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Constitutive Framework for Modeling Incipient Spall Damage in FCC Metals using Microstructurally Explicit 3D Finite Elements

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Shock loading is a complex phenomenon that can lead to failure mechanisms such as strain localization, void nucleation and growth, and eventually spall fracture. Studying spall damage on a microstructural level helps to understand the intrinsic material characteristics that lead to damage localization sites and to formulate continuum models that account for the variability of the damage process due to microstructural heterogeneity. Experimental observations in pure polycrystalline Cu indicate that damage tends to localize at grain boundaries (GB) and triple junctions [1, 2]. However, considerable amount of work still has to be done to determine the physics driving the damage at these "intrinsically weak" sites in the microstructure. The research work presented here focuses on the development of a reliable computational model to predict spall damage on a microstructural level. The development of such a constitutive model to predict damage initiation and evolution under the extreme conditions produced by shock loading requires proper understanding of the physics driving them. A crystal plasticity constitutive model [3] is implemented along with the Mie-Grüneisen Equation of State (EOS) and coupled with different damage criteria via a multiplicative decomposition of the total deformation gradient into plastic, damage and elastic components to study the effects of stress concentration and strain localization at the GBs. Prior to testing the predictive capabilities of the constitutive model, it is put through a series of verification and validation (V&V) tests. An intermediate step of calibration is added to the V&V procedure to obtain the optimal material parameters. The calibration process was done using an optimization technique based on design of experiments (DOE). The constitutive model is then verified using single elements tests and comparisons to known numerical solutions, calibrated using experimental data from single crystal impact experiments, in specimens with both planar and perturbed surfaces. The experiments with the latter type of specimens allowed to sample directly the effect of initial yield strength and hardening rate on the evolution of hydrodynamic instabilities, particularly the Richtmyer-Meshkov [4], which is shown to be affected significantly by material anisotropy and led to additional data to select and calibrate a hardening model. The resulting model is validated using different sets of single crystal and multicrystal impact experiments. The results indicate that strain localization is the predominant driving force for damage initiation and evolution at general GBs with arbitrary misorientations. The results indicate the voids tend to nucleate predominantly at triple points and evolve along the GB. The Taylor factor along the GB normal also plays an important role in the extent of damage along the GB. The finite element simulations show good qualitative as well as quantitative correlation with the experimental results and can be used as the preliminary step in developing accurate probabilistic models for damage nucleation in polycrystalline materials.

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