A Bottom-up Phase-field Approach for Fracture Based on All-atom Simulations

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ABSTRACT

Molecular dynamics (MD) simulations allow studying dynamic events on an atomic level, where events take place in femtoseconds. This technique is based on the numerical solution of Newton's equations of motion and can be effectively used for investigating structural and mechanical properties of macromolecules (see e.g. our previous works, Patil et al. (2014) [1] and Patil et al. (2016) [3]). Thus, using all-atom simulations it is possible to shed light into the enigmatic mechanisms of damage, degradation and fracture. However, the size and time limitations often hinders the application of MD to real-scale problems. On the other hand, mean-field and continuum approaches, such as phase-field models (PFM) for fracture, significantly extend the length and time scales of the considered problem, yet waiving atomic details by mainly focusing on the macroscopic response based on a phenomenological material description.

Here, we bridge this gap by proposing a novel combined approach for fracture of highly brittle materials (Patil et al. (2016) [3]), which provides an efficient and accurate in-sight understanding of multiscale fracture mechanics. In particular, based on MD simulations of a fracturing material, a number of macroscopic constitutive parameters, such as the gradient coefficient associated with the diffusive crack width, the crack resistance and the elasticity modulus, are estimated. Thus, in this combined approach, the results of all-atom simulations provide a more realistic meaning and physical estimation of the phenomenological PFM parameters.

In summary, the proposed computational approach, not requiring any empirical parameters, contributes towards an improved understanding of fracture mechanics on all length scales. Hence, our approach facilitates the optimal design of materials with tailored fracture properties, but may also be applied for the multiscale modeling of any hierarchically structured nano-material.

REFERENCES

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