 6226 - 11, allée de Beaulieu, 35708 Rennes Cedex 7, France

<sup>b</sup> CEMHTI - CNRS UPR 3079 - 1D av. de la Recherche Scientifique, 45071 Orléans Cedex 2, France

<sup>c</sup> Department of Materials Science & Metallurgy, 27 Charles Babbage Road, Cambridge CB3 0FS, UK

### Abstract

Chalcogenide glasses have been widely studied over the past decades due to fact that they possess, among other properties, large infrared transparency windows that extend far beyond the two atmospheric bands (3-5  $\mu\text{m}$  & 8-12  $\mu\text{m}$  - Figure 1). Such features have paved the way to various photonic-related applications, such has remote sensing/*in vivo* investigations by *fiber evanescent wave spectroscopy* or low cost thermal imaging.

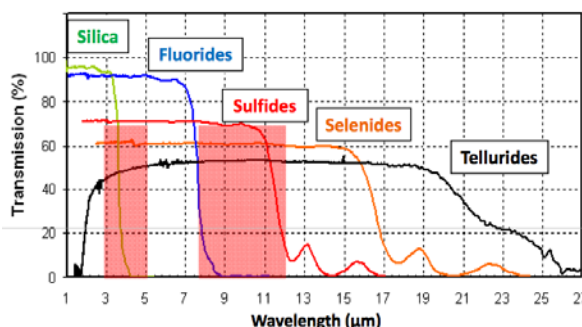


Fig.1: Typical transmittance spectra of silica, fluorides and chalcogenides bulk glasses. The atmospheric transparency windows are depicted by colored orange boxes

The subset of tellurium-based materials is known to exhibit the widest transparency windows. For example, the prototypical  $\text{GeTe}_4$  glass transmits beyond 20  $\mu\text{m}$ . Their synthesis is however difficult, because they are rather unstable being prone to devitrification processes. It is therefore of paramount importance to rationalize the structure of such glasses in order to understand their physical properties, which may subsequently help to improve their stability.

In this context, we wish to present results of recent investigations that have been carried out on telluride glasses, by combining solid-state NMR measurements and NMR parameters calculations on *in silico* samples produced by molecular dynamics simulations.

### Brief Biographical Notes



*Eric Furet obtained in 1993 a Chemistry PhD from the University of Rennes 1 (France). For 16 months, he was then a post-doctoral fellow in the Chemical Physics laboratory of Pr. J. Weber in Geneva (Switzerland), who was one of the pioneer in using Density Functional Theory tools. In 1994, he entered at the Ecole Nationale Supérieure de Chimie de Rennes as an assistant professor. He obtained a Research Habilitation degree in 2006 after joining in 2004 the Theoretical Inorganic Chemistry group of the UMR CNRS 6226. In 2009, he initiated a research project devoted to the investigation of chalcogenides glasses structure using computational chemistry tools. He is the author or co-author of ca. 45 papers (2 Angew. Chem. Int. Ed., 5 J. Am. Chem. Soc., 1 Chem. Mater., 1 Chem. Commun., 3 Chem. Eur. J., 10 Inorg. Chem.) and obtained in 2014 a grant (449 k€) from the French National Agency for a project (IRTeGlass) focusing on tellurides glasses.*

## A Role of Caged Ion Dynamics for the Enhanced Diffusion in Porous Ionic Conductors

Junko Habasaki

*School of Materials and Chemical Technology, Tokyo Institute of Technology*

### Abstract

For several nano-porous materials including composites, enhancement of ionic transport coefficients has been reported, although the origin of it is not necessarily clear [1]. In the present work, ionic motion of porous lithium disilicate was examined by Molecular Dynamics (MD) simulations. Remarkable enhancement of the diffusive motion of Li ions and existence of the maximum value were predicted in the porous lithium disilicate prepared by the gradual expansion of the system in NVE conditions [2]. Characteristic times of the regions found in the mean squared displacement (MSD) is found to be useful to distinguish the mechanism of the enhancement. A shortening of the nearly constant loss (NCL) region of MSD is found in the porous systems with the enhanced diffusion. Corresponding changes are found in structures of the coordination polyhedra. It means that a loosening of the cage is playing roles in the enhancement. With a further decrease of density, tight cages were reformed with formation of larger voids and the diffusion coefficient decreased again. A change of the power law exponent of MSD at longer time scale also contributes to the enhancement especially at the low temperature region. In addition, effects of different extended conditions of MD and some mechanical properties of the systems will be discussed.

1. Dynamics of Glassy, Crystalline and Liquid Ionic Conductors—Experiments, Theories, Simulations, Junko Habasaki, Carlos León, K. L. Ngai, Springer (2016). Chapters 6, 13 and references therein.
2. Molecular dynamics study of nano-porous materials—Enhancement of mobility of Li ions in lithium disilicate, Junko Habasaki, *J. Chem. Phys.*, 145, 204503 (2016).

