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Multiscale Modeling of the Structure-Property Relationship for Semicrystalline Materials

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A micromechanically-based numerical model for the elasto-viscoplastic deformation and texture evolution of semicrystalline materials is developed. A distinction between three different scales is made. The constitutive properties of the material are identified at the microscopic scale for the individual crystallographic and amorphous components. At the mesoscopic scale, an aggregate of individual phases is formed. To bridge between those scales, an elasto-viscoplastic two-phase composite inclusion model is formulated. The microscopic fields are related to the mesoscopic fields of the aggregate by a hybrid interaction law. A full micro-meso-macrolevel bridge is obtained by using an aggregate of composite inclusions in each integration point of a macroscopic finite element model. The full multiscale model is employed to study the mechanics of intraspherulitic deformation for polyethylene, to simulate the influence of a stacked lamellar microstructure on the macroscopic behavior of extruded material, and to investigate the toughening effect of the microstructure in particle-modified materials.

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