On Deformation of A-M Interface in Single Crystal Shape Memory Alloys and Some Related Issues

Recent experimental results on the deformation field of single crystal CuNiAl shape memory alloys (SMA) by using Moiré interference technique are reported and two kinds of austenite-martensite (A-M) interfaces with different deformation features are identified. The experimental discovery questioned the invariant plane hypothesis used in crystallographic theory of martensitic transformation. Some fundamental issues on the property of A-M interface and the related micro- and macro-deformation features are discussed.

1 Introduction
The deformation of single crystal shape memory alloys (SMAs) under externally applied stress is strongly dependent on temperature and crystal orientation, and is normally realized by the formation and propagation of austenite-martensite (A-M) interfaces. Therefore, the nature of the interfaces and the related deformation features have a strong effect on the deformation behavior of single crystals such as one-way and two-way shape memory effects. Even though the material science and metallurgical study on shape memory alloys (SMA) has reached quite a mature level and there has been a significant amount of research dedicated to modeling the thermomechanical behavior of SMA over the last decade (for example, Delaey et al., 1974; Otsuka et al., 1976, 1979; Wayman, 1981; Olson and Owen, 1992; Christian, 1982, 1995; Fisher et al., 1996), systematic investigations on the deformation of interface from continuum mechanics point of view are still very limited in the literature. For example, in almost all investigations on SMA, the A-M interface is assumed to be an invariant plane (IP) (see Otsuka et al., 1976; Patoor et al., 1988; Ball and James, 1987; Bhattacharya, 1991, 1992; Chu, 1993; Zhang et al., 1997; Leo et al., 1993), there is no direct experimental measurement on the deformation of interfaces in SMA to check such a hypothesis.

This paper reports the authors’ recent microstructure-based investigation on austenite-martensite (A-M) interfaces in stress-induced transformation plasticity of single crystal CuAlNi Shape Memory Alloys (SMAs). Attention is focused on the formation of the A-M interface under uniaxial tensile stress and the deformation field in its vicinity. In Section 2, experimental observations on the deformation field of single crystal CuAlNi using high-resolution Moiré technique are summarized and the deformation features near the interfaces are identified. In Section 3, the crystallographic theory of martensite (Wechsler et al., 1953; Ball and James, 1987) used to predict the A-M interface (or habit plane) is briefly described. The deformation features of the interface in shape memory effect (SME, $T < A_S$) and superelasticity (SE, $T > A_T$) and their relevance to the macroscopic deformation modes of single crystal are discussed.

2 The Experimental Phenomena
2.1 Stress-Induced $\beta_1 \rightarrow \gamma'_I$ Transformation at $T < A_S$ (SME). The tensile specimens were cut from the CuAlNi (Cu-13.7%Al-4.18%Ni (wt%)) single crystal ingots using a wire-cutting electrical discharge machine (EDM). The ingots were produced by Prof. Tan Shusong (Central South University of Technology, China) using the improved Bridgeman method. The specimens were differently heat treated to get different transition temperatures. For the SME specimens the characteristic temperatures are measured by Differential Scanning Calorimeter (DSC) as $M_f = 6^\circ C$, $M_p = 3^\circ C$, $A_s = 35^\circ C$, $A_f = 45^\circ C$. The testing temperature is $T = 20^\circ C$, so the initial state of the specimen is austenite ($\beta_1$ phase) and the stress-induced martensite will be retained after unloading ($T < A_S$). The orientation of the tensile axis with respect to the lattice axes of the parent phase is (0.087, -0.796, -0.605). Before the Moiré experiment, tensile tests were performed at $T = 20^\circ C$ on a MTS machine under displacement control with a loading speed of 0.01 mm/s to get the nominal stress strain curve (Fig. 1). The strain was measured by an extensometer. It is well established that the transformation in this temperature range is from $\beta_1$ austenite to $\gamma'_I$ martensite. The serration in the curve is due to the sudden formation of stress-induced martensite plates with sharp A-M interface. At the end of the curve, the stress increases rapidly and when the gauge length is fully occupied by the martensite we stop the machine and unloading. From the unloading curve, it is seen that the modulus of martensite is much less than that of austenite. The martensite is stable at room temperature and remains on removal of the stress.

