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Applications of Phase Field Modelling

A phase field method is in principle able to compute the evolution of microstructure without explicit intervention. The domain of interest is the *field* in which the value of an *order parameter* at a particular location identifies the nature of the phase, the presence of an interface or other parameters such as chemical composition or strain. The heterogeneous system is incorporated into a grand functional representing its free energy. Assumptions are then made about how the field evolves as the free energy is minimized. Interfaces do not need to be tracked but can be inferred from the field parameters during the calculation. The number of equations to be solved can therefore be far smaller than the number of particles which form the structure. The phase field method is also eye-catching because it produces remarkable visual outputs, particularly of morphology, capturing features which are often realistic in appearance.

The motivation for commissioning this special issue was simple, that there is an extensive literature on the virtues of the technique itself, but apparently few applications which have led to tangible products. In particular, for a method which is founded in mathematics, there are few quantitative comparisons with reality, with most applications limited to the observation of shape.

We set about the task of identifying authors by searching the databases for publications focusing on applications which might be construed as tangible outcomes. Fifteen authors were invited to participate; activities such as these take a lot of creative effort and time so we are deeply grateful to those who were able to deliver and to participate in the refereeing process.

Emmerich discusses phase fields in the context of soft matter, specifically, colloids, primarily as a way of getting insight into basic issues of nucleation and dislocation dynamics, exploiting the transparency and convenient event time-scale of colloids as a model system to represent transitions and defects. There is a beautiful explanation of the difficulties in incorporating fluctuations: thermodynamic properties by definition cover averaged values of fluctuating quantities, so an artificial inclusion of fluctuations in effect counts them twice – the further discussion of this and of other open issues makes captivating reading.

Steinbach concludes that phase field theory has been demonstrated to apply quantitatively to solidification problems, but transformations in the solid state are much more difficult to handle because of anisotropies and defects, basically all issues which arise when the phases concerned can support shear stresses. It is arguable whether the simulations even produce images which are visually realistic, in contrast to the intricate and accurate predicted morphologies of dendrites. In the case of the nickel superalloys, progress is evident both in terms of the coherent precipitates and from the wider literature, on elastic strain driven morphological changes.

To the best of our knowledge, Nestler has been one of the pioneers in the commercialization of phase field software. What we find most interesting is the ability of the method to deal naturally with interface instabilities, but treating Widmanstätten ferrite as such an instability ignores the shape deformation as the plates grow; the evidence does not support the evolution of shape by instabilities, but rather by strain energy minimization. This is a thorn that phase field models of transformations need to grasp in order to be useful in the design of materials.

Notwithstanding computational demands, Militzer correctly emphasizes the power of the method in dealing with simultaneous effects, such as coarsening and precipitation, or grain growth in the presence of pinning particles. The method can in principle deal with a large number of interacting phenomena.

Metallic glasses which are below the glass transition temperature suffer from heterogeneous plasticity during compression, and brittle fracture with specific roughness in tension. Zheng exploits the phase field method to dwell deeper into these phenomena, by introducing a displacement field as the order parameter, together with a second such parameter to capture defect density, to describe the formation of the fracture surface. The treatment of interactions between shear bands is quite remarkable in capturing the generation of secondary features.

The evolution of voids and bubbles from radiation-induced changes is dealt with by Millett and Tonks. The theory contains stochastic terms to represent irradiation damage and explicit terms to deal with defect production rates and gas production rates. It is stated that the majority of phase field models in this context are essentially qualitative in their predictions and it will take further effort to make realistic comparisons against experimental data.

Furrer's article shows phase field methods with applications related to real industrial problems. Some of these are the nickel superalloy type calculations dealing with precipitate morphology and coarsening, including the elastic strain driven morphology changes commonly known as rafting. The models are said to reproduce experimentally observed structures, thereby providing confidence in giving specific guidance for altering alloys or processes. However, he too phrases the possibilities in terms of the potential of the method. It would be good to find a real application where phase field models themselves have made a difference to metallurgy or engineering.

To summarise, there clearly is significant activity in the use of phase field methods in understanding phenomena. Our goal with this special issue was to emphasize applications of the method; it seems that the technique is not sufficiently mature to be able to demonstrate that it has led to a significantly novel material or process. If one was to be provocative, then in terms of the NASA technology readiness levels (TRL), phase field modelling is at its lowest stage of evolution (TRL 1), where scientific research begins to be translated into applied research and development. It would be encouraging to promote a transition to TRL 2 where practical applications can, with speculation, be invented or identified. We look forward to this adventure.

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