Dynamics of Material Interfaces

Rohan Abeyaratne
Massachusetts Institute of Technology
Cambridge, MA 02139, USA
&
MIT-Singapore Alliance for Research and Technology (SMART)
Singapore 117543

Abstract

This talk will provide an overview of a series of investigations on the dynamics of a twin or phase boundary beginning at the atomistic scale and leading eventually to the continuum scale.

The underlying mathematics is related to the motion of “shocks” in genuinely nonlinear systems of conservation laws and the so-called “generalized entropy condition”. In a more physics-based characterization this condition is a continuum-scale manifestation of the lattice-scale dynamical processes known as the “kinetic relation”.

First we will describe a molecular dynamic study of interface motion from which we obtain the relationship between the propagation speed of the interface and the driving force on it. This study also identifies “ledge propagation” as the underlying physical mechanism by which the interface propagates.

Based on this atomic-scale observation, we next construct and analyze a mathematical model of ledge motion and use it to derive a relationship between the speed of ledge propagation and the driving force. The resulting relationship, the ``kinetic law'', can be exported to the continuum theory for use there. The kinetic law derived from the model will be compared with the atomistic predictions as well as with various experimental observations.

Several other discrete and continuum models of interface motion based on, for example, a nonlinear lattice chain and peridynamic theory, will be discussed as time permits.