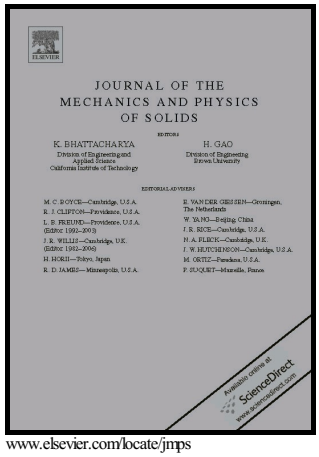

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Crystal Plasticity Finite Element Modeling of Discrete Twin Evolution in Polycrystalline Magnesium

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Abstract

This paper develops an advanced, image-based crystal plasticity finite element (CPFE) model, for predicting explicit twin formation and associated heterogeneous deformation in single crystal and polycrystalline microstructures of hexagonal close-packed or *hcp* materials, such as magnesium. Twin formation is responsible for premature failure of many *hcp* materials. The physics of nucleation, propagation and growth of explicit twins are considered in the CPFE formulation. The twin nucleation model is based on dissociation of sessile dislocations into stable twin loops, while propagation is assumed by atoms shearing on twin planes and shuffling to reduce the thermal activation energy barrier. The explicit twin evolution model however has intrinsic issues of low computational efficiency. Very fine simulation time steps with enormous computation costs are required to simulate the fast propagating twin bands and associated strain localization. To improve the computational efficiency, a multi-time scale subcycling algorithm is developed. It decomposes the computational domain into sub-domains of localized twins requiring very fine time-steps and complementary domains of relatively low resolution. Each sub-domain updates the stress and the deformation-dependent variables in different rates, followed by a coupling at the end of every coarse time step to satisfy global equilibrium. A 6-fold increase in computing speed is obtained for a polycrystalline Mg microstructure simulation in this paper. CPFE simulations of high purity Mg microstructures are compared with experiments with very good agreement in stress-strain response as well as heterogeneous twin formation with strain localization.

Keywords: Explicit Twin Evolution, Crystal Plasticity Finite Element, Magnesium,

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