Atomistic Finite Element Models of Deformation and Fracture at Nanoscales

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Atomistic finite element (AtFE) models with finite element constitutive relations derived from atomistic force laws are developed to address a number of problems of interest to deformation and fracture at nanometer scales. These models are becoming important in modern materials technology such as heteroepitaxial thin films in which extraordinarily large elastic strains occur due to lattice mismatch. The lattice mismatch strains are large compared with strains in common engineering structures and are often further magnified at stress concentration sites such as an island edge and a cusp like surface valley along the film surface. The technological developments are also stimulating the advance of fracture mechanics toward a better understanding of deformation at distances of only a few atomic spacings near a crack tip. AtFE techniques provide a useful approach for these applications. We discuss a few applications of AtFE including formation of dislocation-like defects at an island edge and a cusp like surface valley during growth and anealing of a heteroepitaxial film. The method is also used to study the effects of nonlinear lattice deformation on crack branching and roughening during dynamic fracture.