High temperature solid mechanics: mesoscale continuum describing diffusion, lattice growth and interfaces.

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Abstract

At high homologous temperature, deformation of polycrystalline solids is characterized by diffusion within the crystals, as well as lattice growth/disappearance at the grain boundary. This is further complicated by: formation of new phases (either controlled by differential diffusion of components or by phase transformation), diffusion-controlled dislocation climb, and, nucleation and evolution of voids. The typical example in materials service is creep of metals, alloys and ceramics, including creep fracture. In the manufacturing stage, we have sintering, grain growth and recrystallization. To resolve these phenomena on the mesoscale, i.e., withing crystalline grains and on the grain boundaries, a specialized continuum formulation is needed. Here, the general mathematical formulation for such mesoscale continuum is developed, first assuming sharp interfaces between grains, phases and voids, followed by the diffuse interface (phase field) formulation best suited for computational analysis.
In crystalline solids, when diffusion is operational, the mass velocity is different from the lattice velocity, the mass moves with the lattice, and through the lattice. Since most of the traditional (diffusionless) solid mechanics is based on the deformation/motion of the crystal lattice (e.g., elasticity is based on lattice stretching, while dislocation/crystal plasticity is based on the relative translation of lattice parts), it makes little sense to describe solid kinematics using the mass velocity as the primary field. Instead, we identify the *material* with the *lattice*. The lattice density and mass density are easily connected if the concentration of different components is known. The mass velocity will depend on the lattice velocity and on the fluxes of different components.

In the absence of diffusion, the mass and lattice continua are indistinguishable; the traditional elasticity and crystal plasticity are in fact lattice continua, without distinction between mass and lattice. When diffusion is present such distinction is needed. One important consequence bears emphasis. Solid mechanics traditionally relies on Lagrangean (material) frame, where the fundamental tensor field is the deformation gradient. The reference position is typically taken to be the initial position or the position at some reference time – in any case, it corresponds to a specific real configuration. However, when lattice grows and disappears at the boundary, the reference configuration for the newly created lattice cannot be determined by any physical reasoning. Nevertheless, the deformation gradient is needed for description of lattice elasticity, eigenstrains and dislocation plasticity. Therefore, we adopt the Eulerian frame with deformation gradient now treated as a state variable, moving with the lattice, and being function of current coordinates. At the growing boundary, we assume the continuity of the deformation gradient, which determines its value in newly created lattice in the instant

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of creation, the value in the adjacent old lattice being known.

Much of the sharp interface formulation has been developed in (1, 2, 3). Here, we only summarize the main components as needed for the development of the diffuse interface formulation. Selected computational results are presented.

References

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