Atomistic Simulations of the Mechanical Properties of Silicate Glasses, and of their Interaction with Water

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Abstract:

Being able to understand, at the atomic scale, such fundamental processes as corrosion, dissolution and wetting, on the one hand, and ion and water diffusion on the other, requires a reliable description of the atomic structure of the material, in this specific instance, silicate glasses. Computer simulations have been shown to be capable of providing such a reliable picture and can now be used to calculate, or predict, such physical properties as the elastic moduli, which are derived from the atomic structure. We will present some data in support of this statement.

We will also show how the molecular dynamics simulations can be used to follow structural changes occurring during uniaxial tension, to fracture, in “perfect” glasses.

Molecular dynamics has been used for some time to follow the diffusion of ions in solids including glasses. For this particular workshop, the transport of both ions which constitute the structure, such as alkali ions, and water are of particular interest.

In this presentation, we will present some results on the interaction of water with glass surfaces, using both classical and quantum mechanical simulations. This will include a description of some of the principal features of the surface structure, and of some molecular water dissolution processes. As we will show, a key conclusion is that the chemisorption of water is likely to be an activated process (i.e. subject to an energy barrier), particularly when disruption of the ring structure in the glass, through breaking an Si – O – Si bond, is concerned.

Questions to be answered:

1.) What will be a topic stating an exceptional success to be published in a well known high ranking Research Journal in 2025 concerning your presented R&D field of work? Please think in headlines.

Virtual Reality visualisation of crack propagation seen from a water molecule at the crack tip

2.) Please name up to 10 future key challenges (till 2025) regarding your presented field of expertise and indicate please the specific year when you expect the topic to become a real bottleneck for the future developments.
Text…

Being able to model, atomistically, sufficiently large sub-surface, or near surface, structural regions.

The ability to model the dissociation of water in a classical simulation of silicate glasses is a bottleneck now.

Calculation of Weibull plots from atomistic simulations of glass fibers (2025)

3.)Concerning the topics, what would be

a) the key breakthrough and when is it likely to occur

b) what must happen concerning the research field if this topic will never be successful

Improved accuracy of classical interatomic potential models

Accurate dissociative models of water must become available

The ability to perform routine classical atomistic simulations of 100,000 atoms or more

The ability to perform routine quantum mechanical simulations on thousands of atoms routinely