INTERFACIAL ENERGY EFFECTS IN EVOLVING MARTENSITIC MICROSTRUCTURES

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Summary The incremental energy minimization with the size-dependent contribution of interfacial energy and dissipation is applied to multi-scale modeling of the evolution of stress-induced martensitic microstructures in shape memory alloys. The micro-strain energy at the austenite–twinned martensite interface is calculated by optimizing the interface shape with the use of finite elements. The effect of grain size on the macroscopic pseudoelastic hysteresis loop is determined using a sequential 3D scale-transition scheme.

DESCRIPTION OF THE APPROACH

Evolution of stress-induced martensitic microstructures in shape memory alloys (SMA) is modeled accounting for the accumulation and release of the interfacial energy. In addition to the usual volumetric terms in the three-dimensional setting, the interfacial energy and rate-independent dissipation related to creation, propagation and annihilation of phase interfaces are included. The approach is based on the step-by-step incremental energy minimization [1] in combination with the sequential micro-macro transition [2, 3]. A calculation scheme is proposed that provides multi-scale transition from atomic lattice rearrangements up to the macroscopic behavior of a polycrystal [4].

The interfacial energy of two origins is considered, including the atomic-scale energy of phase or twin boundaries and the elastic micro-strain energy at microstructured interfaces. The micro-strain energy at the austenite-twinned martensite interface is calculated by optimizing the interface shape with the use of finite elements; new results have recently been obtained for NiTi [5]. The interfacial energy factor at a grain boundary of a laminate domain is approximated by an analytic formula of wide applicability [3].

Interfacial energy terms are introduced to the incremental energy functional whose minimization yields the incremental solution [2]. In this way, the phase transformation criterion and microstructure evolution become dependent on characteristic dimensions of the microstructure. The essential feature of the approach is that for a given grain or subgrain size in a polycrystalline SMA, the microstructure dimensions are determined by energy minimization without assuming any artificial length-scale parameter. The whole approach requires specification of just two functions defining the overall free energy and rate-independent dissipation, and is applicable under the symmetry restriction imposed on the state derivative of the dissipation function [1, 2].

It has recently been shown that stability of evolving laminate microstructures depends critically on the interfacial energy contribution and on the laminate domain size [6]. Stabilizing effect of interfacial energy is demonstrated for realistic material parameters. When a domain size enters the nanometer range then instability due to sudden phase transformation of the whole domain can precede the formation of an austenite-martensite laminate.

EXAMPLES

A number of examples have recently been calculated for NiTi, CuAlNi and CuZnAl shape memory alloys; selected results are included here. Figure 1 shows a sample microstructure of the form of a rank-three laminate in a CuAlNi alloy during stress-induced martensitic transformation [3]. The grain thickness of 20 μm has been prescribed, all the remaining dimensions have been calculated by energy minimization.

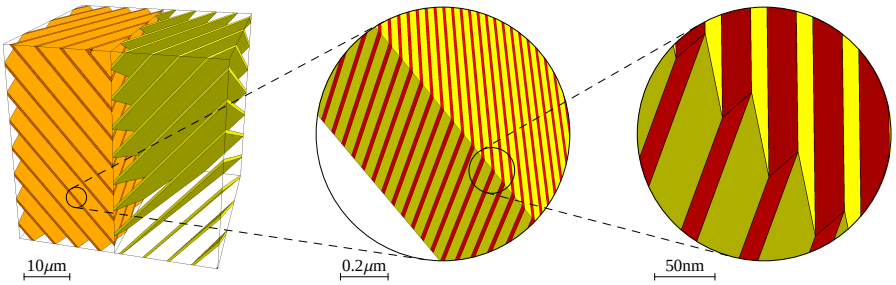

Figure 1. Rank-three laminate microstructure in a CuAlNi SMA during stress-induced martensitic transformation (note the scale markers). The austenite is transparent [3].

