5th International Workshop on Challenges of Atomistic Simulations of Glasses and Amorphous Materials

Abstract Book

Dates: August 6 - 8, 2025

Location: AGC Yokohama Technical Center, Yokohama, Kanagawa, Japan

Website: engineering.unt.edu/mse/research/labs/fgmm/challenge-workshops/2025.html

Organizers

Dr. Shingo Urata (AGC Inc., Japan), shingo.urata@agc.com
Prof. Jincheng Du (University of North Texas, USA), jincheng.du@unt.edu
Prof. Alastair N. Cormack (Alfred University, USA), cormack@alfred.edu

Sponsors:

AGC ICG International Commission on Glass UNT UNIVERSITY OF NORTH TEXAS

Program of 5th International Workshop on Challenges of Atomsitic Simulations of Glasses and Amorphous Materials

Yokohama, Japan. Aug. 6-8, 2025

Oral/Invited talks

8/6/2025			Chair	Subject	Speaker	Affiliation	Title
Reception	9:30	10:00					
Opening	10:00	10:15			Shinya Mine	AGC Inc. Senior Executive Officer	Introduction of AGC, Yokohama Technical Center
	10:15	10:30			Jincheng Du	University of North Texas	Welcome and opening remarks
1	10:30	11:00	Prof. S. Sen	Expt/AI MD	Philip S. Salmon	University of Bath	Titanium phosphate glasses: Beyond tetrahedral network structures
2	11:00	11:30		MD	José Pedro Rino	Universidade Federal de São Carlos	A Reliable Interatomic Potential for Glass simulations
3	11:30	12:00		MD	Kenji Shinozaki	National Institute of Advanced Industrial Science and Technology	Crystal-Like Structure and Nucleation Enhancement in Oxyfluoride Glasses
Lunch	12:00	13:00					
4	13:00	13:30	Prof. N. M. A. Krishnan	MD	Binghui Deng	Huazhong University of Science & Technology	Molecular simulation of subcritical crack growth under dry conditions in a model brittle glass
5	13:30	14:00		MD	Alastair N. Cormack	Alfred University	On the Environment of Alkali Ions in Mixed Lithium-Sodium Silicates from Molecular Dynamics Simulations
6	14:00	14:30		MD	Liping Huang	Rensselaer Polytechnic Institute	Molecular dynamics simulations of glass: from bulk to nanowire

7	14:30	15:00		MD	Federica Lodesani	AGC Inc.	Molecular Dynamics Investigation of Glass–Crystal Interfaces: Structural and Mechanical Characterization
Break	15:00	15:20					
8	15:20	15:50	Prof. A Pedone	MD	Collin Wilkinson	Alfred University	Inter- and Intra- Energy Landscape Basin Dynamics and the Role of the Potential
9	15:50	16:20		MD/DFT	Xusheng Qiao	Zhejiang University	Molecular dynamic simulation and time dependent DFT calculation on silver doped fluoroaluminophosphate glasses
10	16:20	16:50		AIMD	Achille Lambrecht	Université de Strasbourg	Thermal conductivity of amorphous silicon nitride by approach-toequilibrium molecular dynamics
11	16:50	17:20		MD/MI	Lu Deng	Chinese Academy of Sciences	Understanding on the Composition-Structure-Property Relationship of Glasses: A view from General-purpose QSPR Analysis

Dinner	18:00	20:00		

8/7/2025			Chair	Method	Speaker	Affiliation	Title
12	9:15	9:45	Prof. P. S. Salmom	MC	Jean-Marc Delaye	University of Montpellier	Insights from Monte Carlo simulations into the alteration behavior of glasses
13	9:45	10:15		MD/MC	Zhen Zhang	Chengdu University of Technology	Bridging the Gap between Simulation and Experiment: The Case of Metallic Glass-Formers
14	10:15	10:45		MD/MC	Jincheng Du	University of North Texas	Effect of forming procedure on the structures of network forming glasses
Break	10:45	11:05					
15	11:05	11:35	Prof. L	MD/MC	Thibault Charpentier	Université Paris-Saclay	Combining Solid-State NMR with Reverse Monte Carlo Simulations to Elucidate Oxide Glass Structure

16	11:35	12:05	Prof. L. Deng	MD	Takahiro Ohkubo	Chiba University	Molecular Dynamics Study of Crystal Plane-Dependent Growth and Ion Transport at Glass–Crystal Interfaces in Sulfide Glass-Ceramics
Excursion	12:30	20:00					

8/8/2025			Chair	Method	Speaker	Affiliation	Title
17	9:15	9:45	Prof. L. Huang	MI	Xiaonan Lu	Pacific Northwest National Laboratory	Machine Learning in Nuclear Waste Glass Formulation and Property Model Development.
18	9:45	10:15		MI	Leopold Talirz	Schott AG	Bringing atomistic digital twins to specialty glass development
19	10:15	10:45		MD	Masahiro Shimizu	Kyoto University	Molecular Dynamics Simulation of Sodium Silicate Glass using Replica Permutation and Exchange Method
Break	10:45	11:05					
20	11:05	11:35	Prof. T. Charpentier	Expt	Satoshi Yoshida	AGC Inc.	Crack Initiation Load of Glass during a Drop Indentation Test
21	11:35	12:05		Expt	Sabyasachi Sen	University of California Davis	Nature of mixing of modifier cations and tuning its effect on the ionic conductivity of network oxide glasses
22	12:05	12:35		MLIP	Akihiro Nagoya/So Takamoto	Matlantis	Applications and recent developments of universal graph neural network potential for disordered systems
Lunch	12:35	13:30					
Poster	13:30	14:45					We will have 9 poseters from AGC members, and 2 students.

23	14:45	15:15	Prof. A. N. Cormack	MLIP	Volker Deringer	University of Oxford	Machine-Learned Interatomic Potentials for Amorphous Materials
24	15:15	15:45		MLIP	N. M. Anoop Krishnan	Indian Institute of Technology Delhi	Machine Learning Potentials for Glass Simulations
25	15:45	16:15		MLIP	Alfonso Pedone	University of Modena and Reggio Emilia	Exploring Glassy Materials with Machine Learning Potentials: From Oxide Networks to Sodium-based Solid Electrolytes
Break	16:15	16:35					
26	16:35	17:05	Prof. J. Du	MLIP	Marco Bertani	University of Modena and Reggio Emilia	Structural Drivers of Na Diffusion in Amorphous Electrolytes Revealed by Machine Learning Molecular Dynamics
27	17:05	17:35		MLIP	Shingo Urata	AGC Inc.	Certification of boroxol ring population in vitreous B2O3 glass using theoretical simulations
Closing	17:35	17:45			Jincheng Du	University of North Texas	Closing remarks

Poster presentations

No.	Presenter	Affiliation	Title
1	Kohei Numata	AGC Inc.	Construction of Machine Learning Model for Predicting Glass Properties
2	Ryosuke Tobinaga	AGC Inc.	Study on the Mechanism and Construction of an Exhaustive Search Method for SiO2-HF gas Etching Catalysts using Quantum Chemical Calculations.
3	An-Tsung Kuo	AGC Inc.	Structural Insights of Lipid Nanoparticles for mRNA Delivery Revealed by Coarse-Grained MD Simulation: A Comparative Study of Phospholipids DOPC and DSPC
4	Taro Kobayashi	AGC Inc.	Construction of Neural Network Potentials applicable to phosphate glass system
5	Kazuki Kanehara	AGC Inc.	Dielectric response of glass materials in the GHz-THz band
6	Takeyuki Kato	AGC Inc.	Machine-Learning Molecular Dynamics Study on the Structure and Glass Transition of Calcium Aluminosilicate Glasses
7	Tetsuya Nakashima	AGC Inc.	Novel electronic-conductive Nb2O5-BaO-SiO2 glass-ceramics
8	Shunsuke Hiiro	Tohoku Univ.	Decoding Fictive Temperature in Simulated Silica Glass: Implications for Optical Material Design
9	Kei Chiba	Tohoku Univ.	Molecular Dynamics–Based Structural Interpretation of Alkali Borosilicate Glass for Understanding Experimental Results
10	Ryuki Kayano	Chiba Univ.	Investigation of Water-Aluminoborosilicate Glass Interfaces using Machine Learning Potentials

Molecular Dynamics Study of Crystal Plane-Dependent Growth and Ion Transport at Glass–Crystal Interfaces in Sulfide Glass-Ceramics

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Glass-ceramics are promising materials for all-solid-state batteries due to their high lithium-ion conductivity. This study investigates interfacial models composed of $75Li_2S$-$25P_2S_5$ glass and β-Li_3PS_4 crystal with seven different crystal planes using molecular dynamics simulations. The equilibrated structures at 300 K and the crystal growth behavior at 500 K were analyzed in terms of interfacial enthalpy and crystallization rates.

