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

Research project (Master's thesis)

2023-2024

Institute : Mechanics and Glasses Department (Direct. Yann Gueguen), Institut de Physique de Rennes, UR, CNRS, UMR 6251
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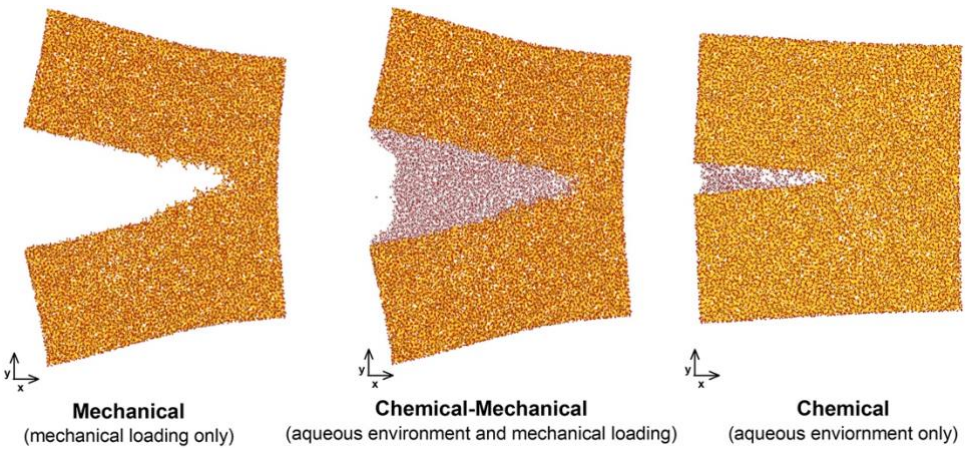
Can we reinforce inorganic glasses using water?

Although studied for decades, glass ageing remains an open question. Whether it's a question of their failure under mechanical loading exceeding their mechanical strength, or of their limited durability induced by their reactivity in an aggressive chemical environment, the complex mechanisms at the origin of glass ageing are not fully understood [1] and could reveal some surprises. These mechanisms are crucial to a wide range of industrial applications, from the design of structural glasses for the building industry to the synthesis of biomaterials for tissue engineering. It is therefore essential to explore the interactions between glass and water at the finest scales!

The aim of the project is to establish a reliable tool for the numerical simulation of glass with atomic resolution. The tool should enable us to generate a glass structure with an adaptable chemical composition (silica, borosilicate, metallic, bioglass, etc.) and then hydrate it. Based on this tool, we will attempt to predict the evolution of glass mechanical properties under mechanical loading. The simulation tool will be based on existing tools: (i) reliable interatomic potentials obtained at the quantum scale to establish interactions between atoms, and (ii) an optimized molecular dynamics simulator (LAMMPS). The simulation tool will be verified and validated against experimental results produced at the Institute, before being documented and published (github). Once the tool has been established, parallelized simulations of cracking under mechanical loading will be carried out on high-performance computers. The simulations' data will enable to investigate situations where water could actually reinforce glasses mechanical properties.

Figure : Simulation of the evolution of the atomic structure of a silica glass under loading: (left) mechanical, (center) mechano-chemical, (right) chemical. Mechanical loading is traction along y, and chemical loading is contact with an electrolyte solution.



[1] Rimsza, Jessica M., Reese E. Jones, and Louise J. Criscenti. "Chemical effects on subcritical fracture in silica from molecular dynamics simulations." Journal of Geophysical Research: Solid Earth 123.11 (2018): 9341-9354.

Methods: LAMMPS, molecular dynamics, high-performance computing.

Preferred skills : materials science, physics, chemistry, mechanics, numerical 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 continue as a PhD student : yes
Funding mechanism : Contrat Doctoral Ordinaire (CDO) at l'Université Rennes