### Brief Biographical Notes

*Dr. Junko Habasaki graduated from Tokyo University of Education and finished a doctor course of Graduate School of Tokyo Metropolitan University. Now she is an assistant professor of Tokyo Institute of Technology. She is a member of editorial boards in two international scientific journals. She was invited as a Professor of Physics (Université de Lille 1, France, 2007-2008). She was awarded the outstanding reviewer status (Physica A in 2015).*





## Development of Potentials for Molecular Dynamics Simulations of Oxide Glasses

Siddharth Sundararaman<sup>a,b</sup>, Simona Ispas<sup>b</sup>, Walter Kob<sup>b</sup> and Liping Huang<sup>a</sup>

<sup>a</sup>Rensselaer Polytechnic Institute, USA

<sup>b</sup>Universite Montpellier, France

### Abstract

Although significant efforts have been made in the past few decades, there is still a lack of reliable, effective, and transferable potential models for multi-component oxide glasses. In this talk, I will first discuss several key questions related to the development of potentials for molecular dynamics (MD) simulations in general:

- 1) *What are the most important interactions to be included in a potential model for the systems under study?*
- 2) *What parameterization procedure to use and what data set (from experiments and/or first principles calculations) should be used for fitting the potential parameters?*
- 3) *From what phases/thermodynamic conditions should the data set be taken for fitting parameters to ensure transferability of a potential model?*

Then, as an example, I will show a new optimization scheme recently developed by us to parameterize effective pairwise potentials for multi-component oxide glasses. This approach is to fit to results from accurate first principles calculations and explicitly incorporate the radial distribution function (RDF) of the equilibrium liquid at multiple temperatures, the vibration density of states (VDOS) and the pressure of glass into the cost function of the fitting scheme. This new optimization scheme has successfully improved potentials for silica glass and alkali silicate glasses, which can not only predict the structure, elastic and dynamic properties at ambient conditions, but also their response to external stimuli like high pressure or high temperature.

### Brief Biographical Notes

*Dr. Liping Huang is an Associate Professor of Materials Science and Engineering at Rensselaer Polytechnic Institute (RPI) in Troy, New York, USA. She obtained her Ph.D. degree from the University of Illinois at Urbana-Champaign. After several years of postdoctoral research experience at the University of Michigan and North Carolina State University, she joined RPI in 2008. Her primary research interest is to investigate the structure-property relationships at the atomic level in amorphous materials by using a combination of in situ light scattering techniques and multi-scale computer simulation methods. Among other awards, she was honored with the Norbert J. Kreidl Award from the Glass and Optical Materials Division in the American Ceramic Society in 2003. In 2009, she was a recipient of the Young Investigator Award from the Defense Treat Reduction Agency in the Department of Defense. In 2013, she won the NSF CAREER award from the Ceramics Program. She was selected as one of the two inaugural Gordon S. Fulcher Distinguished Scholars to conduct her sabbatical research at the Corning Incorporated in Fall 2015. She currently serves as the Vice Chair of the Glass & Optical Materials Division (GOMD) of the American Ceramic Society (ACerS).*

## Structure and physical properties of 56Al<sub>2</sub>O<sub>3</sub>-44Ta<sub>2</sub>O<sub>5</sub> glasses

Hiroyuki Inoue\*<sup>1</sup>, Gustavo A. Rosales-Sosa<sup>1</sup> & Atsunobu Masuno<sup>2</sup>

<sup>1</sup> The University of Tokyo, JAPAN

<sup>2</sup> Hirosaki University, JAPAN

### Abstract

New aluminate glass based on Al<sub>2</sub>O<sub>3</sub> and Ta<sub>2</sub>O<sub>5</sub> was prepared by gas levitation furnace. The glass was colorless and transparent in the visible region and its refractive index was 1.94. The glass also showed the high elastic moduli and hardness. The measured Young's modulus and Vickers hardness were 158 GPa and 9.1 GPa, respectively. These values were comparable to the reported highest ones for oxide glasses.[1]

The structure of the glass was investigated. From <sup>27</sup>Al MAS NMR experiments the coordination number of Al ions were distributed among 4, 5 and 6. The amount of AlO<sub>5</sub> polyhedra was large compared with other aluminate glass systems. The diffraction of the glass was measured by using synchrotron radiation facility, Spring-8. The total correlation function was obtained from the diffraction measurement. The structural models were prepared by classical molecular dynamics simulations. The potential parameters used were determined on the basis of the agreement between the experimental and calculated total correlation functions. Figure shows the experimental and calculated total correlation functions. In the total correlation function there were distinctive peak at 1.96 Å and two peaks at 3.32 Å and 3.74 Å, respectively. The first peak is due to the Ta-O pair and from the area of the peak the coordination number of Ta ions was estimated to be 6. The second peak is due to the Ta-Ta and Ta-Al pairs which are located at the edge-sharing linkage between the coordinated polyhedral and the third one is due to Ta-Ta pairs which are located at the corner-sharing linkage. It was found that coordination number of Al and Ta ions was larger than 4 and the amount of edge-sharing linkage between the coordinated polyhedra was more than 20%. The structure feature is typical characteristics of the structure of the glass prepared by gas levitation furnace. The vibrational spectrum and elastic constants were estimated from the structural models.

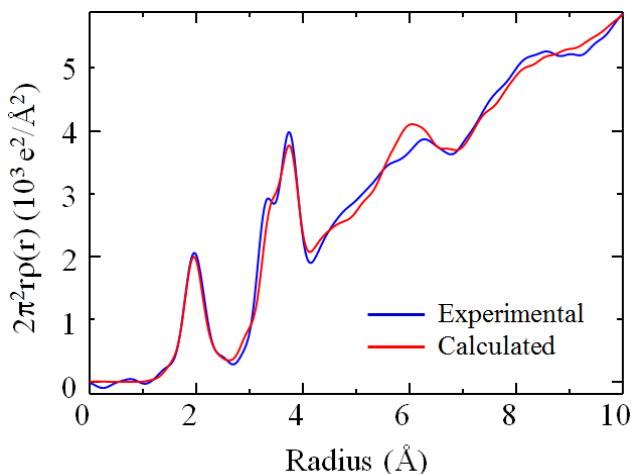


Figure 1 The experimental and calculated total correlation functions of 54Al<sub>2</sub>O<sub>3</sub>-46Ta<sub>2</sub>O<sub>5</sub> glass.