A new method was developed to distinguish PS_4^{3-} units as glassy or crystalline based on their rotational motion, quantified using sulfur trajectories over a 100 ps time window as shown in Fig. 1. The crystallization rate was found to depend on the specific crystalline plane at the interface. Predicted crystal morphology was evaluated using Wulff's theorem, considering interfacial enthalpy and growth rate (Fig. 2).

Li^+ diffusivity was calculated via time integration of velocity autocorrelation functions, revealing that diffusivity in the crystalline region varies with the interfacial model and differs from bulk β-Li_3PS_4. This variation correlates with differences in the rotational motion of PS_4^{3-} units.

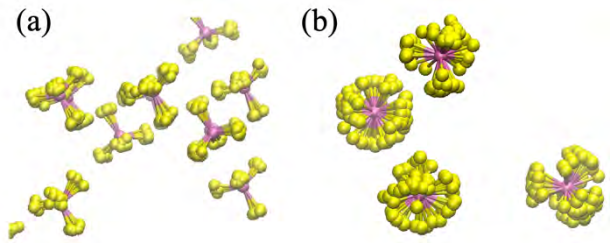

Fig. 1: Visualization of S trajectories around P obtained from the simulations of bulk (a) β-Li_3PS_4 and (b) $75Li_2S$–$25P_2S_5$ glass for 100 ps at 500 K. P and S atoms are represented by purple and yellow spheres, respectively. The S positions on each PS_4^{3-} unit are shown relative to the center of P.

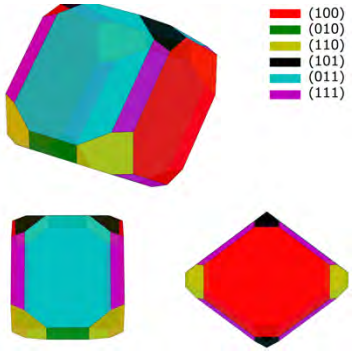

Fig. 2: Wulff shape of β-Li_3PS_4 for the interfacial model derived from interfacial enthalpy with three different viewing angles.

References:

1) K. Fukuda, F. Utsuno, A. Matsuo, T. Ohkubo, J. Phys. Chem. C, 129, 6454-6465 (2025).

Certification of boroxol ring population in vitreous B_2O_3 glass using theoretical simulations

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Population of boroxol rings in vitreous borate glass (v-B_2O_3) is still debated due to several conflicting results from experiments and simulations. To address this issue, we examined structural models of v-B_2O_3 using a combination of classical and *ab initio* molecular dynamics (MD) simulations[1]. For the classical MD simulations, both analytical and machine-learning force fields (MLFF) were utilized to construct multiple v-B_2O_3 models with varying amounts of boroxol rings, followed by ab initio MD and energy minimization using density functional theory. These diverse structures were compared with available experimental data, such as neutron and X-ray diffraction patterns, nuclear magnetic resonance (NMR), and Raman spectroscopy. Consequently, only models with more than 70% of boron atoms within boroxol rings reproduced these experimental data, confirming that a various boroxol rings should exist in v-B_2O_3. Specifically, NMR and Raman spectra of the v-B_2O_3 models with fewer boroxol rings did not show the characteristic spectra observed experimentally even when their structures were sufficiently relaxed. We therefore conclude that the population of boron atoms within boroxol rings should be more than 70%, and could be as high as 80%. Finally, we updated the MLFF using the structural data that included a certain amount of boroxol rings obtained through this work. Consequently, it was demonstrated that accurate MLFF produces a certain amount of boroxol rings, while a quenching rate comparable to experimental condition is required to generate a reasonable population of boroxol rings.

References:

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Machine Learning in Nuclear Waste Glass Formulation and Property Model Development.

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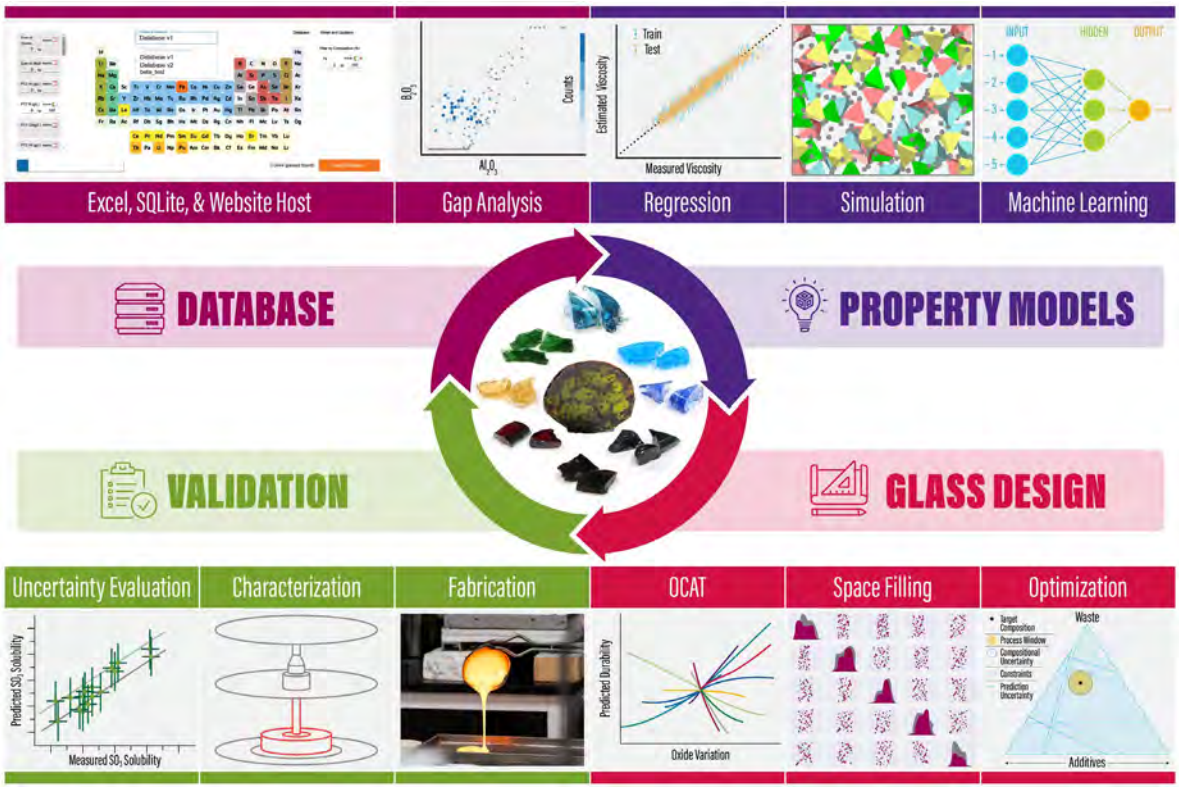
The mission of the US Department of Energy Hanford Field Office is to treat the nuclear waste for disposal. By extracting the low-activity waste (LAW) fraction from the high-level waste and using vitrification to treat each waste stream. Vitrification is the treatment standard of choice around the world for immobilizing highly radioactive waste. Traditionally, LAW glass formulations were developed using methods like partial quadratic mixture models. With the advancing machine learning (ML) methods, ML has emerged as a promising tool for modeling glass properties. This talk reviews recent efforts to integrate ML into nuclear waste immobilization, including database management, model development, uncertainty quantification, glass formulation and experimental validation. Compared to traditional methods, ML-based optimization has shown, in proof-of-principle studies, the potential for improved glass designs and faster, more adaptive formulation workflows. We also highlight advancements in the glass optimization framework, available tools, challenges and future directions for model development and formulation strategies.



