Coupled Nonlinear Ginzburg-Landau and Mechanics Model for Martensitic Transformations in Polycrystals

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ABSTRACT

Martensitic transformation, in a narrow sense, is defined as the change of crystal structure to form a coherent phase or multi-variant domain structures out from parent phase with the same composition by the small shuffles or co-operative atom movements. It often competes with other diffusional transformations in real processes. To elucidate the displacive-diffusion effect recently manifested by atom probe tomographic analysis where atomic relaxation and short range diffusion occur during martensitic transformations while long range atomic movement dominates the diffusional transformations, we develop a 2D multi-field model upon the nonlinear Landau model with irreducible representation formed strains and the inertia dynamics for polycrystals. Incorporated with CALPHAD-based real-time diffusion potentials, chemical mobility and grain boundary relaxing of heterogamous nucleation, our new model represents the microstructure evolution of polycrystalline carbon steels during the quenching and partitioning process [1].

To further account for the morphology in steels different from the shape memory alloys, we put forward to the nonlinear coarse-grained dislocation model in the context of continuum theory of dislocation. With the simulations, we describe the mixed microstructure and composition distribution comparable with the experiments, and demonstrate that the dislocations account for the distinguishing microstructure morphology among carbon steels, nickel steels and shape memory alloys undergoing same symmetry breaking in transformation. We also discern that the difference of diffusion mobility between austenite and martensite primarily contributes to the partitioning in carbon steels. Based on the works, a prototype framework of multi-field model is preliminary built up, which is characterized in covering microstructure and property control and physical inherent communication among some different scales, e.g. thermodynamics and continuum mechanics at the macroscale together with phase field/Landau model at the mesoscale [1].

REFERENCES

[1] Guanglong Xu, Coupled Nonlinear Ginzburg-Landau and Mechanics Model for Martensitic Transformations in Polycrystals, PhD dissertation, Universidad Politécnica de Madrid & IMDEA Materials Institute, Madrid, Spain, 2016.