[1] G. A. Rosales-Sosa *et al. Sci. Rep.* **5** (2015) 15233.

## Brief Biographical Notes

*Dr. Hiroyuki Inoue*

*Integrated Research Center for Sustainable Energy and Materials, Department of Materials and Environmental Science, Institute of Industrial Science, The University of Tokyo*

*4-6-1 Komaba, Meguro-ku, Tokyo 153-8505 JAPAN*

*Email: inoue@iis.u-tokyo.ac.jp*

*Web: <http://www.vetrious.iis.u-tokyo.ac.jp>*

*Phone: +81-5452-6315*

*Fax: +81-3-5452-6316*



### *EDUCATION*

*Dr. Eng., Industrial Chemistry, The University of Tokyo, Tokyo, JAPAN (Mar. 1987)*

### *EXPERIENCES*

*Apr. 2005 - present Professor, Department of Materials and Environmental Science, Institute of Industrial Science, The University of Tokyo, Tokyo, JAPAN*

*Mar. 2003 - Apr. 2005 Associate Professor, Department of Materials and Environmental Science, Institute of Industrial Science, The University of Tokyo, Tokyo, JAPAN*

*Apr. 1997 - Mar. 2003 Associate Professor, Department of Metallurgy and Materials Engineering, The University of Tokyo, Tokyo, JAPAN*

*Apr. 1993 - Mar. 1997 Lecture, Department of Metallurgy and Materials Engineering, The University of Tokyo, Tokyo, JAPAN*

*Oct. 1989 - Apr. 1993 Research Assistant, Department of Metallurgy and Materials Engineering, The University of Tokyo, Tokyo, JAPAN*

*Apr. 1987 - Oct. 1989 Research Assistant, Department of Industrial Chemistry, Metropolitan University, Tokyo, JAPAN*

## First principles modelling of vibrational spectra of silicate glasses

Simona Ispas\*<sup>1</sup>, Dimitrios Kilymis<sup>1</sup>, Bernard Hehlen<sup>1</sup>,  
Sylvain Peuket<sup>2</sup> & Jean-Marc Delaue<sup>2</sup>

Lab. Charles Coulomb, Univ. of Montpellier, UMR 5221 CNRS, Montpellier, France  
<sup>2</sup>CEA DEN/DTCD/SECM, Bagnols-sur-Ceze, France

### Abstract

Raman scattering and Infra-Red absorption are techniques of choice for the structural characterization of glasses in both research and industry. However, owing to the disorder, the spectral responses are complex, combining broad and overlapping peaks, leading to qualitative rather than quantitative interpretations, even for binary compositions.

For example, the decomposition of the well known multicomponent Q<sub>n</sub> feature of the Raman spectra at high frequency in silicate glasses is a long standing issue that could be now tackled by numerical simulations, as emphasized in Fig. 1a. The deconvolution of this broad response is usually performed using a series of Gaussian accounting for the different Q<sub>n</sub> environments (Fig. 1c). Our calculations for some sodosilicate glasses reveal that in fact the individual responses are much broader and highly asymmetric (Fig.1b).

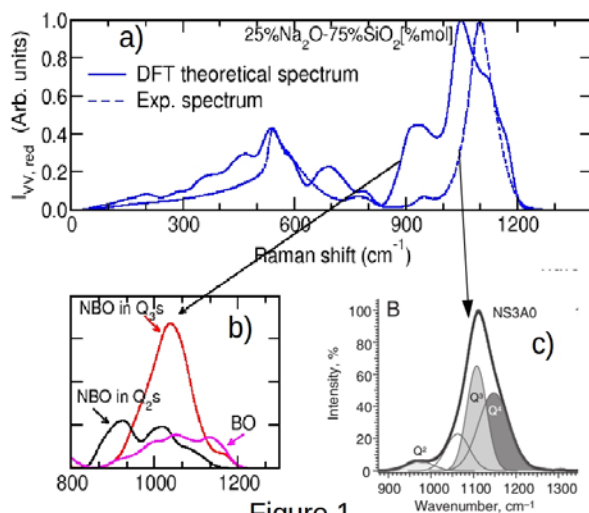


Figure 1

In this paper we will present a thorough description of the various vibrational spectra (VDOS, Raman, IR) of some sodosilicates and their dependence on the alkali content. We have studied the dependence of the mid-part of the spectra with respect to the Si-O-Si angles and have shown that the Si-O-Si bending in bridges with large angles vibrate preferentially at lower frequencies than those with low angles. Additionally, the conclusion that NBOs are essentially the origin of the Q<sub>n</sub> band, alongside the extraction of the exact contributions that lie beneath it, can be proven to be invaluable in the interpretation of experimental results.

### Brief Biographical Notes



Dr. Simona Ispas is an Associate Professor in Physics at University of Montpellier, in Montpellier, France. She obtained her Ph.D. degree in theoretical physics from the University of Montpellier. For her doctoral thesis, she worked on mathematical physics topics related to the image reconstruction in Electrical Impedance Tomography. Following her recruitment as Associate Professor, she changed her research subject and started to set up a research activity centered around first principles modelling of oxide glasses. Her primary research interest is the study of the static and dynamical properties of oxide glasses and liquids, and more particularly that of silicate glasses by means of atomistic simulations. Research areas include: first-principles and classical molecular dynamics simulations of melts and glasses, theoretical Raman and IR spectroscopy, and developing empirical potentials from ab initio simulations for simple and multicomponent oxide glasses.