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1) Lu, X., Weller, Z. D., Gervasio, V., & Vienna, J. D. (2024). Glass design using machine learning property models with prediction uncertainties: Nuclear waste glass formulation. *Journal of Non-Crystalline Solids*, 631, 122907.
2) Allec, S. I., Lu, X., Cassar, D. R., Nguyen, X. T., Hegde, V. I., Mahadevan, T., … Others. (2024). Evaluation of GlassNet for physics-informed machine learning of glass stability and glass-forming ability. *Journal of the American Ceramic Society*.
3) Song, Y., Lu, X., Wang, K., Ryan, J. V., Smedskjaer, M. M., Vienna, J. D., & Bauchy, M. (2024). Unveiling the effect of composition on nuclear waste immobilization glasses' durability by nonparametric machine learning. *Npj Materials Degradation*, *8*(1), 38.
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7) Gunnell, L. L., Lu, X., Vienna, J., Kim, D., Riley, B., & Hedengren, J. (2025). Uncertainty Propagation and Sensitivity Analysis for Constrained Optimization of Nuclear Waste Vitrification. *Journal of the American Ceramic Society*, **DOI:** 10.1111/jace.20446.
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Bridging the Gap between Simulation and Experiment: The Case of Metallic Glass-Formers

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Atomistic simulations—particularly molecular dynamics (MD)—have proven effective in providing atomic-level insights into the properties of glassy materials. However, conventional MD methods invariably employ unrealistically high cooling rates (typically exceeding 10^9 K/s), raising long-standing concerns about the relevance of computer-generated glasses to real-world counterparts formed by liquid solidification. In this talk, I will present our progress in bridging the timescale gap between atomistic simulations and experiments in the case of metallic glass-formers. By coupling MD with Monte Carlo (MC) simulations, we have succeeded in generating glass models with effective cooling rates as low as 500 K/s—comparable to typical experimental conditions. Our results show that these slowly cooled glasses exhibit structural and mechanical properties in excellent agreement with experimental observations. Moreover, we find that the cooling rate plays a critical role in determining the deformation behavior of the glasses, particularly in the initiation of local plastic events and eventual failure. Finally, I will discuss the potential of extending this hybrid MD/MC simulation approach to covalently bonded network glass-formers.

References:

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Effect of forming procedure on the structures of network forming glasses

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Despite tremendous progresses in atomistic computer simulations of glass and amorphous materials, we have been mostly relying on the simulated melt-and-quench method to generate the structures of these materials in atomistic simulations. One of the criticisms of this method, especially from our experimental colleagues, is due to orders of magnitude higher cooling rate than the fastest experimental cooling rate [1]. In this talk, after discussion the cooling rate effect, we will present some alternative methods used to generate glass and amorphous structures [2,3]. This includes methods from bond switching to quasi-static method. Particularly, we propose a hybrid method that combines Monte Carlo, Molecular Dynamics and Reverse Monte Carlo to generate network silicate glasses with targeted Q^n distributions and good agreement with experimental NMR and diffraction data. The short and medium range structural features and the stability of the structures upon relaxation are analyzed in detail. Suggestions will be given on promising alternative approaches of glass formation using atomistic simulations.

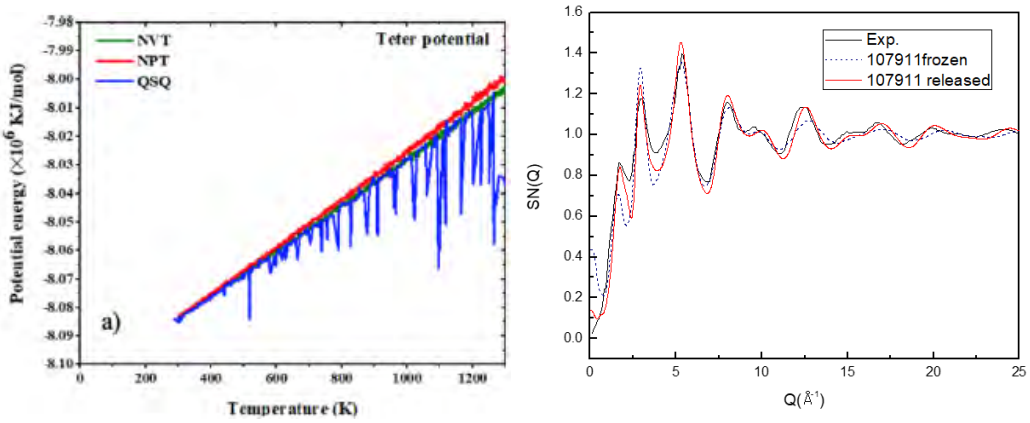

Fig. 1 Effect of simulation procedure on (1) potential energy during cooling with different cooling methods in sodium aluminosilicate glasses [2]. (2) neutron structure factor of MC and MD generated structure models of sodium silicate glasses.

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Molecular dynamic simulation and time dependent DFT calculation on silver doped fluoroaluminophosphate glasses

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Strategies including “solubility control”, “network tetrahedral charge balance” and “non-bridging oxygen coordination” are designed to uniformly disperse a large amount of Ag^{+} / $[Ag_m]^{x+}$ in fluoroaluminophosphate glass. Molecular dynamic (MD) simulation and density functional theory (DFT) calculation are adapted to depict the glass network structure and reveal the molecular fluorescence mechanisms of $[Ag_m]^{x+}$ clusters in glass. The combination of rigid covalent phosphate glass networks and flexible non-directional ionic $[YO_6]$ octahedra structures simultaneously produce a highly stable glass host with $[AlO_4]^{-}$ cross-linked $[PO_4]^{+}$ networks. With extra-generated non-bridging O^{2-} and negatively charged $[AlO_4]^{-}$ units, Ag^{+} further gets a largely increased solubility in glass. It not only enables the uniform dispersion of heavily doped Ag^{+} but also facilitates the generation of Ag clusters under a very low-power fs second laser irradiation at 19 nJ. The glass gets such an excellent chemical and optical stability that it significantly extends the optical storage lifetime up to 1.8×10^{6} years at room temperature. It thus provides a solution to future three-dimensional optical data storage technology with less electricity consumption and space occupation in the forthcoming big data era.

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A Reliable Interatomic Potential for Glass simulations

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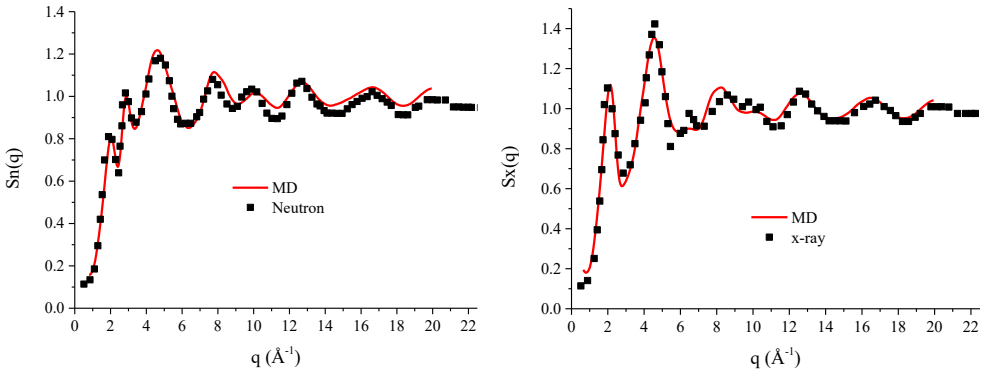
The correct physical description of the properties of a material to be used in a computational simulation depends essentially on the interaction potential employed. Among the interaction potentials proposed in the literature for use in molecular dynamics simulations, the Vashishta-Rahman potential has shown impressive results. It has been used to describe the properties of semiconductors, superionic conductors, crystal growth kinetics in supercooled liquids, amorphous systems, and glasses, among others. This interaction potential consists of the Coulomb interaction due to charge transfer between ions, steric repulsion due to the size of the atoms, charge-induced dipole attraction due to their electronic polarizability, and van der Waals attraction. A description of the structural, dynamic, and thermodynamic properties, as well as growth kinetics, will be presented for some systems described by this interaction potential.



