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, \( \xi \), of the critical mode grows with indenter radius, \( R \). For fixed \( R/L \), \( \xi \) 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, \( r_{\text{meso}} \), centered on the critical mode’s core. The energy of the lowest normal mode \( \lambda_{\text{meso}} \rightarrow 0 \) rapidly as \( r_{\text{meso}} \rightarrow \xi \). The lowest mode shows a spatial extent, \( \xi_{\text{meso}} \), which increases sublinearly for \( r_{\text{meso}} \leq \xi \) and saturates at \( r_{\text{meso}} \approx 1.5 \xi \). We demonstrate that the \( \xi_{\text{meso}}/\xi \) versus \( r_{\text{meso}}/\xi \) curve is universal (independent of \( L \) or \( R \)). Hence small regions, \( r_{\text{meso}} \leq \xi \), can reveal the presence of incipient instability but give excellent estimates for the critical mode’s energy and spatial extent only for \( r_{\text{meso}} \geq 1.5 \xi \). Thus HDN is a quasi-local phenomenon.