Computational Methods for Crystalline Defects: Construction, Analysis, and Benchmarking

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Venue: MAS Executive Classroom 2, MAS-03-07
School of Physical and Mathematical Sciences

Abstract

Defects, defined as irregularities in the periodic arrangement of atoms, determine many important properties of crystalline materials, such as plasticity or failure. Computing defects is often challenging, as the spatial and temporal scales accessible for direct molecular simulations are limited.

My talk will be devoted to efficient methods for computing crystalline defects. I will focus on atomistic-to-continuum (AtC) coupling, a popular approach utilizing atomistic resolution near the defect core while using the continuum model to resolve the elastic far-field. In my talk I will

(1) give a brief introduction to crystalline defects and AtC coupling,
(2) report one of the recent developments in construction of a consistent energy-based AtC coupling method, and
(3) present a theory of how to optimize and compare the performance of existing methods.

Speaker

Alexander Shapeev is a postdoctoral associate in the Department of Mathematics in the University of Minnesota. He obtained his PhD degree from the National University of Singapore.

His research interests lie in applying numerical analysis to materials defect computation (such as dislocations or cracks), or more generally in applying computational mathematics to materials science. He is an author of 11 peer-reviewed papers, one of which has been awarded the 2013 SIAM Outstanding Paper Prize.

Host: Associate Professor Wang Huaxiong, Head of MAS, School of Physical and Mathematical Sciences