MD results for neutron and x-ray scattering static structure factors for amorphous $MgSiO_3$ at 300K, at experimental density. Experimental results are from P. Salmon et al., J. Non-Cryst. Solids: X 3 (2019) 100024.

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1) A. Nakano, R.K. Kalia, P. Vashishta, J.Non-Cryst. Solids **171**, 157 (1994)

Crystal-Like Structure and Nucleation Enhancement in Oxyfluoride Glasses

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Controlling the crystallization process is essential in the development of glass-ceramics; however, predicting nucleation remains a significant challenge. While direct observation of nucleation is difficult both experimentally and computationally, molecular dynamics (MD) simulations offer valuable insights. Recently, Shinozaki et al. reported rapid nucleation and nanocrystallization (~10^3 K/s) in BaF_2–ZnO–B_2O_3 glasses, with nanocrystals of approximately 2 ± 0.5 nm in radius. This system exhibits nanocrystallization even under rapid quenching, making it particularly suitable for MD studies. In this work, we investigated the effects of interfacial energy, structural ordering, and nucleating agents on crystallization behavior in BaF_2–ZnO–B_2O_3 glasses through combined experimental and simulation approaches.

MD simulations were performed using the LAMMPS package with Coulomb–Buckingham potential and machine-learning-potential for a 20BaF_2–40ZnO–40B_2O_3 (mol%) composition. The systems were cooled from 2500 K to 300 K at various cooling rates. The glass sample was also investigated experimentally by high energy X-ray scattering with temperature control in BL04B2 in SPring-8 (Sayo-cho, Japan).

The resulting glass structures exhibited bond selectivity driven by differences in polarizability, with oxygen preferentially bonding with boron and fluorine with barium. Slower cooling enhanced this selectivity and led to glass structures more similar to crystalline phases. Bond-orientational order analysis showed increasing q_6 values with slower cooling rates, indicating structural ordering consistent with the cubic BaF_2 lattice. Furthermore, high-temperature structures exhibited a transition from edge-sharing to corner-sharing Ba–Ba units as shown in Fig. 1, increasing structural similarity to the crystalline phase. Rare-earth ion doping significantly accelerated nucleation, which correlated with increased crystallinity in the glass structure, i.e. fraction of edge-sharing Ba-Ba increases and fraction of fluorine around Ba increases. These findings elucidate the direct role of local structural ordering in nucleation and provide valuable insights for designing nanocrystallized glasses and novel crystallization processes.

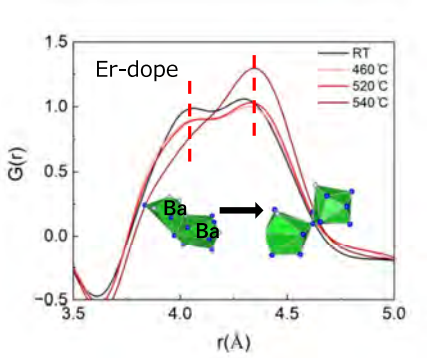

Fig. 1. Temperature dependence of G(r) for the glass sample.

References:

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Understanding on the Composition-Structure-Property Relationship of Glasses: A view from General-purpose QSPR Analysis

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[*] Corresponding Author e-mail: denglu@siom.ac.cn

References:

1) J. Yan, Y. Zhang, F. Wang, C. Shi, F. Jiang, L. Deng, T. Xue, M. Ruan, Z. Li, S. Chen, L. Hu, Effect of Al_2O_3 on the structure–property relationship of sodium aluminophosphate glasses: A combined study of experiments, MD simulations, and QSPR analysis. *J. Am. Ceram. Soc.* **106**, 6510–6526 (2023).

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Glass materials have been widely used in various fields, ranging from daily life applications to high technology optics. The glass compositions for different property requirements are usually designed through the trial and error method, which is inefficient and financially expensive. One potential solution is the quantitative structure-property relationship (QSPR) analysis, a method bridging the results from experimental measured properties and structural information from molecular dynamics (MD) simulations. This approach can correlate the structure and properties of glass, thus promising in predicting unknown glass properties. However, it relies on experimental inputs, which limits its transferability. In this work, an electronegativity-based QSPR method has been proposed without additional inputs from experiments during the descriptor construction process. Experimentally measured density, hardness, glass transition temperature, and elemental leaching rates have been correlated with different structure descriptors. In addition, potential application of the QSPR method together with the machine learning (ML) techniques have been explored. The results show that the new approach can help construct more generalized QSPR models thus provides new ideas for glass design.

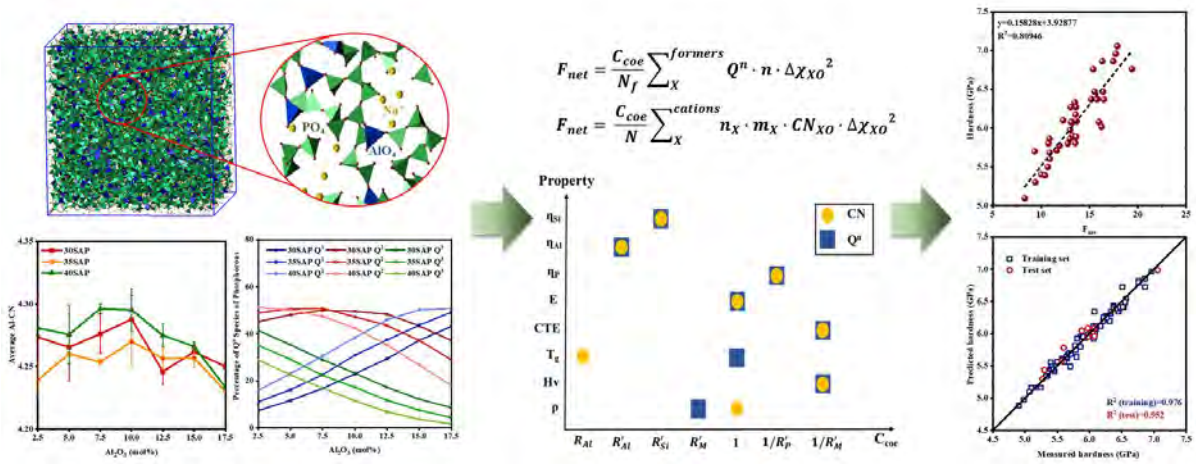

Figure 1. Illustration of the procedure for the QSPR-χ approach

Exploring Glassy Materials with Machine Learning Potentials: From Oxide Networks to Sodium-based Solid Electrolytes

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The integration of artificial intelligence into materials modeling is reshaping glass science, enabling faster and more accurate simulations. Among these advancements, machine learning potentials (MLPs) have emerged as transformative tools, bridging the computational efficiency of classical molecular dynamics and the accuracy of density functional theory.[1] This lecture explores the use of cutting-edge machine learning potentials (MLPs)—specifically DeePMD[2] and MACE[3]—to investigate the structure and properties of oxide glasses and sodium-based solid electrolytes, including thiosulfates and oxysulfates.[4] We assess the capability of these models to capture structural, dynamical, mechanical, and thermodynamic features with near ab initio accuracy and significantly reduced computational cost. A key focus is placed on the inclusion of dispersion interactions, which are often overlooked yet crucial for reproducing glass densities. Incorporating these corrections enhances agreement with experimental data, demonstrating the predictive power of MLPs in modeling complex disordered systems. This work emphasizes the promise of data-driven approaches in advancing our understanding and design of glassy materials for next-generation technologies.