In the Moiré test, the specimens were hand-polished using 600 grit silicon carbide paper, and then a high frequency crossed-line grating of 1200 lines/mm was replicated on the specimen by epoxy cement. The grating deforms together with the underlying specimen. Uniaxial loading is performed by a specially designed loading frame. Figures 2(a) and 2(b), respectively, show the uniform fringe patterns of the $u$ (along $x$-direction) and $v$ (along $y$-direction) elastic displacement fields of the specimen surface before the transformation happens. These fringe patterns represent contours of constant in-plane displacement $u$ and $v$, respectively. From the fringe patterns, the in-plane strain components can be directly calculated (see Post et al., 1994, Zhang et al., 1997). It is seen that there is a shear strain under uniaxial tension. This is because the single crystal is elastically anisotropic and the principle axes of the stress tensor are not coincident with the lattice axes of the material. The three independent elastic constants of this cubic crystal can be accurately determined by Moiré (see Zhang et al., 1997). With the increase of the applied stress, martensite transformation occurs by a sudden formation and propagation of martensite band accompanying a rapid load drop (see Fig. 1). Figures 3(a) and 3(b) are, respectively, the amplified $u$ and $v$ displacement fringe patterns across the A-M interface (see the corresponding point in Fig. 1). It can be seen clearly that...
the A-M interface is inclined in an angle of 55.5 deg with the loading axis in the x-y plane. The calculated total strains $\varepsilon_t$ in the martensite and austenite phase are shown in Table 1. The strain in austenite is the elastic strain and uniform, i.e., $\varepsilon = \varepsilon_t$ and the transformation strain $\varepsilon_t = \varepsilon_t - \varepsilon_t$ inside the martensite is also uniform. Comparing the above results with the strain in Fig. 1, we find that the transformation strain measured by Moiré ($\varepsilon_t = 3.58\%$) is in good agreement with the residual strain ($3.50\%$) in the stress-strain curve. We can also see that the interface is straight and there is a clear strain jump across the interface. After unloading the fringe patterns in austenite totally disappear and the uniform transformation strain in martensite remains, which directly indicates that the martensite formed has an internally twinned structure and the A-M interface is indeed an undistorted invariant plane (IP). The martensite consists of twinned variants and the twinning can be clearly observed under optical microscope.

2.2. The Stress-Induced $\beta_1 \rightarrow \beta_1$ Superelasticity at $T > A_f$. The transition temperatures of the specimen are $M_f = -37^\circ C, M_s = -48^\circ C, A_r = -37^\circ C, A_p = -20^\circ C$. The stress-induced transformation at $T = 20^\circ C$ is from $\beta_1$ austenite to $\beta_1$ martensite phase. The orientation of the tensile loading axis is the same as in SME. Figure 4 shows the measured typical nominal stress strain curve by MTS test machine. It is seen that the macroscopic transformation strain ($\approx 7\%$, where the whole gauge length is occupied by martensite) is much larger than that in SME. Figure 5 shows the fringe patterns of the displacement fields at the initial stage of nucleation where many tiny narrow bands can be observed on the specimen surface. There are weak interactions between the austenite and martensite bands and among the narrow martensite bands at this stage. In addition, the jump of strain across the A-M interface is not as clear as in case of SME (Fig. 3). With further loading, these bands begin to merge into a single band and strains inside the bands increase with loading as shown in Fig. 6. The deformation afterward is mainly accomplished by the steady-state propagation of a single martensite band (like Luder's band propagation in metals), which corresponds to the plateau in the curve of Fig. 4. Macroscopically a sharp A-M interface can be directly observed on the surface of the specimen without grating. The fringe patterns of the displacement fields across this interface in this stage are shown in Fig. 7. In sharp contrast with the case of SME, there is a high strain concentration

<table>
<thead>
<tr>
<th>Point 1</th>
<th>Point 2</th>
</tr>
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<tr>
<td>$\varepsilon$ (%)</td>
<td>-0.07</td>
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<tr>
<td>$\varepsilon$ (%)</td>
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</tr>
<tr>
<td>$\gamma$ (%)</td>
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Fig. 2 Fringe patterns of the $\nu$ (a) and $\nu$ (b) elastic displacement fields at load 248N

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Fig. 3 Fringe patterns of the $\nu$ (a) and $\nu$ (b) displacement fields across the A-M interface at load 280N

Fig. 1 Stress-strain curve under uniaxial tension (Shape Memory Effect case)
in austenite near the A-M interface and no jump in the total strain can be observed across the interface. Because the specimen surface is covered by the grating, what the fringe patterns demonstrated is a diffuse interface (Fig. 7). This indicates that the A-M interface in superelasticity is strongly deformed and no longer an invariant plane. Far away from the interface the strains in both martensite and austenite regions are quite uniform and not disturbed. The uniform fringe patterns in the transformed zone are shown in Fig. 8. Figure 9 and Tables 1 and 2 give the comparison of the measured strain distribution across the A-M interface between SME and SE. In Fig. 9(b) points 1–8 are about 0.5 mm away from the interface. It is noted that the strains at points 1–7 are not the same significance. This is because the constraint effect by the martensite domain is decreasing from point 1 to point 7.

