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Indirect Intergranular Slip Transfer Modeling Through Continuum Dislocation Dynamics

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Abstract : In this study, a mesoscopic continuum dislocation dynamics (CDD) approach is applied to simulate the intergranular slip transfer. The CDD scheme applies an efficient kinematics equation to model the evolution of the "all-dislocation density," which is the line-length of dislocations of each character per unit volume. As the consideration of every dislocation line can be a limiter for the simulation of slip transfer in large scales with a large quantity of participating dislocations, a coarse-grained, extensive description of dislocations in terms of their density is utilized to resolve the effect of collective motion of dislocation lines. For dynamics closure, namely, to obtain the dislocation velocity from a velocity law involving the effective glide stress, mutual elastic interaction of dislocations is calculated using Mura's equation after singularity removal at the core of dislocation lines. The developed scheme for slip transfer can therefore resolve the effects of the elastic interaction and pile-up of dislocations, which are important physics omitted in coarser models like crystal plasticity finite element methods (CPFEMs). Also, the length and timescales of the simulationareconsiderably larger than those in molecular dynamics (MD) and discrete dislocation dynamics (DDD) models. The present work successfully simulates that, as dislocation density piles up in front of a grain boundary, the elastic stress on the other side increases, leading to dislocation nucleation and stress relaxation when the local glide stress exceeds the operation stress of dislocation sources seeded on the other side of the grain boundary. More importantly, the simulation verifiesa phenomenological misorientation factor often used by experimentalists, namely, the ease of slip transfer increases with the product of the cosines of misorientation angles of slip-plane normals and slip directions on either side of the grain boundary. Furthermore, to investigate the effects of the critical stress-intensity factor of the grain boundary, dislocation density sources are seeded at different distances from the grain boundary, and the critical applied stress to make slip transfer happen is studied.

Keywords : grain boundary, dislocation dynamics, slip transfer, elastic stress
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