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## The evolution of compatible microstructures in shape memory alloys

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### Abstract

Shape memory alloys (SMAs) have been extensively used in sensors and actuators. Their behavior is dominated by the microstructures. Observations show that martensite twins usually form laminated patterns with interfaces that satisfy the compatibility equation to minimize the total energy. However, due to high nonlinearity of the material, the relationship between the overall response and microstructure has not yet been revealed. In this study, we identify the set of possible twin structures and the paths along which the microstructure evolves continuously between austenite and martensite phases under loads. The variational principle is used to capture the dissipative nature of interface motion in microstructures when phase transformation occurs. The model is applied to study superelasticity effect in Cu-Al-Ni single crystals. Many subtle features are explained.

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### 1. Introduction

Shape memory alloys (SMAs) have gained increasingly interest because of their outstanding properties, such as superelasticity. The origin of these properties is the phase transformation and the ability to minimize the overall energy of the crystal by phase twinning [1]. The topology of the twin structures is a crucial factor that strongly influences material response and macroscopic properties in SMAs. Thus, it is important for the design of engineering components. Microstructures in SMAs have been extensively studied in recent decades. The formation of the twin patterns is well explained by the constrained theory [2,3]. The orientation of a compatible interface separating distinct phases are also rigorously studied by Bhattacharya [1].

A wide variety of techniques is used for modeling microstructures in SMAs. For instance, phase field approaches can predict the topology of microstructures. They typically use the time-dependent Ginzburg-Landau (TDGL) equations, and describe the microstructure by the order parameter [4–6]. In contrast, sharp interface approach treats phase boundaries as diffuse interfaces, sharp interface approaches treat a phase boundary as a discontinuity, across which the strain may jump. This gives a significant saving of computation. However, particular twin arrangements are commonly assumed [7–9]. For engineering design purposes, larger scale models are needed. Thus, we adopt the sharp

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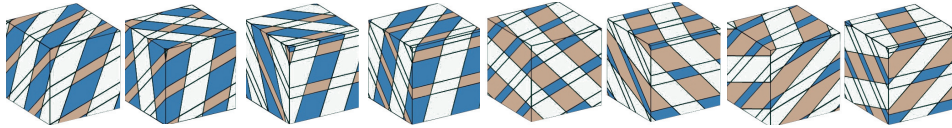


Fig. 1. Eight types of austenite and martensite mixed laminate patterns in the orthorhombic crystal system.

interface approach, but still capture the key microstructural features of SMAs by considering the transition states of microstructure connecting the pure austenite phase and the martensite twins. These states are identified by the non-linear compatibility theory[1]. As the results, the possible microstructural evolution paths for compatible laminates can be revealed. The variational principle is then used to determine which paths are energetically favorable by the applied load. The evolution of microstructure can be modeled, and the macroscopic response can also be predicted. In the current work, we apply the model to simulate the superelasticity effect in Cu-Al-Ni orthorhombic single crystals for illustration purposes. Several subtle features of the response are simulated. The model is ready to extend to other mechanism in SMAs, such as shape memory effect. The results can provide guidelines to engineer the microstructures and to optimize the performance of the applications of SMAs.

## 2. Theory and methodology

### 2.1. The austenite-martensite twin patterns in the orthorhombic crystal system

According to the deformation of the lattices, distinct crystal variants can be specified. Take the cubic-orthorhombic crystal system as an example, there are seven phases in total with deformation  $\mathbf{U}_{(i)}$  ( $i = 1, \dots, 7$ ), given by:

$$\begin{aligned} \mathbf{U}_{(1,2)} &= \begin{bmatrix} \beta & 0 & 0 \\ 0 & \alpha & \pm\gamma \\ 0 & \pm\gamma & \alpha \end{bmatrix}, & \mathbf{U}_{(3,4)} &= \begin{bmatrix} \alpha & 0 & \pm\gamma \\ 0 & \beta & 0 \\ \pm\gamma & 0 & \alpha \end{bmatrix}, \\ \mathbf{U}_{(5,6)} &= \begin{bmatrix} \alpha & \pm\gamma & 0 \\ \pm\gamma & \alpha & 0 \\ 0 & 0 & \beta \end{bmatrix}, & \mathbf{U}_{(7)} &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \end{aligned} \quad (1)$$

