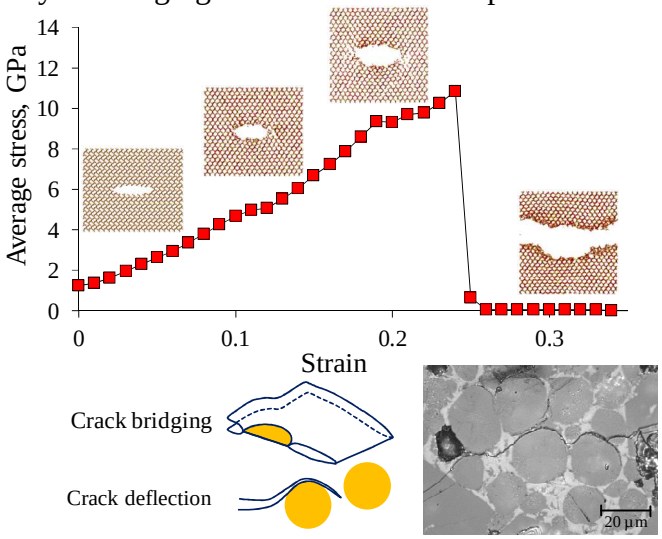
When fracture stems from the atoms

Problem

From an engineering perspective, predicting and controlling fracture properties offer new opportunities to improve concrete structures' reliability and clinker's / raw materials' grinding. At the atomic scale, crack propagation results of complex atomic rearrangements at the crack tip whereas, at the macroscopic scale, one refers to the simplified notions of toughness and ductility. A fine understanding requires an approach at the atomic scale which can capture in detail the role of chemistry and nanotexture. Material heterogeneity of cement and concrete is an additional complexity. An approach at the atomic scale can capture the fracture properties of the elementary constituents and their interface which would be very challenging with conventional experiments.



Top: Strain-stress curve during the propagation of a crack in a silica crystal loaded in mode I. Bottom left: some of the mechanisms involved in the upscaling of fracture properties. Bottom right: example of deflected cracks around belite grains in clinker (courtesy of William Wilson)

Approach

In principle, crack propagation which involves bond breaking / formation can be captured by quantum mechanics only. But, the recent developments of reactive force fields enable us to simulate crack propagation by molecular dynamics techniques. We develop a methodology to estimate fracture properties: we propagate cracks in mode I at the nano-scale by stretching the system, and we use a thermodynamic integration, valid for any material behavior, to derive the fracture properties of bulk materials and their interfaces. We can then upscale the fracture properties at the macroscale by considering different scenarios of fracture of the heterogeneous system: crack front roughening, crack deflection, crack bridging…

Findings

The thermodynamic integration is applied to a brittle material, a silica crystal, for which the classical theory of Linear Elastic Fracture Mechanics (LEFM) is valid. The behavior of this silica crystal should be similar to that of other crystal oxides like alite and belite. The results are consistent with estimations from LEFM and with experimental data. The approach is applied to a polymeric carbon matrix and to its interface with silica. Those systems exhibit a quite ductile behavior which could not be captured by LEFM. At the macroscale, a heterogeneous medium made of the silica matrix with small organic inclusion can have a macroscopic toughness between 1.1 and 3 times the toughness of the silica, depending on the upscaling scenario.

Impact

We propose a new approach to study the fracture properties by molecular simulation valid for both brittle and ductile materials. This research highlights the possibility to understand and engineer the fracture resistance starting from the smallest scale. For instance, it suggests that a binder-mineral interface with high ductility and a significant stiffness contrast may improve significantly the fracture resistance of concrete.

More

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