Département Mécanique et Verres
Institut de Physique de Rennes – Université de Rennes, CNRS

Research project (Master's thesis)

2025-2026

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Exploring the fracture and corrosion of glass-ceramics using molecular dynamics simulations

Controlled crystallization of certain glasses leads to structured materials, designated glass-ceramics (GC), which consist of nano or microcrystals dispersed in a residual glass matrix. GC take advantage of beneficial ceramic and glass properties and have numerous applications to our daily lives, e.g., cookware, bone and dental implants, architecture, cell phone displays, etc. [2, 3]. In literature today, GC datasets concerning physical, mechanical, and fracture properties remain disjointed revealing only a handful of properties on a single GC sample. Furthermore, the susceptibility of glass-ceramics to stress corrosion cracking has been scarcely studied. This phenomenon is highly dependent on the relative humidity and temperature [4], and on material parameters (chemical composition [5] and microstructure [6], herein structure and length scale associated with crystal phases) and can severely restrict GC´s uses due to slow crack propagation leading to the failure of the GC under (apparently) harmless stresses.

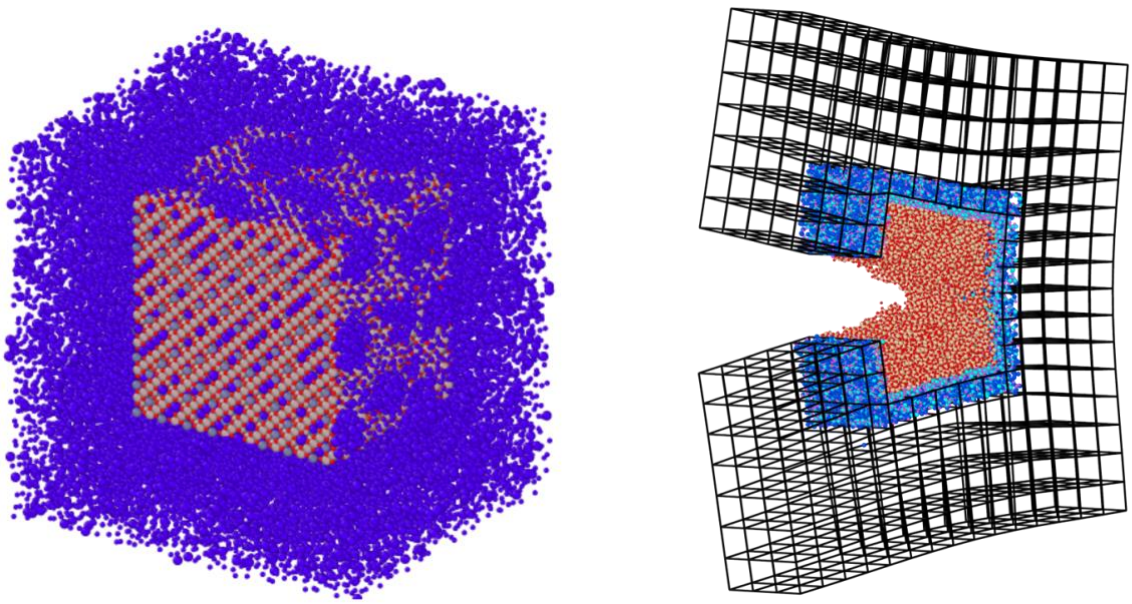

Figure: (a) Molecular model of Zn, Al, Si glass-ceramics featuring a cubic crystalline phase. (b) Mode I fracture crack propagation simulation in silica glass using the CAPRICCIO method [9].

Our long-term goal is to establish the link between the microstructure and the so-called stress corrosion cracking mechanism in glass-ceramics. In general, the stress corrosion cracking behaviour can be modelled by Wiederhorn's formalism [4,7]. In 2020, Grutzik et al. [8] extended Wiederhorn's formulation proposing a single equation to model the crack front velocity in a glass, where the velocity depends on the fracture toughness. The equation is constituting on a parameter set, which also includes the activation energies and characteristic length

scales for both dry and wet environments and the temperature and relative humidity dependencies along with a few macroscopic parameters (Young's modulus, density, etc.). Most of these parameters are from trivial to determine experimentally for a single glass-ceramics microstructure and composition, therefore we want to build chemically-specific molecular models to facilitate these characterizations. We have already established a protocol to construct molecular models of glass-ceramics (see figure, left) but now the resulting structures and mechanical properties need to be validated. The mechanical properties will be probed using all-atom molecular dynamics simulations (elastic properties) and the advanced simulation technique called CAPRICCIO (fracture toughness) [9] (see figure, right). We will perform these calculations for varying glass-ceramics microstructure which will help us understand the influence of crystal phase morphology on the structural and mechanical properties of the resulting glass-ceramics.

The internship will take place in the *Département Mécanique et Verres* of the *Institut de Physique de Rennes*. The department has an original and transdisciplinary position which lies at the crossroads of mechanics, physics and chemistry. Innovative experimentation (from synthesis to testing) coupled with computer simulation have made it possible to develop a recognized research activity on the mechanical behaviour of amorphous materials. The internship is part of a larger ANR-funded project offering a PhD fellowship and involving stress corrosion cracking experts from CEA Saclay (Laure Chomat, Cindy Rountree, Daniel Bonamy) and glass-ceramics synthesis and characterization experts from Universidade Federal de São Carlos in Brazil (Edgar Zanotto, Vinicius Sciuti, Rodrigo Canto).

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[4] Wiederhorn, S. M. Influence of water vapor on crack propagation in soda-lime glass. J. Am. Ceram. Soc., 50(8):407, 1967.
[5] Rountree, C. L. Recent progress to understand stress corrosion cracking in sodium borosilicate glasses: Linking the chemical composition to structural, physical and fracture properties. J. Phys. D: Appl. Phys, 50:34, 2017.
[6] Feng, W. Stress Corrosion Cracking of Sodium Borosilicate Amorphous Phase Separated Glasses. Phd thesis, Université Paris-Saclay, 2022.
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[8] Grutzik, S. J., Strong, K. T., & Rimsza, J. M. Kinetic model for prediction of subcritical crack growth, crack tip relaxation, and static fatigue threshold in silicate glass. J. Non-Cryst. Solids, 16:100134, 2022.
[9] Weber, F., Vassaux, M., Laubert, L., & Pfaller, S. The Capriccio method as a versatile tool for quantifying the fracture properties of glassy materials under complex loading conditions with chemical specificity. arXiv:2501.16537 (preprint), 2025.

Methods (training provided): LAMMPS, molecular dynamics, high-performance computing, CAPRICCIO.

Preferred skills: materials science, statistical physics, physical chemistry, computational methods.

The subject allows a candidate with one of the skills listed to learn about the other skills, as well as to express himself and develop the subject in one of the directions envisaged.

Compensation: approximately 600€/month

Possibility to pursue a PhD thesis: yes