Computational and theoretical aspects of a grain-boundary model that accounts for grain misorientation and grain-boundary orientation

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The miniaturisation of mechanical components composed of crystalline material requires a continuum theory that accounts for the role of the grain boundary and for size-dependent effects. The grain-boundary model should incorporate both the misorientation in the crystal lattice between adjacent grains, and the orientation of the grain boundary relative to the crystal lattice of the adjacent grains. Classical theories of plasticity are unable to describe the well-known size-dependent response exhibited by crystalline material at the micro- and nanometer scale. Numerous extended (gradient and non-local) continuum theories of single-crystal plasticity have been presented in the last two decades to circumvent these limitations. The aim of this presentation is to summarise a recent theoretical and numerical investigation of the infinitesimal single-crystal gradient-plasticity and grain-boundary theory of Gurtin [1]. The governing equations and flow laws are recast in variational form. The associated incremental problem is formulated in minimization form and provides the basis for the subsequent finite element formulation. Various choices of the kinematic measure used to characterize the ability of the grain boundary to impede the flow of dislocations are compared. A series of three-dimensional numerical examples serve to elucidate the theory.