Diffuse-interface modelling of microstructure evolution at micro- and macro-scale

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Formation and evolution of microstructure is a common feature in displacive transformations such as martensitic transformation and deformation twinning. It is accompanied by nucleation, propagation and annihilation of interfaces, either direct phase and twin boundaries or microstructured interfaces such as austenite–twinned martensite interfaces. These phenomena are particularly important in the case of shape memory alloys (SMAs), in which martensitic transformation is the main mechanism responsible for their functional properties, in particular for the shape memory effect and pseudoelasticity. In deformation twinning, the associated microstructure evolution is typically coupled with dislocation slip, and from the modelling point of view, the strong coupling between the two mechanisms of plastic deformation constitutes an additional challenge.

The phase-field method is a powerful computational tool for spatially-resolved modelling of microstructure evolution. Its essence lies in treating the interfaces as diffuse. This is achieved by introducing a continuous phase variable, called the order parameter, so that interface tracing is avoided and computations can be performed on a fixed computational grid. On the other hand, the need for accurate resolution of the diffuse interfaces requires the computational grid to be sufficiently fine with respect to the interface thickness.

At a higher scale, the stress-induced transformation in polycrystalline SMAs often proceeds in a heterogeneous manner, through the propagation of macroscopic transformation fronts that separate transformed and untransformed areas of the sample and often resemble Lüders bands, although more complex patterns are also observed. This is particularly true for NiTi subjected to tension-dominated loading. The associated instabilities result from a non-monotonic (up-down-up) intrinsic stress–strain response. A possible approach to modelling related phenomena is to introduce some kind of gradient enhancement into the model. As a result, the macroscopic transformation front is modelled as a diffuse interface, and the computational framework bears some similarity to the phase-field method. This approach has been used in our recent work on the modelling propagating instabilities and transformation patterns in pseudoelastic NiTi.

The talk will summarize our recent results on diffuse interface modelling of martensitic transformation in SMAs [1], deformation twinning in magnesium [2, 3], both within the phase-field framework, and transformation patterns in polycrystalline NiTi within the framework of gradient-enhanced pseudoelasticity [4, 5].

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