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Structural Drivers of Na Diffusion in Amorphous Electrolytes Revealed by Machine Learning Molecular Dynamics.

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The global growing demand for energy storage is pushing the research for new battery materials with improved performance, safeness, and environmentally friendly synthesis, usage, and disposal. All-Solid-State Sodium Batteries (ASSSB) are attracting increasing attention from both academia and industry as strong candidates for grid-scale energy storage. However, their development requires highly conductive and electrochemically stable Solid-State Electrolytes (SSEs). Among the possible candidates, Glassy Solid Electrolytes (GSEs) are particularly promising as they can potentially meet all the requirements for a good SSE. They can achieve ionic conductivities comparable to those of liquid electrolytes while preventing dendrite growth and fire hazard[1)]. Using sodium as a charge carrier allows avoiding the ethical concerns associated with lithium mining and mitigates possible supply chain issues, thanks to the higher Na abundance. The development of ASSSBs needs a huge effort in the study of a suitable SSE. Most of the GSE studied so far are based on sulfide glasses which offer high conductivity but suffer from high reactivity with atmospheric compounds. Recently, mixed oxy-sulfide (MOS) glasses have been explored as a way to combine the chemical stability of oxide glasses with the conductivity of sulfide ones. From a computational perspective, the lack of classical interatomic potentials for these systems limits their structural investigations, as ab-initio methods are constrained by their computational cost. In this work, we developed a Machine Learning Interatomic Potential (MLIP) to study the structure of MOS glasses and correlated it with the Na diffusion. The accuracy and computational efficiency of the MLIP allow us to perform simulations beyond the capabilities of ab-initio methods, identifying structural units that promote or hinder Na diffusion and relating them to the glass composition, thus paving the way for the design of new GSE with tailored properties.

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Combining Solid-State NMR with Reverse Monte Carlo Simulations to Elucidate Oxide Glass Structure

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Solid-state NMR is now a key spectroscopy for the study of glasses because it offers a multitude of techniques to study their structure at the atomic scale.(1) However, the information acquired is limited to short-range order (structural motifs constituting the glassy network) and medium-range order (connectivity or proximity between these motifs). It does not allow on its own the construction of complete 3D structural models. For this purpose, molecular dynamics (MD) is the reference technique, effective for studying the atomic structure and structural properties of glasses.(2) Thanks to DFT calculations, NMR can now be effectively combined with MD to facilitate the interpretation of experimental data, for example to decipher the origin of the spectral broadening resulting from the geometric and chemical disorder inherent in the glassy state.(3)

To integrate most of the NMR information into MD simulations, we have recently developed a Reverse Monte Carlo (RMC) approach that couples MD, neutron data, and NMR. RMC modeling(4) aims at generating structural models that best reproduce experimental data; its principle is based on random atom displacements using a Metropolis-Hastings algorithm. Our approach will be described and illustrated using several examples: i) the construction of models of aluminosilicate glasses with a constrained population of SiO_4 Q(n)(mAl) tetrahedral units determined by ^{29}Si-^{29}Si J coupling NMR experiments; ii) the construction of borate glasses with 6-atom rings, structural features still debated in these glass compositions; iii) new insights into the structural role of high-coordination states of aluminum in lanthanum aluminoborate glasses. The introduction of machine learning (ML) to calculate NMR properties(5) will be highlighted as a promising approach to predict NMR spectra for models containing thousands of atoms, and accounting for finite-temperature effects such as vibrations or diffusion of atoms.

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On the Environment of Alkali Ions in Mixed Lithium-Sodium Silicates from Molecular Dynamics Simulations.

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The mixed alkali effect, in which there is a non-linear change in the physical properties of, say, an alkali silicate glass when one alkali metal is replaced with another, is well known, having been widely observed experimentally.

Since the transport properties are controlled by the diffusion of the alkali ions, it is obvious that the effect is ultimately controlled by their local environments. Although the last thirty years or so have seen significant advances in our understanding of the atomic structure of glasses, made possible by developments in, *inter alia*, x-ray and neutron scattering, solid state NMR and, particularly, atomistic computer simulations, most attention has been paid to the changes to the tetrahedral network; much less has been devoted to the environments of the alkalis. This is probably because, experimentally it is hard to obtain much more than coordination numbers from pair distribution functions.

Clearly, the local environments, and indeed, transport mechanisms, can be determined from MD trajectories. The challenge, though, is that different sets of interatomic potentials often give apparently differing coordination numbers for the modifiers, even while producing very similar Si-O pair distribution functions. One of the concomitant questions is whether the differences in coordination number imply really different environments.

In this presentation, we will discuss the changes in the environments of the alkali ions in the structure as a function of Li/Na ratio, obtained from molecular dynamics simulations of alkali silicates, using two different potential models.

Several series of mixed lithium and sodium silicates, as a function of both Li/Na ratio and silica content. Di-, tri-, and tetra-silicates have been modelled, with the following Li/Na ratios: 100% Li, 95Li05Na, 75Li25Na, 50Li50Na, 25Li75Na, 05Li95Na and 100% Na.

Insights from Monte Carlo simulations into the alteration behavior of glasses.

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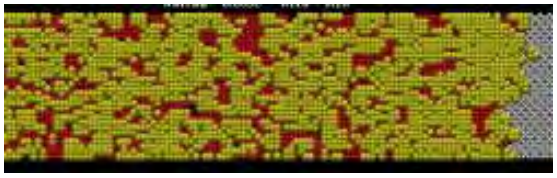
Various Monte Carlo approaches have been proposed in the past to model the alteration behavior of simplified nuclear glasses. However, these approaches have faced certain limitations due to the lack of consideration for the diffusion of aqueous species within the glass. To overcome this issue, a new algorithm has recently been implemented that incorporates both the release mechanisms of solid species into solution and the diffusion of aqueous species within the glass.
This new approach was used to analyze the changes in the alteration behavior of simplified nuclear glasses as the relative intensities of hydrolysis and recondensation mechanisms evolve. In particular, a transition to cluster-based alteration appears when the ratio between the hydrolysis probability and the recondensation probability exceeds a critical threshold. This transition will be compared to the experimentally observed change in behavior as the Al_2O_3 content decreases.
On the other hand, by focusing the computations solely on the simulation of the alteration layer maturation, the formation of pores with increasing sizes within the alteration layer was reproduced, although no visible channels connecting these pores were observed. This finding opens new perspectives for interpreting the nature of diffusion within gels, which experimentally appears to be of a solid-like type.



Simulation of an alteration gel formed on the surface of a SiO_2-Al_2O_3-B_2O_3-Na_2O glass.

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Molecular dynamics simulations of glass: from bulk to nanowire

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Molecular dynamics (MD) simulation of glass is a challenging but effective method to investigate its structure and properties. Among various challenges we are facing, developing accurate potential models to describe the interactions in glass is one of the most difficult tasks. Our study shows that in addition to the construction of the functional form for modeling the interactions between ions without taking explicitly into account the electronic degrees of freedom, the selection of the input data and their associated thermodynamic conditions is critically important for fitting parameters and ensuring the transferability of the potential model. We find that using a higher short-range cutoff is essential for obtaining a more reliable potential, particularly for accurately describing the resistance of the glass structure to compression. The short-range cutoff is a key parameter that should be reported alongside other potential parameters to fully define the model.

Our study also highlights the importance of carefully selecting simulation parameters such as system size, cooling rate, working temperature, and strain rate to correctly reproduce the fracture behavior of glass. While the stiffness of glass is relatively insensitive to these parameters, tensile strength and failure strain are significantly affected. Accurately accounting for sample density and the nonlinear elasticity of glass is crucial for reliable stiffness predictions from MD simulations. With appropriately chosen simulation parameters, glassy nanowires with radii as small as 1 nm still exhibit brittle fracture behavior. However, nanowires prepared by the cutting method show lower stiffness and tensile strength but higher failure strain compared to those prepared by casting. This difference is attributed to the greater number of surface defects introduced during the cutting process at low temperatures. These findings suggest that defect-induced ductility could be an effective strategy for reducing brittleness in glass nanostructures.

