Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Studies of elastic and plastic deformation of nanostructured materials: A continuum approach MIKKO HAATAJA, Princeton University, PETER STEFANOVIC, McMaster University, NIKOLAS PROVATAS, McMaster University — Nanostructured materials can have physical and mechanical properties that are strikingly different from their corresponding bulk counterparts. Consequently, unraveling the physical mechanisms that give rise to their behavior at the atomic scale is essential in order to exploit and harness their unique properties. From a theoretical perspective, capturing dynamic phenomena across very long time scales with direct atomistic simulation methods (e.g., Molecular Dynamics [MD]) becomes a very challenging task due to inherent time scale limitations. Here we present a continuum field theory approach for modeling both elastic and plastic deformations, free surfaces, and multiple crystal orientations in systems with both hexagonal and cubic symmetry in two spatial dimensions. The model is based on a free energy for the local, temporally coarse-grained atomic density, which is minimized by spatially periodic structures. Hence, it incorporates, by construction, both elastic phenomena as well as defects in the form of, e.g., vacancies, dislocations, and grain boundaries. Furthermore, its dynamics is constructed such that it incorporates both diffusive and elastic relaxation phenomena. By introducing a variable elastic time scale, we are able to maintain mechanical equilibrium while simulating microstructural evolution on time scales well beyond those accessible by conventional atomistic MD simulation methods.

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Date submitted: 30 Nov 2005 Electronic form version 1.4