Modeling the Motion of Material Interfaces

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

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, which in this case is the remote shear stress on the specimen. This study also identifies “ledge propagation” as the underlying mechanism by which the interface propagates.

Based on this observation from the atomistic study, we next construct and analyze a mathematical model of ledge motion and use it to derive a relationship between 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 also be discussed.