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Numerical Method for Phase Field Simulation of Polycrystalline Dynamics Based on a Dislocations-Introduced Grain Boundary Model

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A multi-dimensional phase field model with built-in dislocation dynamics has been developed to model nucleation, growth, and deformation of grains in a polycrystalline system. In this model Peierls-Nabbaro's dislocation potential has been engaged to modify the order parameters that govern phase field evolution; grain boundaries are defined as piled-up dislocation-zones that are mathematically expressed as a function of the gradient of Peierls-Nabbaro potential.

The developed phase-field model has been implemented into Moving Particle Finite Element Method (MPFEM) for obtaining numerical solution. MPFEM combines a partition of unity with generalized shape functions, which presents certain advantages for the modeling and simulation of heterogeneity material system such as grain boundary decohesion-induced intergranular fracture. The corresponding 2/3D examples will be given.

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