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Dislocation mechanisms in stressed crystals with surface effects
CHI-CHIN WU, JOSHUA CRONE, LYNN MUNDAY, Army Research Laboratory, DISCRETE DISLOCATION DYNAMICS TEAM — Understanding dislocation properties in stressed crystals is the key for important processes in materials science, including the strengthening of metals and the stress relaxation during the growth of hetero-epitaxial structures. Despite existing experimental approaches and theories, many dislocation mechanisms with surface effects still remain elusive in experiments. Even though discrete dislocation dynamics (DDD) simulations are commonly employed to study dislocations, few demonstrate sufficient computational capabilities for massive dislocations with the combined effects of surfaces and stresses. Utilizing the Army's newly developed FED3 code, a DDD computation code coupled with finite elements, this work presents several dislocation mechanisms near different types of surfaces in finite domains. Our simulation models include dislocations in a bended metallic cantilever beam, near voids in stressed metals, as well as threading and misfit dislocations in as-grown semiconductor epitaxial layers and their quantitative inter-correlations to stress relaxation and surface instability. Our studies provide not only detailed physics of individual dislocation mechanisms, but also important collective dislocation properties such as dislocation densities and strain-stress profiles and their interactions with surfaces.

Chi-Chin Wu
Army Research Laboratory

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