Parameters  $\alpha$ ,  $\beta$ , and  $\gamma$  are material properties characterize the martensitic transformation strain. Phases “1”...“6” are the orthorhombic martensite variants and phase “7” is the unstrained austenite. Consider a pair of phases ( $i, j$ ) with deformation  $\mathbf{U}_i, \mathbf{U}_j$ . A compatible interface with unit normal vector  $\mathbf{n}$  satisfies the compatibility equation [1,3]:

$$\mathbf{Q}_1 \mathbf{U}_i - \mathbf{Q}_2 \mathbf{U}_j = \mathbf{a} \otimes \mathbf{n} \quad (2)$$

for arbitrary vector  $\mathbf{a}$  and rotation matrix  $\mathbf{Q}_1$  and  $\mathbf{Q}_2$ . A compatible interface can be formed whenever a unit vector  $\mathbf{n}$  can be found that satisfies Eqn. (2).

We now assume that the crystal adopts the low energy multi-rank laminates with flat compatible interfaces throughout the procedure of the phase transformation. By solving Eqn. (2) with the concept of tree diagram, which have been commonly used to represent the composition of laminate patterns [8], all possible martensite-martensite and austenite-twinned martensite (A-M) interfaces can be determined. There are in total 96 distinct solutions of pattern in cubic to orthorhombic transformation [10]. However, by removing rigid rotations, reflections and inversions according to the symmetry operations, there are only eight types of A-M pattern, as shown in Fig. 1. As the results, eight types of possible microstructural evolution path connecting pure austenite and martensite twin microstructures are considered in the current study.

### 2.2. The variational approach

Now consider a single crystal shape memory alloy containing twin structures which can evolve with time according to given boundary conditions. The system can be described by a variational functional

$$\Pi = \dot{G} + \Psi \quad (3)$$

where  $\dot{G}$  is the rate of change of Gibbs free energy, and  $\Psi$  is a rate potential associated with the dissipative kinetic process. The Gibbs free energy comprises internal energy and potential energy due to boundary loads.

$$G = \frac{1}{2} \int_V (\phi + \epsilon_p^L c_{pq} \epsilon_q^L) dV + \int_V (-\sigma_p \epsilon_p) dV \quad p, q = 1 \dots 6 \quad (4)$$

where  $\phi$  is the free energy density of phases in stress-free states;  $\epsilon_p^L$  is the elastic energy due to the linear elastic strain field;  $V$  is the volume of the crystal;  $c_{pq}$  is the elastic stiffness matrix. The applied stress is  $\sigma_p$ ;  $\epsilon_p$  is the total strain of each material point.

A rate potential  $\Psi$  is associated with the movement of all the domain walls present in the crystal, given by [11]

$$\Psi = \int_A \int_0^v F(\zeta) d\zeta dA \quad (5)$$

where  $F(v)$  is a mobility function, that is a function of its velocity,  $v$ , in the current configuration. The surface integral in Eqn. (5) is carried out over the area of all interfaces. The system evolves along a path which makes the functional  $\Pi$  stationary with respect to the interface velocities  $v$  [12], that is:

$$\frac{\partial \Psi}{\partial v} = - \frac{\partial \dot{G}}{\partial v} \quad (6)$$

The interface velocities  $v$  can be obtained by solving Eqn. (6). Here we assume the crystal will adopt the laminate patterns with greatest velocity of interface movement. Hence the path of evolution of the laminate pattern can be found.

### 3. The simulation of superelasticity in shape memory alloys

The superelasticity response of a Cu-Al-Ni single crystal subjected to a tensile stress  $\sigma$  along the direction of (0.925, 0.380, 0), motivated by the numeric calculation done by Stupkiewicz and Petryk [10]. The tensile stress is in the form of sin wave with frequency of 1Hz with amplitude of 114MPa, and applied for a half cycle only. The elastic constants of the Cu-Al-Ni single crystal are used as those in the literature. The chemical energy density of austenite phase (variant 7) is set to be zero ( $\phi_A = 0$ ) for simplicity; those of martensite phases (variant 1. . . 6) can then be written as a function of temperature  $\phi_M = 0.1436(T - 278)\text{MJ/m}^3$  [10]. For the simulations, an increment  $\delta a_r = \frac{1}{1000}$  was used to estimate  $\frac{\partial \dot{G}}{\partial v}$ . The velocity of the interface at the current time  $t$  can then be obtained directly. The governing equations were numerically integrated using a forward Euler scheme with time step  $\delta t = \frac{1}{1000}\text{s}$ .

