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Dislocation nucleation in Au nanowires with stress gradients

The dislocation nucleation in face-centered cubic (fcc) defect-scarce Au nanowires (NWs) is a sequence of Shockley partial dislocation nucleation at free surfaces of the facetted nanowires, which is considered as the deformation mechanisms at the onset of plasticity. The yield stresses from MD simulations are usually severely overestimated compared to the experimentally measured stresses. But simple incorporation of the geometrical flaws (e.g. notches) in NWs, the MD flow stresses are comparable to the experimental flow stresses of notched NWs.

In view of notch-effect in Au NWs, the stress gradient will be considered as another parameter in dislocation nucleation by means of a nanohole in the initial NW structure. The resulting MD behavior is evaluated in term of the dislocation nucleation models and their size, strain rate, stress and temperature dependence for artificial Au-NWs with different EAM potentials.

Abstract (optional)

The dislocation nucleation in face-centered cubic (fcc) defect-scarce Au nanowires (NWs) is a sequence of Shockley partial dislocation nucleation at free surfaces of the facetted nanowires, which is considered as the deformation mechanisms at the onset of plasticity. The yield stresses from MD simulations are usually severely overestimated compared to the experimentally measured stresses, which is ascribed to the stress, strain rate and temperature dependence predicted by the classical nucleation theory(CNT) in the line tension model for dislocation nucleation. But simple incorporation of the geometrical flaws (e.g. notches) in NWs, the MD flow stresses are comparable to the experimental flow stresses of notched NWs.

In view of notch-effect in Au NWs, the stress gradient will be considered as another parameter in dislocation nucleation in Au NWs by means of a nanohole in the initial NW structure. The effect of the nanohole size, strain-rate and temperature are evaluated for different Au embedded atom method (EAM) potentials and compared to their respective different elastic constants, theoretical shear strength, generalized-stacking fault energy density. The latter EAM materials'parameters for dislocation nucleation are evaluated and compared to dislocation nucleation in defect-free Au NWs. The resulting MD behavior is evaluated in term of the dislocation nucleation models and their strain-rate, stress and temperature dependence for artificial different Au-NWs with multiple diameters (12nm, 30nm and 50nm, respectively) by means of the different EAM potentials.

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