Two-level models of dynamic plasticity and fracture of magnesium

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Magnesium and magnesium alloys attract increasing attention as lightweight structural materials with high specific strength. Appropriate models of plasticity and fracture of such materials are necessary parts for complete the description of its behavior in addition to the equation of state. Structural models considering evolution of structural defects have obvious advantages in possibility to take into account the initial microstructure and to be valid in a substantially wide range of loading parameters including dynamical regimes with high strain rates. Higher number of parameters can be partially reduced by application of atomistic simulation for their determination as these parameters typically have clear physical meaning.

Earlier we developed structural models of plasticity and fracture of several metals using two-level approach. Here we present their modification for the case of magnesium single crystals. The plasticity model is developed to take into account the crystal anisotropy and the finite deformations. Thermodynamic consistency of the model is discussed. On the atomic level, the molecular dynamic (MD) simulations are used to determine the dislocation motion equation and corresponding parameters, as well as the temperature and pressure dependences of the elastic modules. The obtained data are used on the continuum level to close the plasticity model. The fracture model is developed to take into account the anisotropy of magnesium single crystal; it is also based on MD simulations. The models are verified by comparison with the literature experimental data for the high velocity plate impact.

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