DISLOCATION DYNAMICS SIMULATIONS OF PLASTICITY IN THIN FILMS: DISLOCATIONS INTERSECTING FREE SURFACES

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Dislocation Dynamics (DD) simulations are an effective computational approach for studying physical mechanisms of crystal plasticity based on the collective motion of dislocations. For situations where free surfaces are important, e.g. in thin films, two methodological issues need to be effectively solved. First, image stresses caused by the presence of free surfaces must be accounted for. For this purpose, we employ a FEM code appropriately coupled to the DD model. Second, the singularity at the point of dislocation intersection with the surface must be treated with substantial care. Unlike other existing approaches that resort to a brute force treatment of the apparent singularity through very fine FEM meshes, we employ a special analytical solution to subtract the singular part of the elastic field and treat the remaining, regular field using a much coarser and, hence, more computationally expedient meshes. This enables efficient numerical simulations of dislocation behavior in thin films. Here we discuss a few preliminary applications of this new simulation methodology.