Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A5] Symposium A-5

Chair: Sinisa Dj Mesarovic(Washington State University, United States of America)
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[SY-A5]Lattice continua for polycrystal grains: Climb and glide of dislocations, diffusion and grain boundary kinematics.

○sinisa Dj Mesarovic (Washington State University, United States of America)

At high temperatures, the interior of each grain in a polycrystal suffers: (1) dislocation glide, (2) climb, and (3) diffusion of vacancies. Grain boundaries undergo: (4) growth/disappearance, as a result of vacancy diffusion, and, (5) crystallographic reorientation/mismatch, as a result of dislocations arriving to the boundaries either by glide or by climb. All the above deformation mechanisms are naturally described in the lattice continuum framework, whereby the lattice represents the material. Climbing edge dislocations are lattice sink/source which must be reflected in the continuity equation and the transport theorem. The interacting kinematics of dislocation glide and climb requires dual definition of crystallographic slip fields: the true slip and the apparent slip. The transport theorem for grains with lattice growing or disappearing lattice at different grain boundary faces results in the direct formulation of the boundary condition for vacancy diffusion flux in terms of the boundary velocity (different from the lattice velocity). The field equations for each grain are derived by means of the principle of virtual power. Additional boundary conditions result from the relative motion of the adjacent crystal faces: Change of tilt and twist angle and surface elastic mismatch are derived from the geometry of dislocations arriving to the boundary. The resulting polycrystal initial/boundary value problem consists of elasticity-plasticity-diffusion field equations in each crystalline domain with moving boundaries, coupled through the boundary conditions.

Mesarovic, S.Dj. 2018 Physical foundations of mesoscale continua. In Meso-scale models: From micro-physics to macro-interpretation. Springer lecture notes. To appear.
Mesarovic, S.Dj. 2017 Dislocation creep: Climb and glide in the lattice continuum. *Crystals* **7**(8), 243.
Mesarovic, S.Dj. 2016 Lattice continuum and diffusional creep. *Proc. R. Soc. A* **472**, 20160039.