Machine Learning Potentials for Glass Simulations

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Universal Interatomic Potentials (UIPs) promise to revolutionize atomistic modeling through graph-based neural networks that capture complex interactions across diverse materials. However, their practical utility for realistic molecular dynamics simulations remains poorly understood. This talk presents comprehensive benchmarking results and a novel solution to address fundamental UIP limitations. We introduce AMCSD-MD-2.4K, a rigorous benchmark comprising ~2,400 experimentally validated mineral structures. Our systematic evaluation of six state-of-the-art UIPs reveals striking performance variations: while ORB and SEVENNET achieve >98% simulation completion rates, CHGNET fails in 93% of cases. Critically, even best-performing models exceed experimentally acceptable density variation thresholds (±2.5%), with errors ranging from 8.67% to 76.29%, highlighting a fundamental gap between computational predictions and experimental requirements. To address these limitations, we present a differentiable simulation framework enabling targeted fine-tuning of universal potentials using experimental observables. Our approach leverages automatic differentiation to optimize force field parameters by minimizing discrepancies in radial distribution functions, elastic moduli, and force constants. Applied to silica and silicon systems, this methodology demonstrates significant improvements in reproducing experimental benchmarks while maintaining transferability advantages. This integrated approach offers a pathway toward achieving both broad applicability and material-specific accuracy in machine learning force fields, establishing quantitative metrics for UIP assessment and providing practical solutions for enhanced predictive capabilities.

5th International Workshop on Challenges of Atomistic Simulations of Glasses and Amorphous Materials

Thermal conductivity of amorphous silicon nitride by approach-to-equilibrium molecular dynamics

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This talk will focus on the atomic-scale calculation of thermal conductivity of amorphous silicon nitride (aSiN) using first-principles molecular dynamics (FPMD). Targeted models have been implemented via the melt and quench methodology by attaining sizeable diffusion at high temperatures, a prerequisite to the establishment of a disordered structure at T=300K. To this end, we have introduced at T = 2000 K the Born-Oppenheimer scheme due to a gap closing phenomenon in the electronic density of states. This undermines the adiabaticity conditions inherent in the original Car-Parrinello approach selected from the outset. While amorphous SiN does feature excess silicon atoms relative to the stoichiometric composition it exhibits chemical order[1)]. The availability of a viable model allows us to focus on its thermal conductivity by using the approach-to-equilibrium molecular dynamics (AEMD)[2)]. This methodology is based on thermal transients extending in time on intervals that are affordable for FPMD. By calculating the thermal conductivity on systems of different sizes in the direction of heat transport we are able to follow the corresponding changes,[3)] the observed trends agreeing closely with a thoughtful analytical model[4)]. In order to describe the asymptotic regime leading to bulk values, we have exploited our FPMD temporal trajectories to train an empirical interatomic potential[5)] based on a machine-learning methodology, by gaining access to much larger system size. Overall, by combining FPMD and AEMD, we are in a position to describe quantitatively thermal processes in amorphous nanosystems by bridging the gap between microscopic and macroscopic behaviors.

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Bringing atomistic digital twins to specialty glass development

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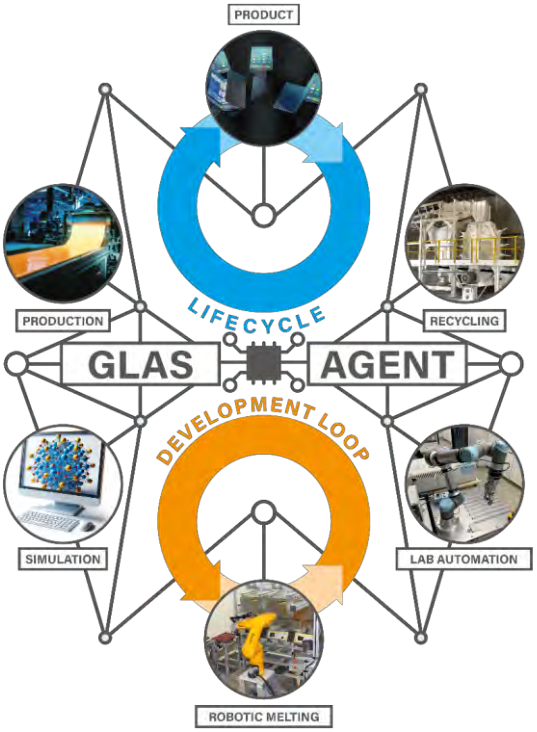
Atomistic simulations face major challenges in industrial glass development. Historically, accurate *ab initio* methods were too computationally expensive and classical force fields often not flexible enough to capture the multitude of interactions in industrially relevant multi-component glasses over a wide range of temperatures. New, flexible machine-learned interatomic potentials with millions instead of tens of parameters and –in principle– coverage of the entire periodic table promise to close this gap for the first time.



The GlasAgent project, co-funded by the German ministry for education and research, encompasses several automation & digitalization efforts in specialty glass development, one of which aims to integrate an atomistic digital twin into the routine glass development process. Over the duration of the project from 2025-29, we plan to make curated atomistic simulation workflows available to experimental glass developers via a natural language interface, starting with classical potentials, but moving to machine-learned potentials as the field matures.

Since the project has just begun, this talk will outline how we plan to get there, hoping to stimulate discussion and inviting feedback and criticism from the audience.

Molecular Dynamics Investigation of Glass–Crystal Interfaces: Structural and Mechanical Characterization

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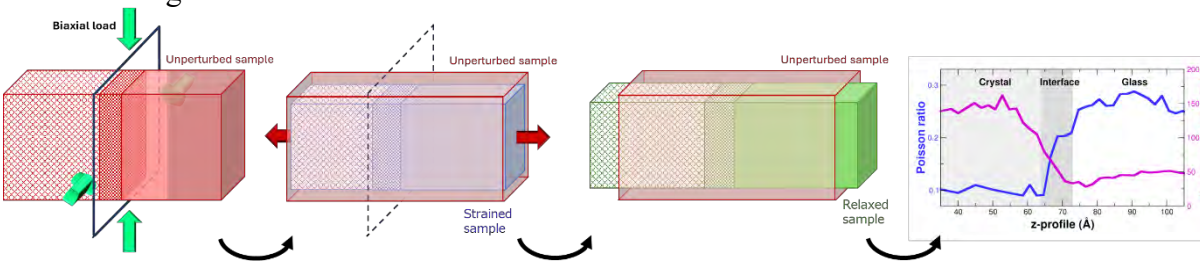
Glass-ceramic materials exhibit superior crack resistance compared to pristine glass[1], making them attractive for advanced engineering applications. A key challenge in this field is the design of new materials with enhanced properties, which requires a fundamental understanding of their mechanical behavior. The finite element method (FEM) is widely used to simulate crack propagation at the macroscopic scale[2,3]; however, the accuracy of the simulation depends on the quality of the material properties assumed in the numerical modeling. While the properties of glass matrices and crystalline regions are well-known from experiments, the glass–crystal interface remains poorly understood due to its nanoscale dimensions, which reduces the simulation accuracy because the strength of interfaces is crucial for crack generation and propagation.

This work aims to address this issue by employing molecular dynamics simulations to unravel the mechanical properties of the glass–crystal interface in lithium silicate glass-ceramics. Interface models were obtained by combining $Li_2Si_2O_5$ crystal and a glass matrix while varying crystal orientation and glass compositions, (xLi_2O–$(1–x)SiO_2$). Structural analyses were conducted to identify the interface region, followed by an evaluation of mechanical properties using the biaxial deformation method[4,5]. We evaluated the profiles of Young's modulus and Poisson's ratio from the glass region to the crystal across the interface. Through an investigation of the influence of the exposed crystalline plane, distinct features of the interfacial region will be discussed.



