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Invited Paper

Insights into Fracture and Fatigue from Machine-Learning Force Fields based Atomistic Simulations

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ABSTRACT

Atomistic simulations can elucidate the effects of chemistry and atomic-scale structures of materials on their mechanical behaviors at large scales. To this end, empirical force fields offer a convenient way to model the interatomic interactions at low cost. However, empirical potential functions face challenges in exploring mechanical processes where the non-equilibrium nature becomes important or an electronic-structure level description of bonding is necessary. In this talk, we will present our recent efforts to develop machine learning force fields for problems of fracture and fatigue. Molecular dynamics simulations using force fields trained from first-principles calculations show that the non-equilibrium nature of fracture controls crack propagation, and the energy densities of edges in equilibrium fail to quantify the fracture resistance. Instead, edge energy densities in the intermediate, unrelaxed states offer a reasonable measure for the fracture toughness and its anisotropy. The first-principles derived force fields can also capture the chemistry of bonding in metallic alloys that is usually not well modeled in empirical force fields, which explain the dependence of plasticity and fatigue resistance of single crystals on the lattice and bonding characteristics.

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