3 Analysis of the Results and Some Discussions

3.1 A-M Interface Property and the Related Macro- and Micro-Deformation Features. The above-experimental results demonstrate different micro- and macro-deformation features of single crystal CuAINi SMA at different temperature regimes. These differences are deemed to be related to the structure and property of the A-M interface and to be intrinsic of the specific material system considered. They are summarized as follows:

(1) Macroscopic deformation mode. In the case of SE, the macroscopic transformation strain is much larger than the case of SME and the superelastic stress-strain curve during forward transformation exhibits stress plateaus after an overshooting at the beginning. (Note: the overshooting peak is more obvious if the martensite band formed in the center of the specimen.) Similar phenomena are also observed for NiTi polycrystals (see Lin et al., 1994, 1996, Shaw and Kyriakides, 1995). The deformation is unstable (inhomogeneous) and realized by the propagation of a macroscopically observable single transformation front (A-M interface here). The deformation is reversed upon unloading with a small hysteresis. It seems that there exists a particular driving force for the forward and reverse motion of...
the interface. Whereas in SME, the macroscopic stress-strain curve exhibits strong serration during forward transformation and no stress plateau and no steady-state single band propagation as in SE can be observed. Instead, several martensite bands formed without preference in the whole length of the specimen if the cross section is uniform. The strains in both martensite and austenite are uniform and the martensite is stable after unloading.

With a certain increase in temperature a large hysteresis with the same transformation strain could be observed (see Otsuka et al., 1976).

(2) Local deformation around the interface. Corresponding to the above different macroscopic deformation modes, the deformation fields around the interface also differ significantly. In SME, the strains in both austenite and martensite are uniform (so the stress is also uniform) and the interface is indeed an invariant plane as shown in Fig. 3. Whereas in SE there is high strain concentration in the austenite near the interface so the A-M interface in Fig. 7 is strongly distorted and thus no longer an invariant plane. Because the strain inside the martensite bands increases with applied stress before and after the bands merged into a big band (Figs. 5 and 6), it is natural to conjecture that the crystal structure change in SE may involve habit plane variant formation followed by detwinning. Direct micro-experimental evidence is required to support such a conjecture.

3.2 Calculation of the Habit Plane for the Case of SME. So far, almost all deformation analysis of the single crystal SMAs is based on the phenomenological crystallographic theory of martensitic transformations (Wechsler, Lieberman and Read, 1953; Ball and James, 1987). Historically, this theory was developed based mainly on the research of martensite in steels and under pure cooling (athermal martensite). According to the theory there are three phenomenological steps describing the total transformation: the Bain distortion, a lattice invariant deformation (inhomogeneous shear like twinning), and a rigid body rotation. There is no time sequence implied in the three steps and the basic hypothesis is that these three steps are so organized that the combined effect of the three operations will make the macroscopic deformation of the martensite domain to

Table 2

<table>
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<tr>
<th>Point</th>
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<th>$e_y$ (%)</th>
<th>$Y_x$ (%)</th>
<th>$e_x$ (%)</th>
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</tr>
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<td>2.31</td>
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Fig. 9 Strain distributions across the A-M interface in the case of SME (a) (the measured strains are listed in Table 1), the case of superelasticity (b) (the strains are listed in Table 2)
be a plane-invariant strain, i.e., the A-M interface (also called habit plane) is an undistorted plane (see Fig. 10). We consider a body that occupies a region \( R \) in three-dimensional space. A deformation of the body is described by the smooth and invertible mapping

\[
y(x) = x + u(x), \quad x \in R.
\]

In the above, \( x \) is the reference position vector of a material point, \( y \) is the corresponding position vector in the deformed configuration, \( u \) is the displacement. The deformation gradient tensor \( F \) is defined as

\[
F = \nabla y, \quad (\text{det } F > 0).
\]

Mathematically the above habit plane description is equivalent to the following statement: If \( F_A \) (for undeformed austenite \( F_a = I \)) and \( F_M \) are the deformation gradients in parent and martensite regions separated by a planar interface with normal \( m \) (in the reference configuration), then the jump of the deformation gradient across the interface must be of the form

\[
F_M - F_A = b \otimes m \quad (3)
\]

or

\[
F_M = I + b \otimes m. \quad (4)
\]

In Eqs. (3) and (4) \( b \) is the shearing vector of the twinned martensite domain, \( F_M = AF_A + (1 - \lambda)F_2 \), \( \lambda \) is the volume fraction of one martensite variant in the twin, \( F_A \) and \( F_2 \) are the deformation gradients of any two correspondent variants in a twin (see Fig. 10). \( F_M \) can be further expressed as (Ball and James, 1987; Shield, 1995)

\[
F_M = R_0[\lambda R_{ab}U_A + (1 - \lambda)U_B] \quad (5)
\]

where \( R_0 \) is the rotation of the average deformation, \( R_{ab} \) is the relative rotation between the two correspondence variants in a twin, \( U_A \) and \( U_B \) are the stretches (Bain strain) of single correspondence variants in a twin. For the \( \gamma \) martensite in CuAlNi single crystal, the substrates \( A, B = 1, 2, \ldots, 6 \) (Shield, 1993). By using the kinematic compatibility across the twin boundary

\[
R_{ab}U_A - U_B = a \otimes n \quad (6)
\]

where \( a \) is the shearing vector and \( n \) is the normal of twin plane, Eq. (4) can be expressed as

\[
R_0(U_A + \lambda a \otimes n) - I = b \otimes m \quad (7)
\]