Newly calculated [5] saw-tooth morphologies that minimize the elastic micro-strain energy at the austenite–twinned martensite interface in a NiTi alloy are shown in Fig. 2 along with the respective values of an interfacial energy factor. That factor enters the size-dependent interfacial contribution to the incremental energy functional and cannot be measured directly.

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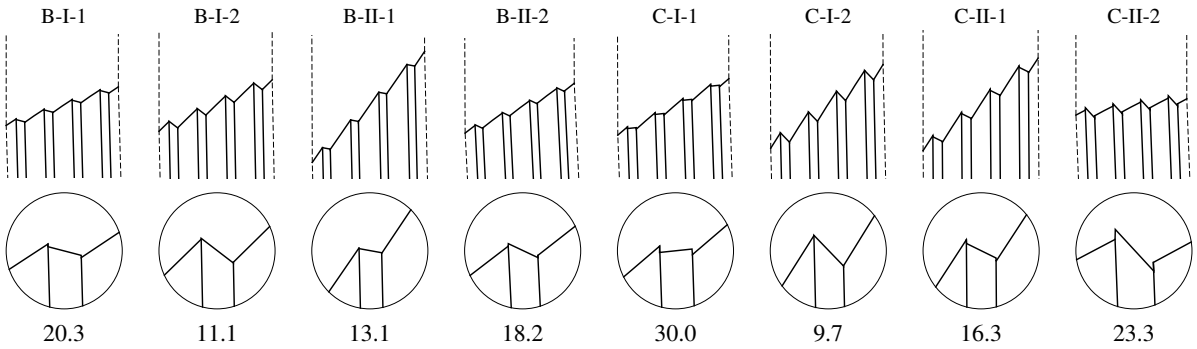

Figure 2. Low-energy saw-tooth morphologies of the eight crystallographically distinct microstructures of the transition layer at the austenite–martensite interface in NiTi. The numbers represent the calculated values of an interfacial energy factor [5].

The predicted effect of grain size on the macroscopic pseudoelastic hysteresis loop for a NiTi polycrystal is shown in Fig. 3; this is a new result which is a refinement of that in [4]. The effect is due to size-dependent accumulation and dissipation of energy related to formation and annihilation, respectively, of microstructural interfaces during both the forward and reverse austenite-to-martensite transformation. The non-monotonic character of the tensile stress-strain curves at a material point level can result in a nonuniform macroscopic transformation pattern in a polycrystalline specimen.

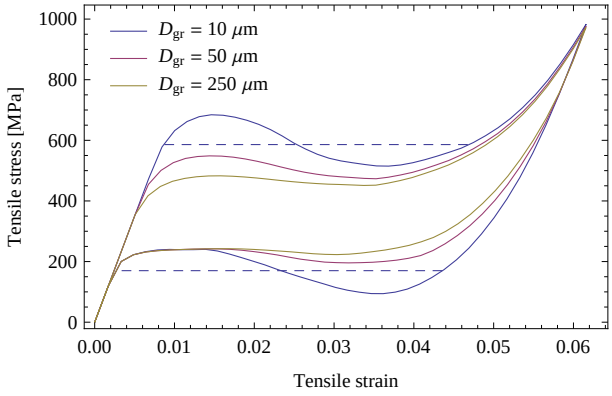

Figure 3. Macroscopic stress hysteresis in tension influenced by grain-size in a 3D multi-scale micromechanical model of NiTi SMA polycrystal.

Further new examples will be presented during the lecture.

CONCLUSIONS

The step-by-step incremental energy minimization with the size-dependent contribution of interfacial energy and dissipation provides an effective tool for multi-scale modeling of evolution of martensitic microstructures in SMA. Three-dimensional stress-induced transformation patterns and their characteristic dimensions within the grains are calculated, and their effect on the macroscopic pseudoelastic behaviour and dissipation in SMA polycrystals is determined. The results can be useful for formulation and calibration of micromechanically-based phenomenological models of polycrystalline shape memory alloys.

References

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