Grain-size dependent elastic properties of bulk nanocrystalline materials

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We present results from a numerical study of the elastic properties of bulk nanocrystalline materials based on a continuum model introduced by Fried and Gurtin [1]. For nanoscale polycrystalline elasticity, the model generates a balance equation that captures length-scale effects via gradient terms and accounts for interactions across grain boundaries via interface and junction conditions. To explore the properties and utility of the model, we developed an efficient non-conforming finite-element method (Kim et al. [2]). We implemented a variational formulation of the method that weakly enforces continuity of derivatives of the displacement field across interelement boundaries and achieves stabilization via Nitsche's method.

Based on the method, numerical studies were performed for a polycrystal subject to an uniaxial deformation. The distribution of the effective stress shows that the model captures high strain gradients near grain boundaries and triple junctions. We considered the influence of the grain-size and the gradient length scale which represents nanoscale effects. With increasing the gradient length scale and decreasing grain-size, the effective Young's modulus decreases and the effective Poisson's ratio increases. This occurs because the length-scale effects and interactions across grain boundaries become significant with increasing the gradient length scale and decreasing grain-size. Importantly, as the gradient length scale approaches to zero, the effective elastic modulus and the effective Poisson's ratio reduce to values consistent with those of conventional grain-sized polycrystal. Numerical results are compared with data for nanocrystalline copper. Our findings indicate a reduction of the effective elastic modulus for nanocrystalline copper of approximately 5%, which compares favorably with experimental results.

References

[1] E. Fried and M.E. Gurtin, Gradient nanoscale polycrystalline elasticity: intergrain interactions and triple-junction conditions, *Journal of the Mechanics and Physics of Solids* **57** (2009), 1749–1779.

[2] T.-Y. Kim, J.E. Dolbow, and E. Fried, Numerical study of the grain-size dependent Young's modulus and Poisson's ratio of bulk nanocrystalline materials, *International Journal of Solids and Structures* **49** (2012), 3942–3952.