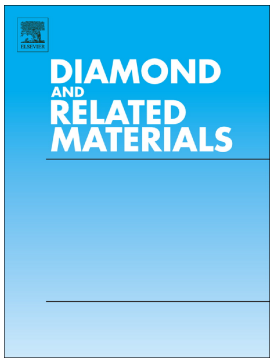

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Homogeneous and Heterogeneous Dislocation Nucleation in Diamond

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Abstract Dislocation nucleation plays a key role in plastic deformation of diamond crystal. In this paper, homogeneous and heterogeneous nucleation nature for diamond $\frac{1}{6}\langle 112\rangle$ glide set dislocation and $\frac{1}{2}\langle 110\rangle$ shuffle set dislocation is studied by combining molecular dynamics method and continuum mechanics models. Our results show that although heterogeneous dislocation nucleation can decrease its activation energy, the activation energy at 0 GPa for diamond heterogeneous nucleation is still in the range of 100 eV. For $\frac{1}{6}\langle 112\rangle$ glide set and $\frac{1}{2}\langle 110\rangle$ shuffle set homogeneous nucleation, their critical nucleation shear stress approaches to diamond's ideal shear strength which implies that those dislocations do not nucleate before diamond structural instability only by a purely shearing manner. While for $\frac{1}{6}\langle 112\rangle$ glide set and $\frac{1}{2}\langle 110\rangle$ shuffle set heterogeneous nucleation, their critical nucleation shear stresses are 28.9 GPa and 48.2 GPa, these values are less than diamond's ideal shear strength which implies that these dislocations may be nucleated heterogeneously under certain shear stress condition. In addition, our results also indicate there exists a deformation mode transformation

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