Abstract Submitted
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Homogeneous Dislocation Nucleation - role of geometrical parameters and interatomic potentials[1] AKANKSHA GARG, ASAD HASAN, CRAIG MALONEY, Carnegie Mellon University — We perform atomistic simulations of dislocation nucleation in defect free crystals in 2D and 3D during indentation with circular (2D) or spherical (3D) indenters of radius R. We study realistic interatomic potentials such as embedded atom method (EAM) potentials for Al in addition to simple pair-wise interactions such as linear springs. The dislocation embryo is localized along a line (or plane in 3D) of atoms with a lateral extent, ξ, at some depth, D, below the surface. For all potentials, in 2D, the scaled critical - load, F_c/R, and contact length, C_c/R, decrease to R independent values in the limit of large R. However, despite the R independence of F_c/R and C_c/R, ξ/R and D/R display non-trivial scaling with R. Although both the interaction potential and the orientation of lattice affect the *prefactors* in the scaling relations (e.g. crystal with springs is much harder than EAM Aluminum), all the *scaling laws* are robust. Furthermore, we show that, despite the excellent prediction for the relation between F and C, Hertzian contact theory fails to correctly predict the strain underneath the indenter. This observation gives us hope that local nucleation criteria based on appropriate local strain may capture the nontrivial scaling laws.

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