Unusual pseudoelastic behaviour of Fe₃Ga shape memory alloys

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Abstract. Pseudoelastic behaviour of Fe-23.8at%Ga single crystals compressed with different loading axes at room temperature was examined focusing on the activated deformation mode. In the crystals, \{101\}<111> slip and \{211\}<111> twin were mainly activated depending on the loading axis. Pseudoelastic behaviour of the crystals depended strongly on the deformation mode. If \{101\}<111> slip was operative, sole and paired 1/4<111> superpartial dislocations moved dragging antiphase boundaries (APB). During unloading, the APB pulled back the superpartials due to its tension resulting in pseudoelasticity. In contrast, twinning and untwinning of \{211\}<111> pseudo-twins also led to large strain recovery accompanying a serrated flow during loading and unloading. It is suggested the energy of the pseudo-twin interface was the driving force for the twinning pseudoelasticity.

1. Introduction

Shape memory alloys generally exhibit the following two phenomena: shape memory effect and pseudoelasticity [1]. By pseudoelasticity, an applied strain during loading recovers during unloading. So, pseudoelasticity is applied to potable phone antenna, eyeglass frame and so on. In general, thermoelastic martensitic transformation is responsible for pseudoelasticity; stress-induced martensitic transformation during loading and the reverse transformation during unloading result in strain recovery. However, Fe₃Al single crystals with the D0₃ structure showed giant pseudoelasticity which is not related to martensitic transformation but peculiar dislocation motion [2-4]. In the crystals, 1/4<111> superpartial dislocations moved individually dragging antiphase boundaries (APB) during loading. During unloading, APB pulled back the superpartials, resulting in strain recovery. Thus, this phenomenon is called “APB pseudoelasticity”.

Recently, we found that Fe₃Ga single crystals with the D0₃ structure also demonstrated giant pseudoelasticity at room temperature [5, 6]. More recently, three kinds of pseudoelasticity were found to appear in Fe-23.8at%Ga single crystals tensile-deformed at room temperature, depending on the degree of D0₃ order [6]. So, we call the phenomena “multimode pseudoelasticity” which has not been observed before. Figure 1 shows a schematic illustration of the mechanism of the pseudoelasticities. In
Fe$_3$Ga single crystals, APB pseudoelasticity took place associated with {101}<111> slip, which is similar to Fe$_3$Al single crystals (figure 1 (a)). The APB tension on {101} plane was large enough to pull back the 1/4<111> superpartial dislocations during unloading. {211}<111>-type twins were also formed in the course of tensile deformation in the crystals fully ordered to the D0$_3$ phase as shown in figure 1 (b). In general, an atomic shuffling occurs to maintain the mirror symmetry. However, the atomic shuffling never took place in Fe$_3$Ga crystals. Christian et al. [7] defined the {211} twins as 2.2 T-type pseudo-twins. The interface energy of the pseudo-twins was higher than that of perfect twins. Thus, the energy of the twin boundaries was the driving force for untwining during unloading. Furthermore, if the degree of D0$_3$ order in Fe$_3$Ga was low, stress-induced transformation of 14M martensites with 14-layered periodic structure occurred in the crystals (figure 1 (c)). The reverse transformation during unloading led to the shape recovery of Fe$_3$Ga single crystals. The free energy difference between the parent and martensite phases resulted in the pseudoelasticity.

It is well known that twinning deformation depends strongly on loading axis and stress sense such as tension and compression. In the present study, the pseudoelastic behaviour of Fe$_3$Ga single crystals compressed with different loading axes at room temperature were investigated focusing on the orientation dependence and tension-compression asymmetry of the pseudo-twins.

