AN ATOMIC LEVEL MATERIAL STABILITY THEORY – FAILURE ANALYSIS OF NANOSTRUCTURES

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Local elastic instability of crystal lattices is a source of defect nucleation and material failure. The stability analysis of an initially pristine lattice is a well-developed subject, on which many approaches and results have been reported. However, there is no unified approach for detecting the local instability in a non-homogeneous atomic system.

In this paper, we develop an atomic level material stability theory which is the atomic counterpart of the material stability theory in continuum elasticity for atomic structures. We define the "atomic acoustic tensor" as an indicator in the stability criterion to detect material failure at the atomic level. The atomic material stability criterion is based directly on the atomic energetic response, in particular the non-convexity of which is the counterpart of the non-elliptic constitutive behavior in continuum elasticity. The theory does not resort to continuum homogenization and does not require the lattice to be pristine. Thus, we expect it to be applicable in defective nanoscale structures provided that the atomic energy can be reasonably defined. In addition, the criterion can be easily implemented in the framework of molecular dynamics/mechanics.

To test for validity, we have applied this stability theory to defective simple crystals and found that the atomic acoustic tensor can be used to characterize the instability modes of the defective region. We have also performed local instability analysis on the initially defective carbon nanotubes. The tensile limits predicted by this theory are in good agreement with those reported in the literature.

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