## Probing the Structure of Glasses: More Order than expected

Walter Kob\*, Zhen Zhang & Simona Ispas  
*Laboratoire Charles Coulomb, University of Montpellier and CNRS  
34095 Montpellier; France*

### Abstract

Characterizing the structure of amorphous systems has been one of the main applications of computer simulations since the precise knowledge of the position of all the atoms permits to predict the properties of glasses. Of particular interest are the partial radial distribution functions since they allow to get some understanding of the relative position of the various type of atoms in real space. The corresponding partial structure factors can be used to calculate the total neutron or X-ray structure factor which in turn can help to interpret the meaning of the peaks found in the structure factors obtained in experiments. However, it is evident that in the simulation data there is way more information than just these simple two-point correlation functions. In this talk I will thus discuss our recent efforts to measure higher order correlation functions for silicate glasses. We find that these glasses show order on length scales that are significantly larger than expected from the mentioned two-point correlation functions and discuss how the chemical composition affects this order.

### Brief Biographical Notes

*-Studied in Basel, Switzerland  
-Postdoc at Stanford University, USA  
-Assistant professor in Mainz, Germany  
-Since 2000 full professor at the University of Montpellier, France  
-uses computer simulations (molecular dynamics, Monte Carlo, ab initio) to investigate the properties of disordered systems such as oxide and metallic glasses, gels, granular materials, polymers*



## Glass-forming ionic liquids under high pressure

Arnold A. Veldhorst, Luiz F. O. Faria, Tatiana C. Penna,  
Thamires A. Lima, Vitor H. Paschoal, Mauro C. C. Ribeiro\*  
*Laboratório de Espectroscopia Molecular,  
Instituto de Química, Universidade de São Paulo, Brazil*

### Abstract

Many room-temperature molten salts (*ionic liquids*) are good glass-forming liquids. Glass transition of ionic liquids takes place typically at  $T_g \sim 190$  K at atmospheric pressure, and also at room temperature under high pressure ( $\sim 2$  GPa). In this talk, some results from molecular dynamics (MD) simulations of ionic liquids under high pressure will be discussed. I will first show how the pressure of glass transition can be obtained by spectroscopic methods. Then, the models used in MD simulations of ionic liquids will be presented. Isotherms of density as a function of pressure,  $\rho(P)$ , calculated by MD simulations are compared with empirical equation of states proposed on the basis of volumetric data of ionic liquids. The correctness of simulated  $\rho(P)$  curves is also evaluated from vibrational spectroscopy of ionic liquids under high pressure. The pressure dependence  $T_g(P)$  calculated by MD simulation of a molten salt is compared with theoretical  $dT_g/dP$ , were the glass transition a second order transition following the Ehrenfest equations. The pressure effect on the structure of ionic liquids is revealed by the static structure factor,  $S(k)$ , calculated by MD simulations. Curves  $T_g(P)$  are discussed by the so-called thermodynamic scaling of transport coefficients on the basis of both spectroscopic and MD data. Concerning dynamical properties, collective dynamics is addressed by MD calculations of time correlation functions of mass current. These calculations provide the excitation energies of longitudinal and transverse acoustic modes (LA and TA) as a function of the wavevector,  $\omega(k)$ , *i.e.* the dispersion curve of sound mode within high- $(k, \omega)$  range. The relevance of MD calculations of high-frequency sound modes to our understanding of Raman spectra of glass-forming ionic liquids will be stressed.

### Brief Biographical Notes

*Mauro C. C. Ribeiro (email: mccribei@iq.usp.br) is an Associated Professor at the Chemistry Institute of the Universidade de São Paulo, IQ-USP. Mauro obtained his Bachelor degree in Chemistry in 1989 from Universidade Santa Cecília (Santos-SP). He obtained his master degree in 1992 and his PhD degree in 1995, both from USP under supervision of Prof. Paulo S. Santos. His master studies concerned calculations of resonant Raman spectra and his PhD thesis on Raman spectroscopy and molecular*

*dynamics of liquids. He started teaching at IQ-USP in 1996. Mauro spent one and a half years (1996-1998) as a pos-doc in the group of Prof. Paul A. Madden at Oxford University, UK, working with molecular dynamics of high-temperature molten salts. After returning to São Paulo he started working with vibrational spectroscopy and molecular dynamics simulation of room-temperature ionic liquids. His research concerns structure and dynamics of ionic liquids with particular focuses on changes observed along glass transition and crystallization taking place under low temperature or high pressure.*



## The atomic-scale structure of the glassy $\text{Ge}_2\text{Sb}_2\text{Te}_5$ phase change material: a via first-principles molecular dynamics study

Assil Bouzid<sup>1</sup>, Guido Ori<sup>2</sup>, Mauro Boero<sup>2</sup> and Carlo Massobrio<sup>2\*</sup>

<sup>1</sup>Chaire de Simulation à l'Echelle Atomique (CSEA), Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

<sup>2</sup>Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, F-67034 Strasbourg, France

### Abstract

$\text{Ge}_2\text{Sb}_2\text{Te}_5$  (GST hereafter) is the most established and successful phase change material (PCM) due to its high switching speed and its remarkable optical contrast between the amorphous and the crystalline phases. To exploit GST properties and optimize applications, a precise understanding of its atomic scale structure is highly desirable. Despite the known dependence of the local order of amorphous GST on the sample processing, the structure of the GST network (mostly octahedral, tetrahedral or containing both) and its bonding nature remain elusive. We employ first-principles molecular dynamics within density functional theory to elucidate the network topology of glassy GST, for which controversial structural models have been proposed so far. To this end, we take full advantage of a thoughtful, well established choice of the exchange-correlation (XC) functional (Becke-Lee-Yang-Parr, BLYP), combined with appropriate options for the non-local part in the pseudopotential construction for Ge.

