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Influence of different interatomic potentials in void growth, dislocations emission and temperature evolution

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ABSTRACT

We have studied the process of void growth by dislocation emission in Cu and Al under different loads using a nonequilibrium thermodynamic QC method. In addition, we have compared the results with different interatomic potentials to understand the influence of them in dislocation emission, void growth, and temperature evolution during the ductile failure of the material. We have observed that Mishin's potential predicts the formation of shear and prismatic dislocations loops due to cross slip. On the contrary, Johnson's potential predict a local change in the microstructure making a self-locking structure near the void that allows its grow only in the load direction. Because of the self-locking structure, a linear behavior of the material up to high levels of deformation is observed. Interestingly, because the different set the dislocations emitted from the void surface, the temperature evolution has also shown a different behavior for both potentials modifying the heat conduction process during the ductile failure. In fact, our simulations have shown that with the flux of material due to the dislocation emission there is a heat flux which is strongly connected to the plastic work generated in the material.