

Physical Modeling of Fracture Mechanics in Complex Materials

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The mechanical behaviour of brittle materials is very sensitive to microstructure defects, like point or extended lattice imperfections, elastic inclusions, voids. Since the local stress conditions (i.e. the conditions nearby a defect) may largely differ from their average values, the prediction of the overall mechanical response to external loads results to be a tough theoretical problem. This is, for instance, the case of the stress threshold at which a microcrack starts propagating, or the interaction features between a defect and an incoming crack. In this work, we investigate at the proper nanoscale the interaction between a crack tip and elastic inclusions by combining a hierarchy of different computational tools, namely atomistic simulations (carried out at the molecular dynamics level) and statistical mechanics models (based on replica-symmetry breaking). The investigated material is silicon carbide, i.e. the prototypical example of brittle material with directional and covalent bonding.

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