

Interfacial energy and size effects in multiscale modelling of shape memory alloys

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Shape memory alloys (SMA) undergo phase transformation of martensitic type which is the main mechanism responsible for the interesting effects, such as the shape memory effect and the pseudoelastic effect, observed in these materials. The transformation is accompanied by formation and evolution of martensitic microstructures which govern the functional properties of SMA. Evolution of microstructure occurs at different scales, and micromechanical models have been developed aimed at description of this multiscale phenomenon. A promising new area of research is to include into such models the effects of interfacial energies present at different scales of martensitic microstructures.

In this work, interfacial energy of two origins is accounted for, namely the atomic-scale energy of phase boundaries (taken from the materials science literature) and the elastic micro-strain energy at microstructured interfaces (e.g. at the austenite–twinned martensite interface). The latter is a bulk energy at a finer scale, however, at a higher scale it can be interpreted as the interfacial energy. This energy is predicted using micromechanical considerations. A suitable scale transition scheme is developed for that purpose which employs finite element analysis, carried out for a class of interface shapes, combined with shape sensitivity analysis and gradient-based minimization of elastic strain energy.

Size-dependent interfacial energy contributions introduce size effects into the multiscale modelling framework. Evolution of microstructure is then determined by applying a general evolution rule in the form of minimization of incremental energy supply. The incremental energy, being the sum of the increments in the free energy and dissipation, comprises both the bulk and the interfacial energy contributions at all levels of the microstructure.

As an example, size effects are studied for the pseudoelastic CuAlNi and NiTi shape memory alloys. In particular it is shown that characteristic dimensions of the microstructure can be predicted without introducing any artificial length-scale parameters.

References

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