

DEFECTS IN CRYSTALLINE SOLIDS: MANIFESTATION OF QUANTUM MECHANICS AT CONTINUUM SCALES

Kaushik Bhattacharya

**Department of Mechanical and Civil Engineering, California Institute of Technology, Pasadena,
USA**

E-mail: bhatta@caltech.edu

Defects such as vacancies, impurities, dislocations and grain boundaries have a profound effect on materials properties of solids even at dilute concentrations. This is because defects intimately couple quantum chemistry, atomistic physics and continuum mechanics. Thus a predictive understanding of the role of defects in determining macroscopic properties requires the resolution of quantum mechanics at macroscopic scales. This talk will describe the need for such modeling, the opportunities it offers, the challenges it poses, the state-of-the-art, and conclude with some new promising approaches.

Keywords: Defects; Multi-scale modeling;