Our results feature unprecedented quantitative agreement with experimental structural findings. The atomic structure of glassy GST is characterized by Ge atoms lying in a predominant tetrahedral network, albeit a non-negligible fraction of Ge atoms are also found in defective octahedra.

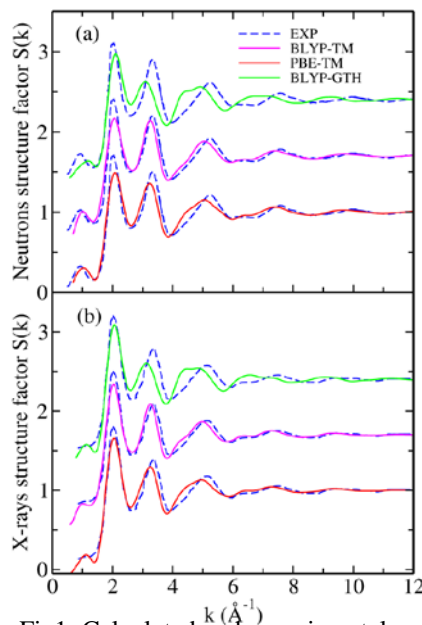


Fig1: Calculated and experimental neutrons (a) and X-ray (b) total structure factor  $S(k)$  of amorphous  $\text{Ge}_2\text{Sb}_2\text{Te}_5$ . The BLYP-TM (magenta line), PBE-TM (red line) and BLYP-GTH (green line) are compared to experimental data (dashed blue line).

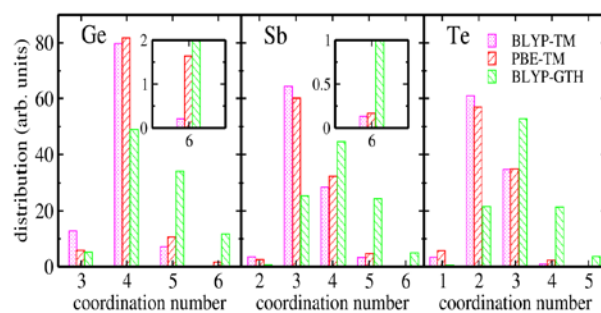


Fig2: Fractions of  $n$ -fold Ge, Sb and Te atoms ( $n=1, 2, 3, 4, 5$  or  $6$ ) for the BLYP-TM (black bar), PBE-TM (red bar) and BLYP-GTH (green bar) models.



## Brief Biographical Notes

**Carlo Massobrio**, 7-4-1958 (Milan, Italy)

*First class Research Director CNRS*

*(French Center for Scientific Research)*

*Data on March 24, 2017*

*Scientific production : 180 papers and book contributions*

*ISI Web of Knowledge: 3299 citations, h-index= 33.*

*Professional experience, accomplishments and status*

*1983-Physics Diploma, University of Rome (Italy)*

*1984-1987 Post-doctoral Researcher*

*(UC Davis, Clemson University (USA), CEA Saclay  
(France))*

*1988-Research Associate Ecole Polytechnique Fédérale de Lausanne (Switzerland)*

*1989- CNRS first class researcher*

*1998-“Habilitation” University of Strasbourg*

*2000- CNRS Research Director (second class)*

*2011- CNRS Research Director (first class)*

*2013- Deputy Director of the Institute of Physics and Chemistry of Materials,  
Strasbourg*

*2016- Appointed Member of CNRS panel expert on Chemistry of Materials*



## Local electronic redistribution and chemical bonding of vanadium oxides polyhedra in amorphous vanadates by first-principles molecular dynamics

Guido Ori, Mauro Boero, and Carlo Massobrio

*Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, F-67034 Strasbourg, France*

### Abstract

Glass-based materials containing transition metal (TM) oxides with TM in different oxidation states and modifier ions give rise to a multifunctional platform with tunable ionic-electronic conductivity properties, which are particularly suitable as electrolytes and high capacity cathodes. The absence of a long-range order allows for subtle structural adaptation during ions charge/discharge processes, which can overcome the heavy capacity loss observed during the first cycles due to irreversible phase transformations occurring in other materials. Glass systems containing vanadium oxides are receiving a renewed attention in this field due to their tunable conductivity properties on the basis of the employed synthesis conditions. With this contribution, we show how first-principles molecular dynamics combined with density functional theory can foster our comprehension of the chemical order and chemical bonding properties of the building blocks constituting amorphous vanadates. The output of this work complements the structural knowledge obtained by classical molecular dynamics and fosters our understanding to disentangle the factors governing the complex scenario of the structure - properties relations for this type of glasses. The structure around oxygen atoms of vanadium oxides polyhedra in amorphous vanadates is evaluated by first-principles molecular dynamics simulation. Thanks to the use of maximally localized Wannier functions to represent the electronic ground state of the simulated system, one is able to quantify the redistribution of electronic density around oxygen atoms as a function of the cationic environment and amorphous system. The structure of the glass network in the immediate vicinity of the oxygen atoms modulates the distribution of the Wannier centers associated with oxygen atoms. In particular the evaluation of the distances between the oxygen-core and the Wannier centers and their evolution with the nature of the surrounding ions unravels the degree of ionic or covalent nature of the involved chemical bonding.

