Nonlocal Continuum Modeling of Crystalline Plasticity

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Ongoing efforts devoted to the development of physics-based nonlocal models of crystalline plasticity are discussed with respect to modeling the mechanical response of copper-niobium (Cu-Nb) lamellar nanocomposites. Two different modeling strategies are put forward, and results demonstrating the scale-dependent mechanical behavior of an idealized polycrystalline material are presented. The results indicate a "smaller is stronger" trend and offer promise that these methods can be successfully adapted to model the Cu-Nb lamellar composite material system.

The limitations of classical (local) continuum modeling approaches under certain conditions have been established for quite some time now. For example, there are pathological mesh sensitivity issues that arise when material softening and/or geometric constraints lead to strain localization and models are unable to predict the size-dependent mechanical behavior that is often observed in submicron-sized material systems. These shortcomings of local continuum models are the direct consequence of the scale invariance of the governing equations, that is, fundamental length-scale parameters are absent. Several methods of incorporating nonlocality into continuum models have been proposed and pursued to various extents in an effort to address these limitations. Nonlocal continuum modeling approaches may be broadly classified into three major categories: 1) integral formulations (strongly nonlocal), 2) gradient formulations (weakly nonlocal), and 3) multiphysics formulations. In the present work, we are developing both gradient and multiphysics models for crystalline plasticity.

The primary application of interest for our model development efforts is the simulation of the synthesis and mechanical response of bimetallic lamellar nanocomposites. The initial material system being studied is a copper-niobium (Cu-Nb) composite that has been a material of interest at LANL for the past 10 to 15 years [1]. The earlier studies were conducted on composites that were synthesized using physical vapor deposition (PVD), whereas current efforts are focused on samples that are produced using an accumulative roll-bonding (ARB) technique [2]. By employing the ARB manufacturing process, larger sample sizes can be produced and layer thicknesses ranging from 10 nm to several microns can be achieved with relative ease, thereby enabling the study of the overall deformation response of the composite as a function of layer thickness. As the layer thickness is refined below the submicron level, this material system exhibits elevated strength and radiation damage resistance as compared to composites with larger layer thicknesses. We hypothesize that the transition in deformation modes is inherently related to the Cu-Nb interfaces and their increased participation in the overall inelastic deformation of the composite as the layer thickness is reduced. For larger layer thicknesses, dislocation motion in the bulk dominates the total material response; however, as the layer thickness is refined, the ability of the interfaces to absorb, transmit, and block dislocations plays the dominate role. The underlying physics of dislocation interactions at the bimaterial interfaces, while different, is analogous to what transpires at grain boundaries in polycrystalline metals. The most physical and accurate way to model these processes is through the development of a multiphysics type of nonlocal model that couples standard continuum crystal plasticity theory with an additional conservation equation governing dislocation transport. The length scales that enter this model formulation are directly related to the dislocation transport. The development of the coupled plasticity/dislocation transport model capable of describing the complex dislocation-interface interactions in the Cu-Nb lamellar composites is a work-in-progress.

Ongoing research is also working to extend current nonlocal modeling capabilities by adapting them to the application of interest. In this vein, a nonlocal crystal plasticity model that treats lattice curvature (a second gradient of deformation) in addition to the lattice strain as a fundamental deformation measure and constitutive response variable is being tailored to model the Cu-Nb composite material system. This type of weakly nonlocal model is a more coarse-grained description as compared to the dislocation transport model and is more computationally efficient,

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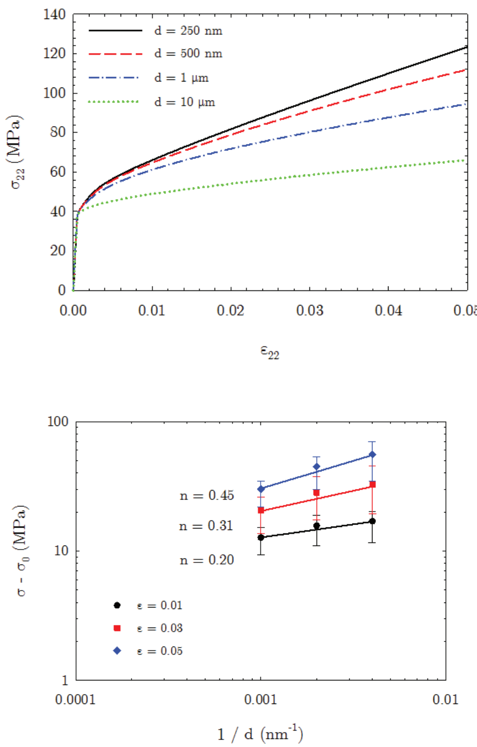

Fig. 1. (a) Nominal stress-stress curves for an SVE. (b) Scaling of nominal stress as a function of grain size for various levels of applied strain.

but makes some sacrifices with regard to its true predictive capabilities. The importance of accounting for the effects of lattice curvature and geometrically necessary dislocations (GND) on the mechanical response of small scale material systems has long been established [3], and there are many different approaches for capturing these effects. The grain size-dependence of the stress-strain response of an idealized polycrystalline material is investigated to demonstrate the capabilities of our approach. Small statistical volume elements (SVE) containing 30 randomly oriented grains are subjected to remote uniaxial loading under plane strain conditions. Periodic boundary conditions have been employed within the plane. The grains are modeled as regular hexagons and four different grain sizes are considered, d = 250 nm, 500 nm, 1 mm, and 10 mm. The nominal stress-strain curves for the four different grain sizes are given in Fig. 1a for one of the SVEs considered; Fig. 1b shows the scaling of the flow stress with the inverse grain size at different levels of applied far-field strain. The expected “smaller is stronger” type of behavior is predicted by the model, and the scaling exponents of the flow stress are observed to increase with deformation. The scaling exponents range from n = 0.2–0.45 for the range of applied strains considered, and are within reasonable proximity of the traditional Hall-Petch flow stress scaling exponent of n = 0.5. In Fig. 2, the magnitude of the GND density is plotted for two different grain sizes and we observe that the intensity of the GND fields increase with diminishing grain size and are concentrated within the grain boundaries. This is exactly the response characteristics that would be expected based on prior experimental and analytical results, and also on the fact that lattice curvature (GNDs) is most pronounced at grain boundaries. These results capture the correct trends in scale-dependent mechanical response and offer promise that these methods can be successfully adapted to model the Cu-Nb lamellar composites.

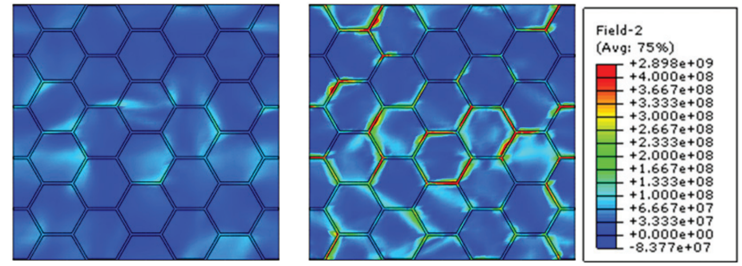

Fig. 2. Contours of geometrically necessary dislocation density in units of mm-2 (left) d = 10 mm (right) d = 250 nm.

[1] Misra, A. et al., *Scripta Mater* **39,** 555 (1998).
[2] Mara, N. et al., *Scripta Mater* **50,** 803 (2004).
[3] Ashby, M.F., *Phil Mag 21,* **399** (1970).

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