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FIRST-PRINCIPLE BASED ATOMISTIC CALCULATIONS AND MESOSCALE MODELING TO INVESTIGATE MATERIAL FAILURE

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ABSTRACT

Capturing the physics of material fracture at multiple scales is a vital component of Integrated Computational Materials Engineering (ICME), an emerging, physics-based approach to investigate material behaviour [1]. While methods are available for modelling at scales from atoms to structural parts, the intrinsic deficiency of atomic level simulation for complex dislocation patterns and inaccurate description of arbitrary crack paths via classical continuum mechanics based modeling as well as its dependency on empirical fitting of material properties from experimentations, makes such methods prohibitive to problems characterized by complex fragmentations or the cases where cracking interweaves with the evolution of material microstructure/properties.

In this work, we present our effort to integrate quantum mechanics (QM) and peridynamics (PD) to develop a coupled approach for better understanding of crack growth in complex materials. The QM-based first-principle calculations are carried out within the formulation of the density functional theory (DFT) to explore chemical composition effects on the material properties otherwise impossible to be investigated with experimental means [2]. The material properties from first-principle calculations are passed into mesoscale models to simulate the material fracture propagation. The mesoscale simulations are performed via the PD framework, a nonlocal theory of mechanics that uses displacements instead of displacement derivatives in its formulation and allows description of discontinuities in materials [3,4]. With the validation of experimental fracture testing [5], we show that our approach is capable of capturing the bondline failure of co-cured composite-metal hybrid materials and the sensitization induced cracking in 5XXXX series Aluminum (Al) alloys, suggesting the efficiency of the developed approach for investigating material fracture with arbitrary cracking paths and complex patterns.

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