### Brief Biographical Notes



*Guido Ori became CNRS (French National Center for Scientific Research) researcher on a permanent position at IPCMS in December 2014. He holds a Ph.D. in experimental and computational approaches for the study of functionalized materials (2009, UniMORE, ITA) along which he extended his background at the Dept. of Materials Engineering of the Imperial College of London through the EU funded Network of Excellence-Knowledge based Multifunctional Materials (NoE-KMM) focused multifunctional nanocomposites (2008). He deepened his expertise on the study of ionic liquid - solid interfaces at the international UMI CNRS-MIT joint lab located in Cambridge (USA) "MultiScale Materials Science for Energy and Environment" in the period 2012-2014. He has been awarded in 2014 a grant IDEX from the University of Strasbourg to support his research on nanomaterials through the purchase of computational units and he is currently involved in a regional project (2016-2019) focused on the study of hybrid interfaces for optoelectronic applications..*

## Simulation of the thermal properties of glasses by first-principles molecular dynamics via the "approach-to-equilibrium" methodology

E. Lampin<sup>a,\*</sup>, A. Bouzid<sup>b,c</sup>, H. Zaoui<sup>a</sup>, P. L. Palla<sup>a</sup>, G. Ori<sup>b</sup>, M. Boero<sup>b</sup>, C. Massobrio<sup>b</sup>  
and F. Cleri<sup>a</sup>

<sup>a</sup>IEMN – Lille – France

<sup>b</sup>IPCMS – Strasbourg- France

<sup>c</sup>Present address: EPLF – Lausanne - Switzerland

### Abstract

The thermal conductivity of phase change materials (PCMs) is a key property that controls the heat transport and dissipation during the writing/reading processes of memories. Since nanoscale effects impact the value of this property, atomic-scale theoretical approaches are ideally suited to address its microscopic foundations. Recently, we developed a new method to study thermal properties, the approach-to-equilibrium molecular dynamics<sup>1</sup> (AEMD), based on the analysis of a temperature transient. In this presentation, we will show that a transient thermal regime can be achieved in glassy GeTe<sub>4</sub> by first-principles molecular dynamics (FPMD) following the AEMD methodology<sup>2</sup>. We demonstrate that the time scales required to create the hot and the cold parts of the system and observe the resulting approach to equilibrium are accessible to FPMD. The temporal and spatial evolution of the temperature do comply with the time-dependent solution of the heat equation. Therefore the characteristic decay time is used to provide the thermal conductivity. Finally, the impact of the initial temperature difference, the equilibration duration, and the main simulation features are rationalized in detail.

<sup>1</sup> E. Lampin, P. L. Palla, P.-A. Francioso and F. Cleri, *Thermal conductivity from approach-to-equilibrium molecular dynamics*, J. Appl. Phys 114, 033525 (2013)

<sup>2</sup> A. Bouzid, H. Zaoui, P. L. Palla, G. Ori, M. Boero, C. Massobrio, F. Cleri and E. Lampin, *Thermal Conductivity of glassy GeTe<sub>4</sub> by First-Principles Molecular Dynamics* to be published in Phys. Chem. Chem. Phys.

### Brief Biographical Notes

*Dr. Evelyne Lampin is a CNRS Researcher in Computational Materials Science at the IEMN (Institute of Electronics, Microelectronics and Nanotechnologies) in Lille (France) and the head of the modeling team NAMASTE (NANoMATERIALS and Soft matTER). Her interest lies on the physical understanding of micro/nanotechnology by means of dedicated atomic-scale modeling. She is currently studying heat transport at the nanoscale and the applications for thermal management in nanoelectronics and thermoelectricity. She develops simulation methodologies, like the approach-to-equilibrium molecular dynamics (AEMD) for thermal properties, using classical and first-principles methods. The approaches are applied to silicon-based nanostructures and disordered materials. Evelyne Lampin has authored 40 articles for publication in international peer-reviewed journals and books. She has been involved in several european (FP5 Friendtech, FP6 PullNano and NANOCMOS, FP7 NANOPACK) and national projects (ANR QUASANOVA and NOODLES). She has been the main organiser of the Symposium on "Heat transfer at short time and length scales" at eMRS 2015 fall meeting in Warsaw and she is a member of the eMRS executive committee.*



## Molecular dynamics simulation of spontaneous nucleation and grain growth in melt BaS

José Pedro Rino<sup>1\*</sup> & Sandra Cristina Costa Prado<sup>2</sup>

<sup>1</sup>*Departamento de Física, Universidade Federal de São Carlos, Via Washington Luiz km235, 13565-905 São Carlos SP-Brazil,*

<sup>2</sup>*Faculdade de Tecnologia de Mococa, 13736-260, Mococa, SP-Brazil,*

### Abstract

Molecular dynamics simulations were performed using an effective pair potential proposed to describe barium sulfide<sup>1</sup>. The interatomic potential takes into account Coulomb interactions due to charge transfer between ions, steric repulsion, charge-induced dipole attractions due to the electronic polarizability of the atoms, and the attractive van der Waals interaction between barium and sulphur. The beginning of spontaneous nucleation and the grain growth at fixed temperature at supercooled region were observed and monitored. The number of grains varies with the cooling rates. Simulations at different temperatures showed that the initial time for nucleation and the velocity of grain growth are different.

