Abstract Submitted
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Homogeneous Dislocation Nucleation ASAD HASAN, CRAIG MALONEY, Carnegie Mellon University — We perform atomistic computer simulations to study the mechanism of homogeneous dislocation nucleation (HDN) in a 2D hexagonal crystalline film under circular indentation. The nucleation process is governed by vanishing of energy associated with a single normal mode. For fixed film thickness, L, the spatial extent, ξ, of the critical mode grows with indenter radius, R. For fixed R/L, ξ scales roughly as $\xi \sim L^{0.4}$. We perform a *mesoscale* analysis to determine the lowest energy normal mode for regions of varying radius, $r_{\rm meso}$, centered on the critical mode's core. The energy of the lowest normal mode $\lambda_{\rm meso} \to 0$ rapidly as $r_{\rm meso} \to \xi$. The lowest mode shows a spatial extent, $\xi_{\rm meso}$, which increases sublinearly for $r_{\rm meso} \leq \xi$ and saturates at $r_{\rm meso} \approx 1.5\,\xi$. We demonstrate that the $\xi_{\rm meso}/\xi$ versus $r_{\rm meso}/\xi$ curve is *universal* (independent of L or R). Hence small regions, $r_{\rm meso} \leq \xi$, *can* reveal the presence of incipient instability but give excellent estimates for the critical mode's energy and spatial extent *only* for $r_{\rm meso} \geq 1.5\,\xi$. Thus HDN is a *quasi-local* phenomenon.

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