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Microscopic Mechanism of Void Nucleation at Dislocation Boundaries: A Discrete Dislocation Dynamics Simulation Study

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ABSTRACT

Void nucleation is of great significance in understanding ductile fracture of many important engineering materials. Recent experiments have shown that voids are nucleated via vacancy condensation and dislocation boundaries are the main nucleation sites. However, it is still unclear what role is played exactly by dislocation boundaries in promoting void nucleation and what kind of defect configuration is involved. Here we propose a new mechanism for dislocation boundary-induced void nucleation and develop accordingly a vacancy condensation model based on the classical nucleation theory. The model suggests that vacancy condensation to form void is impossible in the absence of external driving force and there is a nonlinear negative correlation between the activation free energy barrier for void nucleation and the local hydrostatic tensile stress. It is also shown that the relaxation of elastic strain energy of vacancies, absent in the previous void nucleation models and introduced in ours, can greatly lower the activation energy barrier and thus cannot be ignored. The kinetic feasibility of the newly proposed mechanism is examined and explored using three-dimensional discrete dislocation dynamics simulations. Our simulation results show that vacancy condensation occurs more likely near the dislocation boundary than in the dislocation cell and the synergy of *multiple* dislocation pile-ups is the key to enabling dislocation boundaries to serve as the preferential sites for void nucleation, which cannot be achieved by a single dislocation pile-up alone.

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