[1] J.P. Rino, *Comput. Mat. Sci.* 92 (2014) 334-342

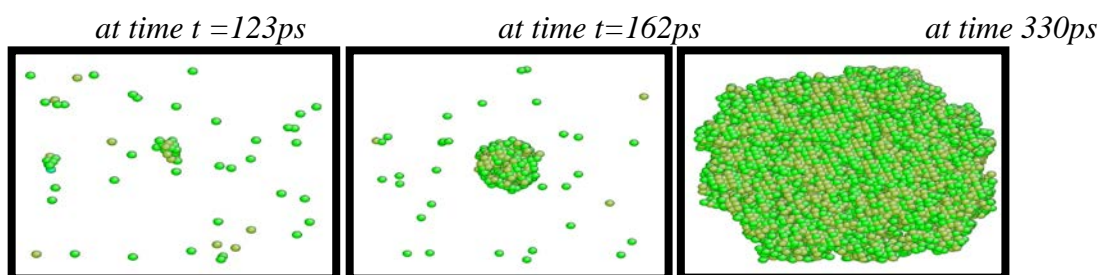


Fig.1: Snapshots of atomic configuration at different time steps. Only particles with coordination number 6 are shown.

### Brief Biographical Notes



*José Pedro Rino ([djpr@df.ufscar.br](mailto:djpr@df.ufscar.br)) is a Full Professor at Physics Department of the Federal University of São Carlos. He obtained his Master Degree (1978) and his PhD (1983) from Universidade de São Paulo at São Carlos. The Master degree deal with the influence of geometry in the Bose-Einstein condensation of a charged Boson gas, and the PhD thesis on Theories of Classical Liquids. He spends 2 years as a Pos-Doc fellow at Argonne National Laboratory under the supervision of Prof. Priya Vashishta which whom he has been working since then on the development of interatomic potential for semiconductors. His actual research concern with development of interatomic potential for simple oxides and perovskite to be used in molecular dynamics study.*

## Identifying and characterizing the different structural length scales in glass-forming materials

Philip S. Salmon\* & Anita Zeidler

Department of Physics, University of Bath, Bath BA2 7AY, UK

### Abstract

The ordering that occurs in glass on different real-space length scales manifests itself by the appearance of distinct peaks in the structure factors  $S(k)$  that are measured by diffraction. For a network-forming glass such as  $\text{SiO}_2$  or  $\text{GeSe}_2$ , three peaks generally occur with positions  $k_i$  ( $i = 1, 2, \text{ or } 3$ ) that scale roughly with the nearest-neighbour interatomic distance  $d$ , such that  $k_1 d \approx 2-3$ ,  $k_2 d \approx 4.6-4.9$  and  $k_3 d \approx 7.7-8.9$  (Figure 1). The real-space periodicities associated with  $k_3$ ,  $k_2$  and  $k_1$  are commensurate with the nearest-neighbour atomic separations, with the size of network-forming  $\text{AX}_4$  motifs ( $\text{A} = \text{Si}$  or  $\text{Ge}$ ;  $\text{X} = \text{O}$  or  $\text{S}$ ), and with the arrangement of these motifs on an intermediate range, respectively. In contrast,  $S(k)$  for a metallic glass is dominated by a first peak at a scaled peak position  $k_3 d \approx 7-8$ , which reflects a close-packed atomic structure. The structure-related properties of network-forming systems are influenced by a competition between the ordering on the different length scales, which can be manipulated by changing the chemical identity of the atomic constituents or by varying state parameters such as the temperature and pressure. The decay of the pair-correlation functions at large- $r$  can be represented by making a pole analysis of the Ornstein-Zernike equations.

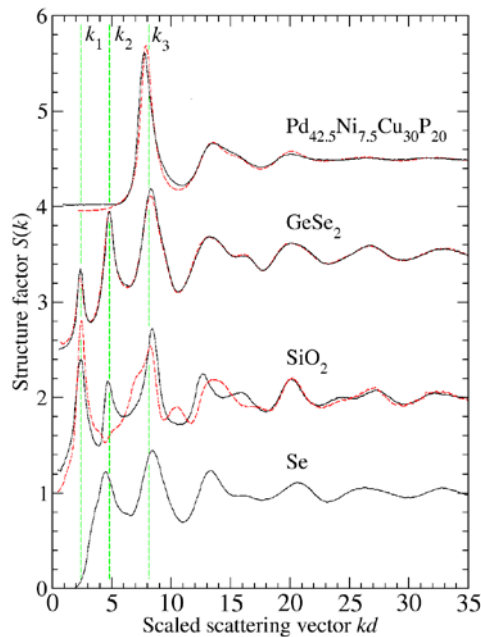


Figure 1. The structure factors  $S(k)$  measured by neutron (solid curves) and x-ray (broken curves) diffraction for several glass-forming materials, plotted as a function of the scaled scattering vector  $kd$ .

### **Brief Biographical Notes**

*Phil Salmon received his B.Sc. and Ph.D. degrees from the University of Bristol. He did postdoctoral work at the University of Exeter, before moving to a “New Blood” Lectureship at the University of East Anglia. He has been at the University of Bath since 1998.*

*Professor Salmon has spent sabbatical periods at the Institut Laue-Langevin; University of Oxford; Kyushu University via an Invitation Fellowship for Research in Japan; Yamagata University; and the Université de Montpellier II. He was a recipient of Corning Incorporated’s Gordon S. Fulcher Distinguished Scholarship in 2016.*



## The effects of time step length and force field accuracy in the application of Molecular Dynamics in multicomponent glasses

Adama Tandia

Corning Incorporated, 1 Riverfront Plaza  
Corning, NY 14831 USA

Molecular Dynamics methods have played key roles in the field of glass and amorphous materials. When coupled with accurate force field parameters, the methods have successfully helped characterize complex structures, compute elastic properties, and even some mechanical properties related to response to indentation and scratch. Molecular Dynamics is equipped to handle properties such as glass transition temperature, viscosity and diffusion, but current motion integration methods are limited by small time step in the order of 1-2 fs. Force field generalization for industrial applications to a wide range of properties is also another limitation factor which we will also discuss.

