Atomistic Study of Dislocation Loop Emission from a Crack Tip

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A central issue in understanding the ductile versus brittle behavior of solids is the local response of an atomically sharp crack at critical loading. While it is widely recognized that cleavage decohesion and dislocation emission are the two major competing modes of response, atomistically accurate analysis of dislocation loop emission in the presence of a crack-tip stress field has not been carried out. We report in this work the first atomistic calculation of the saddle-point configuration and activation energy for the nucleation of a 3D dislocation loop from a stressed crack tip in single crystal Cu. The transition state is found using reaction pathway sampling schemes, the nudged elastic band and dimer methods. For the $(111)[\bar{1}10]$ crack, loaded typically at 75% of the athermal critical strain energy release rate for spontaneous dislocation nucleation, the calculated activation energy is 1.1eV, significantly higher than the continuum estimate. Implications concerning homogeneous dislocation nucleation in the presence of a crack-tip stress field are discussed [1].

References

[1] T. Zhu, J. Li and S. Yip, "Atomistic study of dislocation loop emission from a crack tip," *Physical Review Letters*, **93**, 025503, 2004.

Keywords: fracture, atomistic simulation, dislocation loop emission