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Meso-scale harmonic analysis of homogeneous dislocation nucleation. ASAD HASAN, CRAIG MALONEY, Carnegie Mellon University — Atomistic computer simulations are performed using empirical potentials to study the process of the nucleation of dislocations in a perfect thin-film under a smooth nano-indenter. In particular, we study the energy eigenvalue spectrum and spatial structure of the energy eigenmodes of **mesoscale** regions in the crystal on approach to nucleation. We show that: i) the local strain rate diverges along an **extended** disc-like region ii) the divergence of the strain rate is in accordance with the classical scaling expected from a saddle-node instability corresponding to a **single** reaction pathway iii) stresses and strains in the crystal are not particular large near the nucleation site at the time of nucleation iv) the stiffness of meso-scale regions provides good predictive capabilities for identifying the core of the embryonic defect and, moreover, allows one to unambiguously define a characteristic length-scale. These observations point to the shortcomings of several recent approaches and highlight the collective nature of homogeneous dislocation nucleation, while at the same time, they show how a quasi-local approach may be useful as a predictor of dislocation nucleation.

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