Figure 2 shows the stress and strain curve of the superelasticity effect, where the solid line represents the result generated by the current model and the dotted line represents that in the literature [10]. Figure 2(a)–(f) are the patterns present in the crystal generated by the current model. It starts from the pure austenite phase (Fig. 2(a)) and the onset of the austenite to martensite transformation occurs when the magnitude of stress reaches 103MPa. The applied load induces four A-M patterns in the crystal: two of them consist variants “1”, “3”, “7” and the others consist variants “2”, “3”, “7”, as shown in Fig. 2(b). They are in good agreement with those in the literature. At point (c) in the stress and strain curve, austenite phase vanishes; the A-M phase transformation is completed. It is worth noting that variant “3” (colored in brown) is energetically favored by the applied load compared with variants “1” and “2”, and thus further M-M phase transformation takes place resulting in a de-twinned, single phase state as shown in Fig. 2(d). However, the model in the literature (dotted line) assumes there is no further de-twin process. Thus, the dotted line saturated at point (c) with maximum strain of the crystal less than 5% while the solid line has maximum strain around 5.7% . As the magnitude of the stress decreases, the current model suggests that the crystal adopts a different microstructural evolution path and only two patterns are present (Fig. 2(e)). Finally, the austenite phase (variant “7”) grows gradually by consuming the martensite variants “1”, “2” and “3”, and the microstructure returns to its initial state (Fig. 2(a)). It can be observed that there is a significant difference between the two strain and stress curves when the applied stress decreases. This is because the model in the literature assumes the crystal adopts the same evolution path for both A to M and M to A phase transformations.

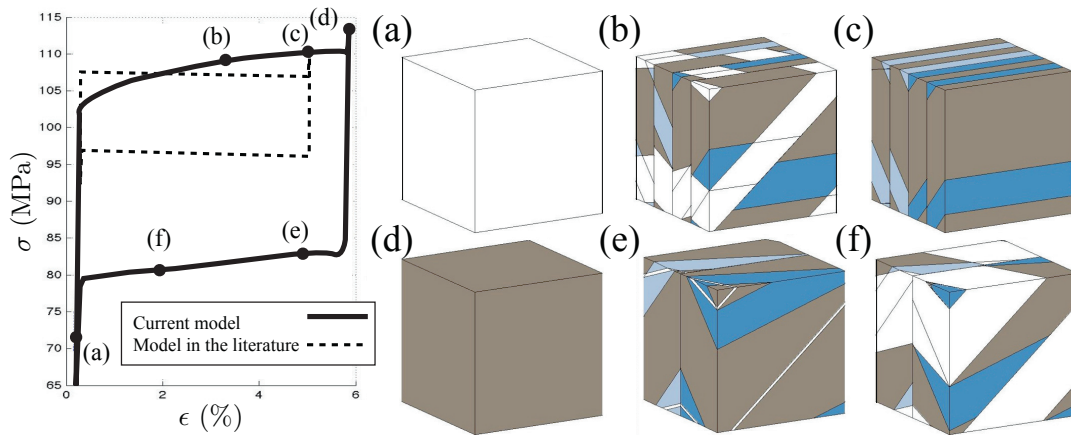


Fig. 2. The predicted stress and strain curve for the superelasticity effect, where the solid line represents the result generated by the current model; the dotted line represents that shown in the literature [10] and the corresponding microstructural evolution. Where different colors in the unit cell represent the distinct crystal variants.

#### 4. Conclusions

A kinetic model of laminate microstructure evolution in shape memory alloy single crystals has been developed, based on non-linear compatibility theory, evolving according to the variational principle. Eight transitional patterns which connect pure austenite and martensite twins are identified. The model was applied to study the response of superelasticity in Cu-Al-Ni single crystals. The results reproduce and explain several significant features. The model provides a rapid estimate of the microstructural evolution in SMAs and is ready to extend to study other crystal systems and other materials.

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