INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

ICAMS Seminar

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Phase field and plasticity

When dealing with phase transformations at the solid state, it seems difficult to neglect the influence of mechanics, i.e. elasticity and plasticity, even in the case of diffusion-controlled transformations. If the influence of elasticity on kinetics and morphologies has been studied for a long time (see e.g. the pioneer work of F. Larché and J.W. Cahn [1] and subsequent extensive works of P.W. Voorhees and W.C. Johnson [2,3]), the influence of plasticity has rarely been addressed. It is indeed difficult to obtain analytical solutions in relevant cases, and the resort to numerical calculations is mandatory. Despite the extensive use of phase field models to investigate the interplay between phase transformation and elasticity for nearly 20 years, it is only recently that the phase field approach has been coupled to plasticity (e.g. [4-8]).

In this talk, I will first present such a coupling between a simple phase field model and a simple J2 plasticity model, relying on a particular interpolation scheme within the diffuse interface. Using this model, I will show how the dissolution of a spherical precipitate is influenced by an applied shear stress. In particular, I will show that plasticity may lead to some morphological bifurcations. In a second part, I will present very briefly a new route toward modeling plasticity at the atomic scale in the framework of a continuum model, which is ultimately intended to be coupled to phase field models. I will then focus on the process of coherency loss of misfitting precipitates that we have been able to investigate with this new model.

[1] A linear theory of thermochemical equilibrium of solids under stress, F. Larché and J. W. Cahn, Acta Metallurgica 21 1051-1063 (1973).
[2] Interfacial equilibrium during a first-order phase transformation in solids, P. W. Voorhees and W. C. Johnson, Journal of Computational Physics 84 5108-5121 (1986).
[3] On the morphological development of second-phase particles in elastically-stressed solids, P. W. Voorhees, G. B. McFadden and W. C. Johnson, Acta Metallurgical and Materialia 40 2979-2992 (1992).
[4] Combining phase field approach and homogenization methods for modelling phase transformation in elastoplastic media, K. Ammar, B. Appolaire, G. Cailletaud and S. Forest, European Journal of Computational Mechanics 18 485-523 (2009).
[5] Phase field modeling of elasto-plastic deformation induced by diffusion controlled growth of a misfitting spherical precipitate, K. Ammar, B. Appolaire, G. Cailletaud and S. Forest, Philosophical Magazine Letters 91 164-172 (2011).
[6] Coupling phase field and viscoplasticity to study rafting in Ni-based superalloys, A. Gaubert, Y. L. Bouar and A. Finel, Philosophical Magazine 90 7-28 (2010).
[7] Viscoplastic phase field simulation of microstructural evolutions under complex loadings in Ni-base superalloys, A. Gaubert, Y. L. Bouar and A. Finel, Advanced Materials Research 278 216-221 (2011).
[8] A phase field model incorporating strain gradient viscoplasticity: Application to rafting in Ni-base superalloys, M. Cottura, Y. L. Bouar, A. Finel, B. Appolaire, K. Ammar and S. Forest, Journal of the Mechanics and Physics of Solids (2012).