2. Experimental procedure

Fe$_{23.8}$at%Ga single crystals were grown by a floating zone method at a growth rate of 5 mm h$^{-1}$. After homogenisation at 1373 K for 48 h, the crystals were annealed at 873 K for 10 h for D0$_3$ ordering. By the ordering treatment, possible activated deformation modes in compression were limited to {101}<111> slip and {211}<111> pseudo-twins while martensitic transformation never occurred [6]. The compression specimens with gauge dimension of 2.5×2.5×5.5 mm$^3$ were prepared by spark machining. The loading axes of the compression specimens were selected to be [149] (A), [358] (B) and [441] (C) as shown in Figure 2. Schmid factors (SF) for (011)[111] slip and (211)[111] pseudo-twin are listed in table 1. It should be noted that twinning deformation generally shows tension-compression asymmetry, (211)[111] pseudo-twin is activated in compression. From the previous study, the critical resolved stresses ($\tau_{\text{CRSS}}$) for (011)[111] slip and (211)[111] pseudo-twin were determined to be 224 and 225 MPa, respectively. If the Schmid law hold true, the yield stress ($\sigma_Y$) corresponding to each deformation mode can be predicted by the following equation,

$$\sigma_Y = \frac{\tau_{\text{CRSS}}}{\text{SF}}.$$  (1)
Table 1. Schmid factor (SF) for \(\{101\}[111]\) slip and \(\{211\}[111]\) twin at different loading axes.

| Orientation | SF for \(\{101\}[111]\) slip | SF for \(\{211\}[111]\) twin |
|-------------|-------------------------------|--------------------------------|
| A           | 0.500                         | 0.433                          |
| B           | 0.458                         | 0.457                          |
| C           | 0.433                         | 0.500                          |

Using equation (1), one can predict loading axis favorable for the activation of \(\{101\}[111]\) slip and \(\{211\}[111]\) pseudo-twin as shown in figure 2. Near [011] orientation, \(\{211\}[111]\) pseudo-twin is activated before \(\{101\}[111]\) slip. Compression tests were done in air at room temperature at a cross-head speed of 0.05 mm/min corresponding to an initial strain rate of \(1.7 \times 10^{-4}\) s\(^{-1}\). After loading to a plastic strain (\(\epsilon_p\)) of 5 %, the load was subsequently released at the same cross-head speed. After the compression tests, surface relief due to the slip or pseudo-twin was observed by an optical microscope. Deformation substructure was also observed using a transmission electron microscope (TEM) at an accelerating voltage of 300 kV.

### 3. Results

Figure 3 shows stress-strain (S-S) curves of Fe-23.8at%Ga single crystals compressed to a plastic strain of 5 % at room temperature. The pseudoelastic behaviour of these crystals depends strongly on loading axis. At A orientation where \(\{101\}[111]\) slip is active, perfect pseudoelasticity appears showing smoothly curved S-S curve. This means no twinning occurred at A orientation which is consistent with theoretical calculation shown in figure 2. Moreover, there is also no evidence that proves occurrence of pseudo-twinning at B orientation. It is also noted that strain recovery at B

Figure 3. Stress-strain curves of Fe-23.8at%Ga single crystals compressed to \(\epsilon_p = 5\) % at A, B and C orientations at room temperature.
orientation is quite small compared with A orientation. On the other hand, a serrated flow is observed in the S-S curve for C orientation. It is also interesting to note that the serration also appears in the unloading curve. This suggests twinning and untwinning during loading and unloading resulted in pseudoelasticity at C orientation though the strain recovery was not perfect.

Optical micrographs of specimen surface at A, B and C orientations are shown in figure 4. At A orientation, fine slip traces parallel to primary (011) slip plane are observed as shown in figure 4 (a). The contrast of the slip traces is very low since the slip traces considerably disappeared during unloading. On the other hand, (011) coarse slip traces remain after compression at B orientation (figure 4 (b)). In contrast, there exists coarse bands associated with (211) pseudo-twins in addition to (211) and its cross slips (figure 4 (c)). Thus, (011)[111] slip and (211)[111] pseudo-twin were activated depending on loading axis, which is in good agreement with figure 2. Thus, APB pseudoelasticity appeared at A and B orientations while the crystals compressed at C orientation revealed twinning pseudoelasticity. Strictly saying, the Schmid law (i.e. equation (1)) did not fully hold for (011)[111] slip due to the complicated core structure of <111> screw dislocations. However, one could roughly estimate the activated deformation mode from figure 2.

4. Discussion

In the present study, APB and twinning pseudoelasticities were observed to appear in F-23.8at%Ga single crystals compressed at room temperature. The mechanism of pseudoelasticities was discussed in detail.