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Inter- and Intra- Energy Landscape Basin Dynamics and the Role of the Potential

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In this talk we will discuss the interconnectivity between the vibrational properties and the configurational properties of the energy landscape of common oxide glasses. A particular focus will be placed on understanding the role of the interatomic potential and the methods used to calculate the dynamics. The landscape properties discussed include heat capacity, relaxation, and crystallization with the goal being an informed discussion on energy landscape techniques for studying glassy systems.

Titanium phosphate glasses: Beyond tetrahedral network structures

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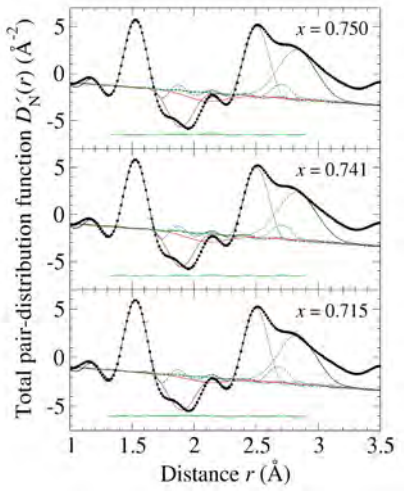
The structure of titanium phosphate glasses $(TiO_2)_x(P_2O_5)_{1-x}$ with $0.70 \leq x \leq 0.75$ was investigated by combining neutron and high-energy x-ray diffraction with solid-state ^{31}P nuclear magnetic resonance (NMR), Raman and electron paramagnetic resonance spectroscopy. The results were interpreted with the aid of an analytical model that delivers the composition dependence of the structural motifs. The structure of these materials was also simulated using *ab initio* molecular dynamics. ^{31}P static NMR spectra show that orthophosphate groups predominate, and the diffraction results find a Ti-O coordination number of 5.32(7) at $x = 0.715$ that increases to 5.49(7) at $x = 0.750$. The findings show the prevalence of five- and six-coordinated titanium atoms and the coexistence of two-coordinated O(II) and three-coordinated O(III) oxygen atoms. The Ti-centred polyhedral units contribute towards a network in which the orthophosphate groups form P-O(II)-Ti and P-O(III)-2Ti connections, with signatures that are evident in the ^{31}P magic angle spinning NMR spectra. The results suggest that structural variability is a key factor in promoting the vitrification of this atypical glass-forming system. The findings will provide a benchmark for investigating the structure of other glass-forming materials based on networks of higher-coordinated polyhedral units.



Nature of mixing of modifier cations and tuning its effect on the ionic conductivity of network oxide glasses

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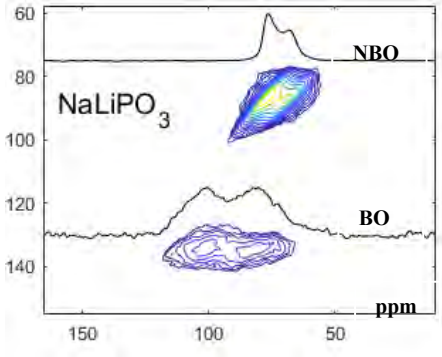
The distribution of modifier cations around non-bridging and bridging oxygen (NBO and BO) atoms in mixed-modifier metaphosphate glasses is investigated using ^{17}O NMR spectroscopy. The results demonstrate that an ordered distribution of these cations is favored in mixed-alkali systems, which is likely responsible for the pronounced non-linear compositional variation of ionic conductivity in these glasses. In contrast, the mixed alkali-alkaline-earth glasses display a monotonic compositional variation of ionic conductivity corresponding to a random distribution of the modifier cations around the NBO atoms. Structural relaxation of these glasses during isothermal aging significantly reduces their ionic conductivity. While the activation enthalpy ΔH_m of ionic conduction remains constant after aging, the entropy of migration ΔS_m decreases, leading to a corresponding reduction in the hopping rate of mobile alkali ions. This behavior is observed to be associated with a spatial redistribution of the modifier cations in the glass structure during aging. These findings, when taken together, suggest that significant increases in the ionic conductivity of a glass, even by orders of magnitude, can be achieved by raising its fictive temperature. The possible consequences of this effect will be discussed.



Crack Initiation Load of Glass during a Drop Indentation Test

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I am happy to welcome all of you to AGC Yokohama Technical Center, which is the main hub for AGC's technology development activities. In this talk, I'd like to introduce you our recent topics on fundamental glass research, especially on indentation responses of silicate glass. Unfortunately, my talk focuses only on experimental works, but I hope you will find some interesting in unsolved issues on permanent deformation and cracking in glass.

The indentation test in glass is widely used not only for measuring hardness but also for evaluating susceptibility to crack initiation in glass. In fact, it has been well known that the crack initiation load (CIL) determined from the indentation test depends on glass compositions. Although CIL is one of the good measures to compare resistance to indentation-induced cracking among various glass compositions, one's attention should be paid to the fact that CIL is the parameter obtained from the quasi-static indentation test. So far there's been very limited information on the mechanical response, especially cracking behavior, of glass under the indenter at higher impact velocities. In this study, therefore, the dynamic indentation behavior (See Fig. 1) of some silicate glasses is evaluated by using a lab-made drop indentation set-up[1]. From in-situ observation images and the obtained load-depth curve during the test, the dynamic CIL and the dynamic indentation toughness are determined.

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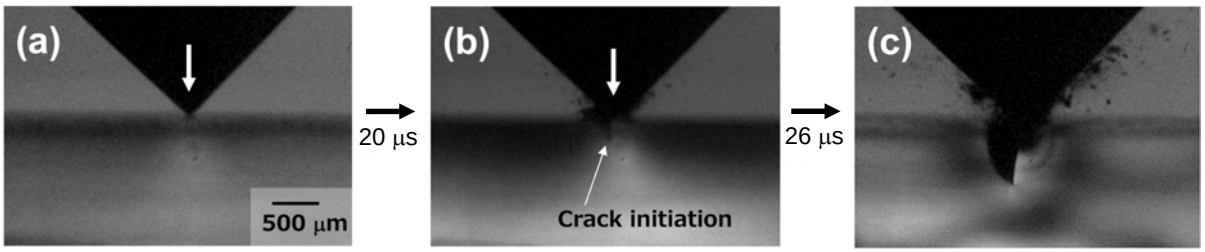

Fig. 1 Snapshots of the high-speed camera image during the sample-drop test using the indenter with a tip-radius of 0.05 mm. (a) The indenter touches the glass surface. (b) The moment the crack initiates. (c) The maximum load (~160 N) is applied to the glass. The times shown between the photos denote the elapsed times.[1]

Machine-Learned Interatomic Potentials for Amorphous Materials

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Machine-learning-based interatomic potentials (MLIPs) are now becoming increasingly popular simulation tools in chemistry and materials science. In this presentation, I will highlight some recent advances in the MLIP-driven modelling and understanding of amorphous solids. These studies range from fundamental research questions – such as the atomic structure of amorphous silicon monoxide[1] – to device-scale simulations of phase-change memory materials which encode digital "ones" and "zeroes" in data-storage devices.[2] I will discuss future perspectives for both purpose-specific and generally applicable MLIPs, and the role they might play in the computational "design" of amorphous materials with target properties.[3]

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Molecular Dynamics Simulation of Sodium Silicate Glass using Replica Permutation and Exchange Method

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Cooling rate of molecular dynamics simulation (MD) in silicate glass(10^9~10^{13} K/s) is much faster than experimental melt-quenching method($<10^3$ K/s). The fictive temperature of $15Na_2O$-$20CaO$-$65SiO_2$(mol%) obtained by classical MD with 10^{11} K/s is 1304 K, which is higher than experimental T_g (845 K)[1)]. Considering the structural change below glass transition temperature affects structure and volume[1,2)], the discrepancy would be an obstacle to precisely predict structure and property of silicate glass using MD. Some methods have been reported to obtain an energetically stable glass: stress perturbation[3)], QSQ[4)], and replica exchange method(REM)[5)]. Here, we check the efficiency of REM and replica permutation method(RPM)[6)], which is a modified version of REM, for obtaining steady-state glassy structure of sodium silicate glass.

