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Investigation of extended stacking fault emission from grain boundaries using a density functional theory -informed 3D phase field dislocation dynamics model

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ABSTRACT

As characteristic length scales shrink (<100 nm) in fcc metals, alternative deformation mechanisms not seen in bulk and course-grained material counterparts emerge. In particular in grain sizes on the order of 10s of nanometers, plasticity is mediated by the motion and interaction of partial dislocations and extended stacking faults. Typically, partial dislocations nucleate at grain boundary defects and propagate into the grain interior, leaving stacking faults behind. The extent that these faults expand before a trailing partial dislocation emits generally does not equal the equilibrium separation distance of the corresponding full dislocation. This research uses a density functional theory informed phase field dislocation dynamics model to study the effect of applied stress, 3D grain size, material stacking fault energies, and grain boundary ledge size on the stress-driven emission of leading and trailing partial dislocation from grain boundaries. Most notably, we find that there is a regime in which the stacking fault size increases with increasing grain size until saturation is reached. Furthermore, the extent that the stacking fault region can propagate into the grain has an enormous dependence on the material surface.