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Universal Scaling Laws for Homogeneous Dislocation Nucleation During Nanoindentation

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We perform atomistic simulations to study the mechanism of homogeneous dislocation nucleation in two dimensional (2D) hexagonal crystals during nanoindentation with a circular indenter of radius R. We study both a realistic embedded atom method (EAM) potential for Al in addition to simple pair-wise potentials: Lennard-Jones, Morse, and Hookean springs. The nucleation process is governed by the vanishing of the energy associated with a single energy eigenmode. The critical eigenmode, or dislocation embryo, is found to be localized along a line of atoms with a lateral extent, ξ , at some depth, Y^* , below the surface. For all interatomic potentials, the scaled critical load, F_c/R , and scaled critical contact length, C_c/R , decrease to R-independent values in the limit of large R. However, despite this, ξ/R and Y^*/R display non-trivial scaling with R. We show that although both the interaction potential and the orientation of the lattice affect the prefactors in the scaling relations, all the scaling laws are robust. Furthermore, we show that a stability criterion proposed by vanVliet et. al. based on the minimum eigenvalue, Λ , of the local acoustic tensor predicts the location, orientation, and polarization of the dislocation embryo with a high degree of accuracy for all potentials and crystallographic orientations. However, we also show that, for all crystallographic orientations and interaction potentials, Λ erroneously indicates instability before the true instability occurs.

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