The determination of habit planes is to find quantities of \( a, n, b, m, R_0, R_{ab}, \) and \( \lambda \) such that Eqs. (6) and (7) are satisfied for a given choice of \( A \) and \( B \) (see Shield, 1995; Zhang et al., 1997). Using this theory, the A-M interface orientation and transformation strains can be predicted and quite good agreement is obtained between theory and experiment for the case of SME (see Zhang et al., 1997). In Fig. 4 the invariant plane can be observed clearly from the fringe patterns. The domains with dense and sparse fringes are the martensite and austenite, respectively. The strains in both phases are uniform and the strain jump is very sharp. Due to the plane invariant nature of the interface, the stress \( \sigma \) is uniform for the whole domain so the Gibbs free energy difference between parent phase and martensite can be simply expressed as

\[
\Delta G(\sigma, T) = G_p - G_m = \sigma e_n + \Delta G_{\text{SME}}(T) \quad (8)
\]

which is known as transformation driving force. So the driving force for transformation is uniform everywhere for the SME specimen at a given \( T (M_S < T < A_S) \). This explains why in SME several martensite bands always can form without preference in the whole length of the specimen under uniaxial tension.

3.3 On the Non-Plane-Invariant Nature of the A-M Interface in SE. Different from the case of SME, so far there is no satisfactory theory to predict the transformation strain in the case of SE (see Otsuka et al., 1976) because the A-M interface is not an invariant plane (even though the measured A-M interface orientation in SE is very close to that in SME). A model on the deformation of detwinning is recently developed by Buchhert and Wert (1996). But the A-M interface structure is still not clear. Due to the strong mismatch between the deformed martensite and the austenite there is a triangle region in the austenite near the interface where the strains are much larger than the remote uniform elastic strain (see upper-right part of Fig. 7). The further growth of martensite or nucleation of new bands always happens in this triangle region. Compared with the remote region of uniform stress and strain, this high strain concentration (therefore high stress) near the interface energetically serves as the additional driving force for the formation of martensite. This explains why after the formation of martensite band by nucleation a stable propagation of a single macroscopic A-M interface can be maintained and be observed during the whole deformation (plateau in Fig. 4). Therefore, the nature of A-M interface and the resulted deformation features (such as transformation strains) has a strong effect on thermodynamics, kinetics, and macroscopic deformation mode. Similar effect also exists in polycrystalline SMAs (see the work of Lin et al., 1994, 1996, Shaw and Kyriakides, 1995). The calculation of the driving force for single P-M interfaces propagation in SE is not as simple as in case of SME because the stress is not uniformly distributed as in SME and jumps across the A-M interface. Detailed analysis on this issue is in progress.

4 Conclusions

In this paper, an experimental study on the moving strain discontinuities in single crystal CuNiAl SMA is performed by using the full-field Moiré interference technique, two kinds of interfaces—invariant plane (IP) and non-invariant-plane (NIP)—are identified and their deformation features are revealed. The experimental results demonstrate that the invariant plane assumption on the A-M interface agrees very well with the Moiré measurement in the temperature range of SME but does not hold in case of SE at temperature \( T > A_S \). For the non-invariant plane (in the case of SE) so far there is no satisfactory theoretical modeling to predict its formation and the corresponding transformation strain.

The energetic aspects for the formation of the interface are briefly analyzed. It is shown that the thermodynamic driving forces of transformation near the interface for the case of non-invariant plane is much higher than that of invariant plane, which may be the reason for the stable propagation of single interface observed in SE.
The experimental discovery raises doubt to the plane invariant strain assumption that is used for calculation of transformation strain in so far almost all theoretical models. Satisfactory answers to this question are of significance in both checking the established theoretical models and the analysis and evaluation of the internal stress and strain energy. It is believed that the interface properties at different temperature regimes are intrinsic of particular SMA systems and are responsible for different macroscopic deformation modes in these systems.

Propagation of interfaces or instability is a fascinating and widely observed phenomenon in materials and structures (Abeyaratne and Knowles, 1990; Kyriakides, 1993). The present study demonstrated the deformation field during the nucleation and growth of martensite under uniaxial tension. A micro-scale accurate validation of the present discovery by combined use of TEM and AFM under in-situ loading will consist of the work in the future.

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References


