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Quantum Mechanical Simulations of Nanoindentation of Al Thin Film with Mg imurities QING PENG, XU ZHANG, CHEN HUANG, Department of Physics and Astronomy, California State University Northridge, Northridge, CA, USA, EMILY A. CARTER, GANG LU — QCDFT is a multiscale modeling approach that can simulate multi-million atoms effectively via density functional theory (DFT). The method is based on the framework of quasicontinuum (QC) approach with DFT as its sole energetics formulation. The local QC energy is calculated by DFT with Cauchy-Born hypothesis. The nonlocal QC part is treated by a self-consistent embedding approach, which couples DFT nonlocal atoms to the vertices of finite-elements at the local QC region. The QCDFT method is applied to a nanoindentation study of an Al thin film in the presence and absence of Mg impurities, as well as the cluster of the impurities. The results show that the randomly distributed Mg impurities can significantly increase the ideal and yield strength of the Al thin film, while the Mg impurities clustered in tension field will reduce the yield strength of the Al thin film.

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