In the presentation, after we shortly introduce the analysis of structural change below T_g with experiment and DFT, we show the results of RPM and REM. The target composition was $30Na_2O$-$70SiO_2$(mol%), and the total number of atoms was 750. We used Coulomb-Buckingham type potential parameterized by Teter and Du[7)]. The velocity rescaling method and Berendsen barostat were employed. For MD without replicas, after keeping the 1600 K and 0.1 MPa for 0.25 ns for equilibration, we changed the temperature to 1400 K discontinuously. For MD with REM and RPM, after the 1600 K annealing, we put 20 replicas from 1400 K to 2407 K, and started replica exchange and permutation. Fig. 1 shows the potential energy at 1400 K. MD without replicas took 17.0 ns to reach the minimum potential energy. MD using REM and RPM took 7.5 ns and 4.1 ns to obtain the minimum potential energy, which means the efficiencies are 2.2 and 4.1 times, respectively, compared to the standard MD.

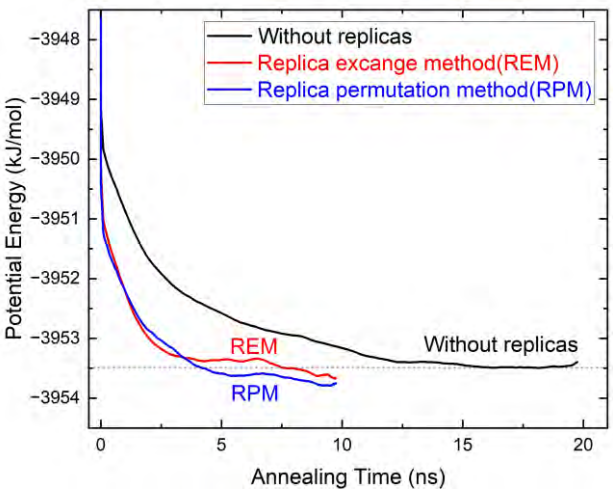

Fig. 1 Potential energy at 1400 K. Dotted line is the minimum of MD without replicas

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Applications and recent developments of universal graph neural network potential for disordered systems

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Machine learning interatomic potentials (MLIPs) have emerged as powerful tools for enabling large-scale, accurate atomistic simulations[1]. Among them, the PreFerred Potential (PFP) is a universal MLIP developed to achieve DFT-level accuracy without system specific fine-tuning[2,3]. It has been successfully applied to a wide range of materials—including batteries, semiconductors, catalysts, metal-organic frameworks (MOFs), and polymers—highlighting its effectiveness for practical applications. These results demonstrate the robustness and universality of PFP, making it a promising tool for systems with significant chemical and structural complexity. This includes amorphous and glassy materials, where atomic-scale modeling remains challenging due to the lack of long-range order and the need for statistical sampling of disordered structures. The versatility of PFP opens new opportunities to investigate the formation, structural motifs, and dynamic properties of glasses through scalable, ML-accelerated molecular dynamics simulations.

As part of our recent development, we performed extensive validation studies, demonstrating that PFP accurately predicts a broad range of properties, such as melting points, amorphous structures, specific heats of organic liquids and crystalline solids, and ion diffusion coefficients, in good agreement with both DFT-PBE and experimental data. This confirms PFP's universality in describing not only equilibrium structures but also thermodynamic and dynamic behaviors across diverse systems. To further improve accuracy in temperature-sensitive systems, we developed a new PFP mode trained on the meta-GGA R2SCAN functional, recently released in PFP v8. This model significantly enhances the prediction of melting temperatures for water and ceramics, addressing systematic errors inherited from PBE. Moreover, to enable large-scale and long-timescale simulations, we developed LightPFP, a moment tensor potential (MTP) trained on PFP data. LightPFP achieves simulation speeds approximately ten times faster than PFP while maintaining comparable accuracy, making it ideal for melt-quench simulations and glass modeling at practical scales.

These recent advancements represent significant steps forward in expanding the capabilities of MLIPs. They enable high-throughput, accurate simulations of glasses and amorphous materials, bridging the gap between ab initio precision and industrial-scale modeling.

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Molecular simulation of subcritical crack growth under dry conditions in a model brittle glass

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Subcritical crack growth refers to continuous crack extension under a constant applied load below the threshold value for catastrophic failure, also known as static fatigue. Here we report how a crack grows under a combination of stress intensity factor (K) and temperature in a model brittle glass using molecular dynamics simulation. The model glass is under dry conditions thus avoiding the complexity of corrosion chemistry. Crack growth rate is shown to be inconsistent with the commonly used subcritical crack growth model rooted in the transition state theory (TST), in which the applied stress intensity factor reduces the transition barrier. A new subcritical crack growth model is proposed with a constant barrier and a K-dependent prefactor in TST, representing the size of the region for potential bond breaking. The thermomechanical condition for subcritical crack growth is also mapped in the K-T domain, in between elastic deformation and catastrophic fracture regimes. Finally, we show substantial crack self-healing once the applied load is removed, under the thermodynamic driving force of surface energy reduction. Our findings provide new insights into the mechanochemical coupling during static fatigue and call for experimental investigation of whether the activation energy is K-dependent.We encourage including a figure relevant to the abstract.

Crystal-Like Structure and Nucleation Enhancement in Oxyfluoride Glasses

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Controlling the crystallization process is essential in the development of glass-ceramics; however, predicting nucleation remains a significant challenge. While direct observation of nucleation is difficult both experimentally and computationally, molecular dynamics (MD) simulations offer valuable insights. Recently, Shinozaki et al. reported rapid nucleation and nanocrystallization (~10^3 K/s) in BaF_2–ZnO–B_2O_3 glasses, with nanocrystals of approximately 2 ± 0.5 nm in radius. This system exhibits nanocrystallization even under rapid quenching, making it particularly suitable for MD studies. In this work, we investigated the effects of interfacial energy, structural ordering, and nucleating agents on crystallization behavior in BaF_2–ZnO–B_2O_3 glasses through combined experimental and simulation approaches.

MD simulations were performed using the LAMMPS package with Coulomb–Buckingham potential and machine-learning-potential for a 20BaF_2–40ZnO–40B_2O_3 (mol%) composition. The systems were cooled from 2500 K to 300 K at various cooling rates. The glass sample was also investigated experimentally by high energy X-ray scattering with temperature control in BL04B2 in SPring-8 (Sayo-cho, Japan).

The resulting glass structures exhibited bond selectivity driven by differences in polarizability, with oxygen preferentially bonding with boron and fluorine with barium. Slower cooling enhanced this selectivity and led to glass structures more similar to crystalline phases. Bond-orientational order analysis showed increasing q_6 values with slower cooling rates, indicating structural ordering consistent with the cubic BaF_2 lattice. Furthermore, high-temperature structures exhibited a transition from edge-sharing to corner-sharing Ba–Ba units as shown in Fig. 1, increasing structural similarity to the crystalline phase. Rare-earth ion doping significantly accelerated nucleation, which correlated with increased crystallinity in the glass structure, i.e. fraction of edge-sharing Ba-Ba increases and fraction of fluorine around Ba increases. These findings elucidate the direct role of local structural ordering in nucleation and provide valuable insights for designing nanocrystallized glasses and novel crystallization processes.

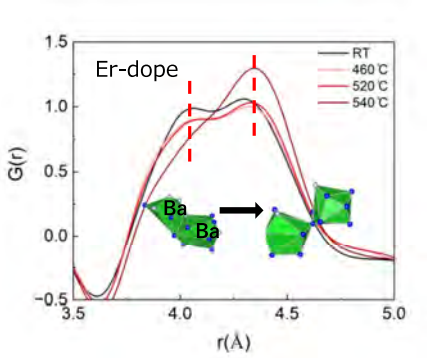

Fig. 1. Temperature dependence of G(r) for the glass sample.

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