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Cloud computing in nanoHUB powering education and research

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ABSTRACT

We present a tool that uses a phase field approach to simulate plastic deformation in nanocrystalline materials. It captures the competing grain-boundary and dislocation-mediated deformation mechanisms that govern plastic deformation in these materials. The model is based on a multiphase field approach in which dislocations and grain boundary sliding are represented by means of scalar phase fields described in “The role of grain boundary energetics on the maximum strength of nanocrystalline Ni”, Koslowski, Lee and Lei, *Journal of the Mechanics and Physics of Solids*, 59 1427–1436, 2011. The tool enables users to quantify how uncertainties in the input parameters (materials properties such as elastic constants, Peierls energy barrier for dislocation glide, and activation barrier for grain boundary sliding) affect the prediction of the yield stress. In addition, it provides a sensitivity analysis that quantifies the relative importance of each input variable. In order to achieve this, the phase field simulation code is orchestrated by the PRISM Uncertainty Quantification tool that enables users to select various state-of-the-art methods for uncertainty propagation.