At A and B orientations, only APB pseudoelasticity appeared. Figure 5 shows dislocation configuration and atomic arrangement of APB in the D0₃ structure. From TEM observation, two types of dislocation configuration were observed. Uncoupled and paired 1/4[111] superpartial dislocations moved dragging the nearest-neighbour and next-nearest neighbour APB (NNAPB and NNNAPB), respectively as shown in figure 5 (a) and (b). The atomic arrangements on {101} plane for perfect crystals, near the NNAPB and NNNAPB are shown in figure 5 (c), (d) and (e), respectively. The energies of NNAPB ($\gamma_{NN}$) and NNNAPB ($\gamma_{NNN}$) depend strongly on the number of wrong bonds and are given by, [8]

$$\gamma_{NN} = \frac{2\sqrt{2}}{a_0^2} \left[ 4V_1S_1 + V_2 \left( S_2^2 - 4S_1^2 \right) \right]$$

And

$$\gamma_{NNN} = \frac{2\sqrt{2}}{a_0^2} \left[ 2V_2S_2 \right]$$

where $a_0$ is the lattice constant, $V_1$ and $V_2$ are the first- and second-nearest ordering energies and $S_1$ and $S_2$ are the first- and second-nearest degrees of order, respectively. It should be noted that $S_1$ and $S_2$ are
0.5 and 1 for the perfect D0₃ lattice, respectively. In addition, tensions of NNAPB (τ_NN) and NNNAPB (τ_NNN) are written as [4]

\[ \tau_{NN} = \frac{\gamma_{NN}}{b}, \]  
\[ \tau_{NNN} = \frac{\gamma_{NNN}}{2b}, \]  

where \( b \) is the magnitude of \( 1/4[111] \) superpartials. Substituting each parameter for equations (2)–(5), \( \tau_{NN} \) and \( \tau_{NNN} \) were calculated to be 268 and 204 MPa, respectively. Since the APB tension was much higher than frictional stress of \( 1/4[111] \) superpartials, APB could pull back the superpartials during unloading, which resulted in APB pseudoelasticity. In fact, to-and-fro motion of \( 1/4<111> \) superpartials during loading and unloading was confirmed to occur by in-situ TEM observation [6].

At A orientation, perfect pseudoelasticity appeared while strain recovery at B orientation was small, though \( (011)[111] \) slip was a major deformation mode at both orientations. Frequency of cross-slip of \( 1/4[111] \) screw dislocation is higher at B orientation than at A orientation. The cross-slip segments suppressed the reversible motion of the dislocations resulting in the decrease in strain recovery.

Twinning pseudoelasticity associated with twinning and untwinning of \( (\bar{2}11)[111] \) pseudo-twins appeared at C orientation. The \( (\bar{2}11)[111] \) pseudo-twin showed tension-compression asymmetry; the twins were formed only in compression. It is also noted that \( (1\bar{1}2)[\bar{1}11] \) pseudo-twins were observed to appear in the crystals tensile-deformed at A orientation. Such tension-compression asymmetry is the common feature of \( \{211\}<111>-type \) twins in bcc metals. The interface energy for the pseudo-twins (\( \gamma_T \)) and the tension (\( \tau_T \)) are given by, [8]

\[ \gamma_T = \frac{2\sqrt{2}}{\sqrt{3}a_0^2} \left\{ \left| \varepsilon_1 \right| \left( 4S_1^2 - S_2^2 \right) + V_2 \left( 2S_2^2 - 5S_1^2 - 0.25 + S_1 \right) \right\}, \]  
\[ \tau_T = \frac{\gamma_T}{t}, \]

where \( t \) is the twin shear for \( (\bar{2}11)[111] \) pseudo-twin. \( \tau_T \) was calculated to be 275 MPa, comparable with \( \tau_{NN} \) and \( \tau_{NNN} \). Therefore, it is strongly suggested that the high interface energy of the pseudo-twins resulted in the twinning pseudoelasticity.

5. Conclusions
APB and twinning pseudoelasticities in D0₁-ordered Fe-23.8at%Ga single crystals compressed at room temperature were investigated. The operative pseudoelastic mode could be controlled by changing the compressive axis. The tensions of APB and twin interfaces were the driving force for APB and twinning pseudoelasticities in Fe-23.8at%Ga single crystals, respectively.

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