
Structural Heterogeneity in the Shock-induced Plastic Deformation Mechanism of Nanocrystalline High-Entropy Alloys

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Abstract

The grain size distribution greatly influences the macroscopic mechanical and functional characteristics of polycrystalline materials. However, comprehending the distinct characteristics of nanocrystalline metals under dynamic loading poses challenges due to stringent spatio-temporal resolution requirements. In this study, the shock response of nanocrystalline CoCrCuFeNi high-entropy alloys (HEAs) with varied sizes of both homogeneous and heterogeneous grain microstructures are systematically investigated through molecular dynamic simulations. Our findings reveal that the shock front width, Hugoniot elastic limit (HEL), and shock wave velocity all exhibit an increase with larger grain sizes. Under shock loading, the dominant plastic mechanism transitions from grain-boundary-accommodated processes to dislocation-mediated (dislocation, twin, L-C lock, and HCP phase) ones with increasing grain size, resulting in the shear strength increases with the increase in grain size. In comparison, heterogeneous structures enhance plasticity through a synergistic deformation model, efficiently distributing loads between grains of varying sizes. Additionally, it is found that the smaller grain sample performs a higher spall strength due to its higher fracture surface energy. The damage mechanism transforms from multiple nucleation of voids and individual growth to intergranular damage and void coalescence as the grain sizes increase. An energy balance fragmentation model considering void damage evolution and fracture surface energy is adopted to accurately predict the spall strength of nanocrystalline HEAs. Compared with the traditional metal Ni, HEA performs a higher HEL, spall strength, and twinning tendency due to the low stacking fault energy and pronounced lattice distortion. These atomistic insights contribute to the identification of practical applications for HEAs as structural materials in extreme loading environments.

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