Contribution ID : **102** Type : **Poster Presentation**

The Hard Truth: How Composition and Structure Shape the Mechanics of Aluminosilicate Glasses

Hardness [1] is a key property that determines how solid materials respond mechanically to applied stress. Understanding the mechanisms underlying hardness at the atomic scale is crucial for designing materials with enhanced mechanical performance. In this work, we employ molecular dynamics (MD) simulations to perform nano-scale indentation tests, offering new insights into the fundamental processes that influence hardness in oxide glasses. Our study specifically investigates how the atomic structure of aluminosilicate glasses is modified during their interaction with a diamond cone-shaped indenter. We focus on the albite–anorthite compositional series, which spans from sodium-rich albite ($NaAlSi_3O_8$) to calcium-rich anorthite ($CaAl_2Si_2O_8$). This compositional variation enables us to explore how the replacement of monovalent sodium ions with divalent calcium ions affects the charge compensation of AlO_4^- tetrahedra and the resulting reorganization of the glass network. In addition to nanoindentation, we present a detailed analysis of the surface characteristics of the glasses, including surface roughness and topographical evolution before and after deformation. The simulations reveal how surface morphology is influenced by composition and mechanical loading. To further complement the mechanical characterization, we also perform two additional sets of simulations: hydrostatic compression and uniaxial elongation [2]. These tests allow us to evaluate the elastic and plastic response of the glass networks under different stress states, providing a more complete picture of the mechanical behavior. By combining these simulations, we assess changes in structural parameters such as bond angles, coordination numbers, and network connectivity across different loading conditions. The effects of densification, both at the surface and in the bulk, are systematically examined across the compositional series. Variations in elastic moduli, residual stresses, and permanent deformation are linked to the underlying atomic rearrangements induced by mechanical stress. This investigation offers a comprehensive understanding of the nanoscale mechanical behavior of aluminosilicate glasses. By exploring the interplay between chemical composition, atomic structure, and mechanical performance, our study provides valuable insights for the rational design and optimization of glassy materials for advanced technological applications, including protective coatings, optical devices, and micro-electromechanical systems.

[1] Liu, H., Deng, B., Sundararaman, S., Shi, Y., & Huang, L. (2020). Journal of Applied Physics, 128(3). [2] Pallini, A., Ziebarth, B., Mannstadt, W., & Pedone, A. (2025). Journal of Non-Crystalline Solids, 647, 123267.

Primary author(s) : Ms. PALLINI, Annalisa (University of Modena and Reggio Emilia, DSCG)

Co-author(s) : Mr. PEDONE, Alfonso (University of Modena and Reggio Emilia, DSCG); Mr. TALIRZ, Leopold (SCHOTT AG); Mr. MANNSTADT, Wolfgang (SCHOTT AG)

Presenter(s) : Ms. PALLINI, Annalisa (University of Modena and Reggio Emilia, DSCG)