### Brief Biographical Notes



*Adama Tandia holds a Ph.D. degree in Applied Math/Applied Physics from Paul Sabatier University (France). He worked as a Research Associate at Northwestern University (USA) in the department of Applied Math from February 1998 to December 2000 as an active member of a DARPA project for crystal growth using Level Set and Monte Carlo methods. He joined Corning Incorporated in December 2000 and led the optical fiber micro-bending modeling effort until June 2002. He then transferred to the department of Modeling & Simulation where he introduced the use of atomic scale modeling, and very recently Machine Learning. Adama is currently involved in process optimization, materials modeling and machine learning. He is the Corning subject matter expert in machine learning and atomistic materials modeling.*

## Pressure induced structural changes in oxide glasses

Anita Zeidler\*, Philip S. Salmon

Department of Physics, University of Bath, Bath, BA2 7AY, UK

A prerequisite for designing glassy materials with new functional properties is an understanding of their structure, and the evolution of this structure with composition, temperature and pressure. In particular, it is desirable to develop models that have the power to predict the structure-related properties of glassy materials.

This talk will focus on the use of pressure as a freely tuneable parameter for inducing structural transformations in glass, which can be abrupt as in polyamorphic phase transitions. In particular, the results from diffraction and other experimental methods have been combined with molecular dynamics simulations to help elucidate the mechanisms of structural transformation in network-forming systems such as glassy SiO<sub>2</sub>, GeO<sub>2</sub> and B<sub>2</sub>O<sub>3</sub>. For these materials, the oxygen-packing fraction is found to be the driving force for structural transformation of the network-forming motifs. This observation also holds for other oxide materials under extreme conditions, including magma-related liquids.

### Brief Biographical Notes

*Anita Zeidler is a Royal Society – EPSRC Dorothy Hodgkin Research Fellow at the University of Bath. She obtained her Diploma in Chemistry from the University of Marburg in 2004, and her PhD in Physics from the University of Bath in 2009. She was the recipient of the 2015 Pilkington Award from the Society of Glass Technology, the 2014 BTM Willis Prize from the Royal Society of Chemistry and the Institute of Physics (IoP), and the 2013 Liquids and Complex Fluids Early Career Award from the IoP. In 2016 she was Corning Inc.'s Gordon S. Fulcher Distinguished Scholar.*





## Structural, Chemical and Topological Disorder- Experimental Results and New Challenges for MD Simulation

Sabyasachi Sen

*Dept. of Material Science & Engineering, University of California at Davis, Davis, CA 95616, USA*

### Abstract

Major developments in the field of classical and ab initio molecular dynamics simulations of glasses and supercooled liquids in recent years have led to significant advances in our current understanding of the amorphous state. Regarding structural studies, the 'gold standard' for the validation of the simulation methodology has been a comparison between the experimental and simulated structure factors and radial distribution functions. However, such a comparison between directionally averaged structural parameters largely ignore the topological complexities. Recent developments in correlated two-dimensional NMR spectroscopic techniques often allow for a detailed parametrization of the nature of topological disorder and its correlation with structural and/or chemical disorder. We will present recent experimental results obtained in three such areas, namely: (i) correlated bond length- bond angle distribution in vitreous silica and simple binary alkali silicates; (ii) steric constraint induced topological effects in amorphous silicon oxycarbide polymer-derived ceramics; and (iii) size-induced structural disorder and consequent amorphization in MgAl<sub>2</sub>O<sub>4</sub> spinels. We will demonstrate that these experimental results present novel challenges for developing molecular dynamics simulation techniques to establish the currently missing links between the structure and topology of glassy materials.

### Brief Biographical Notes

#### SABYASACHI SEN

Department of Materials Science & Engineering, Univ. of California, Davis, CA 95616  
Ph: 530-902-2802; Fax: (530) 752-1031; email: sbsen@ucdavis.edu

#### PROFESSIONAL PREPARATION

Presidency College, India	BSc, Honors, 1987
University of Calcutta, India	MSc, 1989
University of Houston, Texas	MS, 1991
Stanford University	Post-doctoral fellow, 1997
Stanford University	



#### APPOINTMENTS

7/2010-present Professor, Department of Materials Science & Engineering, University of California, Davis

11/2004–6/2010 Associate Professor, Department of Chemical Engineering & Materials Science, University of California, Davis  
2/1999–10/2004 Senior Research Scientist, Glass and Glass-Ceramics Research Division, Corning Inc., Corning, New York  
1997–1/1999 Lecturer, Department of Physics, University of Wales, UK  
1996–1997 Post-doctoral Research Associate, Stanford University

### **Other Activities & Accomplishments**

Varshneya Frontiers of Glass Science Lecture Award of American Ceramic Society (2015)

Member of the editorial boards of:

Journal of Non-Crystalline Solids (2011-present) Materials Research Express (2014-present); Earth and Planetary Materials (2014-present)

Invited Professorship, University of Claude Bernard Lyon1, France, 2011

Honorary Lecturer, Department of Physics, University of Wales, UK (2000-2005)

W. A. Weyl International Glass Science Award (1998)

H. Hoots Fellowship, Stanford University (1992 - 1996)

Phillips Petroleum Research Fellowship, University of Houston (1989 - 1991)

Council of Scientific and Industrial Research Fellowship, India (1989)

Mining and Metallurgical Institute of India Award (1985)

### **Granted 7 US patents**

### **Author of 195 peer-reviewed scientific papers and book chapters**