Role of deformation twinning and plastic anisotropy on void growth in HCP Mg polycrystals: A crystal plasticity finite element study

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Ductile damage in HCP metals is governed by a complex interaction between plastic anisotropy, deformation twinning, and the void evolution. Despite this complexity, studies that investigate damage mechanisms in porous HCP polycrystals remain scarce. Most existing investigations based on the crystal plasticity finite element method (CPFEM) have focused on single-crystal unit cell models. For instance, void growth under plane strain conditions using cylindrical voids in 2D [1], and spherical void growth in 3D unit cells [2], both in the context of HCP Mg single crystals. Although these unit cell studies provide valuable insights into the fundamental mechanisms governing void evolution in HCP crystals, they do not capture key microstructural features of polycrystalline materials. In particular, they neglect grain-to-grain interactions, crystallographic heterogeneity, and the competition between differently oriented grains that strongly influence damage development in real polycrystals. To address this gap, the present study conducts a full-field CPFEM analysis on a RVE of porous HCP Mg polycrystal, constructed by periodically translating a cubic unit cell containing a centrally positioned spherical void along all three orthogonal directions, yielding an aggregate of multiple grains. Crystallographic orientations are independently assigned to each grain using a single realization of randomly sampled Bunge Euler angles, introducing grain-to-grain orientation variability while maintaining the overall statistical homogeneity of the polycrystalline aggregate. To ensure mechanical consistency with the periodic microstructural construction, periodic boundary conditions are imposed on all external faces of the RVE.

The constitutive framework employed in this study is a rate-dependent crystal plasticity model formulated within a Lagrangian framework, incorporating both slip and deformation twinning. Twinning-induced lattice reorientation is treated using the Probabilistic Twin Volume Consistent (PTVC) scheme [3], which ensures consistency between the evolution of the twin volume fraction and the probability of grain reorientation. The hardening formulation accounts for the interactions among deformation systems, including slip-slip, slip-twin, and twin-twin interactions, thereby capturing the anisotropic hardening behavior characteristic of HCP crystals. Within this framework, the present study systematically investigates the influence of the initial basal slip resistance, neighboring grain orientations, and stress triaxiality on void evolution in an elasto-viscoplastic porous HCP Mg polycrystal. Both local and macroscopic responses are analyzed in detail, with particular emphasis on the underlying microstructure evolution, including twinning-induced lattice reorientation and the spatial distribution of accumulated slip/twin. This analysis elucidate the roles of slip and twinning mechanisms in governing the path to ultimate failure in HCP polycrystals.

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