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A grain boundary formulation for crystal plasticity

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Abstract

A three-dimensional grain-boundary formulation for *small strains* crystal plasticity is presented for the first time. The method is developed and implemented for both single grains and polycrystalline aggregates and it is based on the use of a suitable set of boundary integral equations for modelling the individual grains, which are represented as *anisotropic* elasto-plastic domains. In the boundary integral framework, crystal plasticity is modelled resorting to an *initial strains* approach and specific aspects, related to the integration of strongly singular volume integrals in the anisotropic elasto-plastic grain-boundary equations, are discussed and suitably addressed for the first time. In the polycrystalline case, Voronoi-type micro-morphologies are discretised using robust non-structured *boundary* and *volume* meshes. A general grain-boundary incremental/iterative algorithm, embedding rate-dependent flow and hardening rules for crystal plasticity, is developed and discussed. The method has been assessed through several numerical simulations, for both single and polycrystalline aggregates, which confirm its robustness and accuracy and suggest directions for further developments. The key feature of the formulation is the expression of the micro-mechanical problem in terms of grain-boundary variables only, namely

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