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Pattern formation during cubic to orthorhombic martensitic transformations in shape memory alloys

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Abstract

The superelasticity and shape memory effect of shape memory alloys originate from martensitic transformations (MT) that produce self-accommodated polydomain structures. In order to understand the formation mechanism of various domain patterns, a phase field model of cubic to orthorhombic MT in NiTiPt and NiTiCu is formulated, through which microstructure evolutions dominated by long-range elastic interactions are simulated. A rich variety of morphological patterns are predicted and analyzed. In particular, autocatalytic events leading to multi-variant "pyramidal triangular" and "nested triangular" configurations in NiTiCu are revealed. These morphological patterns are beyond the reach of the classical phenomenological theory of martensitic crystallography (PTMC). The simulation predictions agree well with experimental observations. By distinguishing deformation variant from orientation variant, the theoretical connection and distinction between PTMC and phase field microelasticity theory are discussed, and their predictions are compared with experimental observations.

Keywords: Martensitic phase transformation; Microstructure; Shape memory alloy; Phase field model; NiTi-based alloys

1. Introduction

NiTi-based shape memory alloys (SMAs) are the most widely used commercial SMAs for various applications [1–3]. From a crystallographic point of view, their good mechanical and functional properties are not only related to B2 ordering in austenite, but also determined by the group–subgroup relationship between the symmetry groups of the parent and product phases [2,4–6]. For example, the B2 to B19 (orthorhombic) or B19′ (monoclinic) martensitic transformation (MT) offers considerable recoverable strain, and the six or twelve correspondence variants generated as a result of symmetry reduction provide enough fundamental building blocks for the formation of self-accommodated multi-variant domain structures, especially in polycrystals [2,7,8]. However, the transformation pathways in NiTi-based SMAs, in which multiple martensitic phases (including R (rhombohedral) in addition to the B19 and B19′ mentioned above) and domain structures (including long-range ordered, internally twinned multi-variant plates, herringbone structure, pyramidal triangular and nanodomains of individual variant of the martensite) are involved, are rather complex. It has been shown that the transformation pathways could be altered through the control of ternary addition and extended defects such as dislocations and precipitates and, as a consequence, their mechanical and functional properties could be

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tailored [2,9–11]. For example, by adding Pt, Pd or Hf, the MT starting temperatures of the system can be elevated by several hundred degrees, making them suitable for high-temperature applications [12,13]. Slim hysteresis can be achieved by introducing point defects that stabilize nanodomains of martensite [14,15]. Through sophisticated design of training to introduce special defect structures, a two-way shape memory effect can be realized [16–18].

Because of such complicated transformation pathways, most existing investigations on MT in these alloys are limited to crystallographic analysis and do not provide direct predictions on detailed microstructural evolution during the MT. However, it is the evolution of polydomain structures that determines the mechanical and functional properties of these alloys, such as the stress–strain curve and hysteresis. The present study employs the phase field approach based on Landau theory of MT [19], Khachaturyan–Shatalov's microelasticity theory (KS theory, also called phase field microelasticity theory) of arbitrary two-phase microstructures [20], and gradient thermodynamics [21,22] to study pattern formation and evolution in NiTiPt and NiTiCu SMAs in an attempt to provide fundamental guidance to transformation pathway engineering of the systems for desired properties. As a kinetic model, the phase field approach has been applied successfully to cubic → tetragonal and cubic → trigonal MTs [20,23,24], where direct connections among crystallography, microstructure and mechanical behavior are characterized and analyzed. However, owing to the limited number of variants, tetragonal and trigonal martensites could not provide the desired shape memory properties, especially in polycrystalline systems.

For a generic cubic to orthorhombic MT, all three principal values of the transformation strain are non-zero, and the NiTiPt system can be chosen as a typical example. In this case, lattice invariant shear (twinning or slip) (LIS) is required to satisfy the invariant plane condition [25,26]. However, when one of the principal strains vanishes, the invariant plane condition could be satisfied between the austenite and a single variant of the martensite, and LIS becomes unnecessary [25,26]. As a result, different types of morphology are expected in such a special system. Coincidentally, NiTiCu is one of such systems that satisfy approximately this condition and, thus, it is chosen as an example to show the special effect. In order to make a comparison between the phase field model and the classical phenomenological theory of martensite crystallography (PTMC) [7,25–27], a crystallographic analysis is first provided, followed by construction of phase field model. Simulation results and their implications are presented and discussed in Sections 5 and 6, respectively. The major findings are summarized in Section 7.

2. Transformation path degeneracy based on group theory

In order to determine transformation path degeneracy, or number of deformation variants, point groups of the parent and product phases cannot be represented independently because the two phases are related to each other by a MT through lattice correspondence (LC) that describes a uniform deformation connecting the two lattices [28].

Assuming that the point groups of α and β phases are denoted by $H^{\alpha}_{C_\alpha}$ and $H^{\beta}_{C_\beta}$, respectively, where the subscripts C_α and C_β indicate the bases in which the α and β phases are represented. In principle, any basis can be chosen as C_α and C_β. However, if the two lattices are related to each other by an LC, and one would like to express such a relationship through their point groups, then $H^{\alpha}_{C_\alpha}$ and $H^{\beta}_{C_\beta}$ need to be represented in a common basis, which means that a change in basis is necessary [5,29]. For simplicity, C_α is taken as the common basis. Then any vector $\mathbf{r}$ in C_β can be represented in C_α through

$$\mathbf{r}_{C_\beta} = \mathbf{A}\mathbf{r}_{C_\alpha} \tag{1}$$

where $\mathbf{A}$ is a matrix describing the change of basis between C_β and C_α, and the point group of β can be represented in basis C_α as

$$H^{\beta}_{C_\alpha} = \mathbf{A}^{-1} H^{\beta}_{C_\beta} \mathbf{A} \tag{2}$$

All the symmetry operations in $H^{\beta}_{C_\beta}$, expressed in a matrix form, are changed by similarity transformation through $\mathbf{A}$.

Consider a structural transformation from α to β: if their LC is considered as the relationship between C_α and C_β, the so-called correspondence matrix [26,27] in MT crystallography becomes the $\mathbf{A}$ matrix. The point groups of α and β, expressed in the common basis, can then be used to determine the degeneracy of transformation path (i.e. number of crystallographically equivalent deformation pathways or deformation variants) according to the Lagrange Theorem

$$N_{\alpha\to\beta} = \frac{|H^{\alpha}_{C_\alpha}|}{|H^{\alpha}_{C_\alpha} \cap H^{\beta}_{C_\alpha}|} \tag{3}$$

where $|H^{\alpha}_{C_\alpha}|$ is the order of group $H^{\alpha}_{C_\alpha}$, and ∩ is the intersection operator. In parallel, if the orientation relationship (OR) between α and β is considered as the relationship between C_α and C_β, then $\mathbf{A}$ becomes a rotation matrix, and the number of crystallographically equivalent OR (i.e. orientation variants) can be determined by the above equations, as shown previously in the literature [30].

Based on the above group description, pathway degeneracy for all structural transformations can be determined through Eq. (3). The numbers of deformation variants for both face-centered cubic (fcc) to body-centered cubic (bcc) and bcc to fcc transformations are three, according to the Bain LC. Note that such a description can capture symmetry reduction of not only the uniform lattice deformation, but internal shuffle as well if any, leading to a distinction between deformation variant and "correspondence variant" commonly referred in the literature. In the B2 to B19 MTs in NiTiPt and NiTiCu, for example, the number of deformation variants increases from six to twelve when internal shuffle is taken into account. Considering the six