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Spallation in metallic systems: Effects of microstructure, and loading pulse shape, rate and orientation[1]

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The dynamic nature of spallation and the ubiquitous presence of microstructure may give rise to significant dependences on microstructure and loading, as indicated by indirect experimental observations. We present systematic, direct molecular dynamics (MD) simulations of spallation in metallic systems represented by Cu and a CuZr glass. The "microstructure" includes various defects in Cu, porous Cu, atomic-level inhomogeneities in the CuZr glass, and the Cu crystal−CuZr glass interfaces. We explore supported and decaying shock loading pulses, as well as different loading orientations. Tensile loading rates are changed via varying the flyer and target thicknesses in shock simulations, and more significantly (down to $\sim10^6$ s^{-1}), with accelerated MD simulations of single-void growth in Cu (mimicking shock). Our direct simulations reveal strong dependences of spallation on microstructure and loading, and quantitative dynamics of void nucleation/growth as well as mechanisms for plasticity, void nucleation and their interactions in the absence or presence of defects or interfaces. The future task of incorporating statistically the microstructure effects and their rate dependences into analytic models is of great interest to shock physics but a challenge.

[1]Work done in collaboration with T.C. Germann, D. Perez, Q. An, B. Arman, W.Z. Han, D.L. Tonks, J.E. Hammerberg, A.F. Voter, Los Alamos National Laboratory; W.A. Goddard III, Caltech; and T. Cagin, Texas A&M University.