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Effect of Al concentration on pseudoelasticity in Fe_3Al single crystals

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Abstract

Pseudoelasticity in Fe_3Al single crystals with different Al contents was investigated focusing on the dislocation configuration and the ordered domain structure. Giant pseudoelasticity only appeared in the $D0_3$-ordered Fe_3Al single crystals, while the B2-ordered crystals and those with the disordered α phase exhibited small strain recovery. The amount of shape recovery in the $D0_3$-ordered crystals showed a maximum near 23.0at.%Al and decreased with increasing deviation from this Al concentration. In the $D0_3$ phase at 22.0–25.0at.%Al, 1/4[1 1 1] superpartial dislocations moved individually dragging the nearest-neighbour antiphase boundaries (NNAPB), while couplets of the superpartials were observed to bow out, dragging the next-nearest-neighbour antiphase boundaries (NNNAPB) in Fe–28.0at.%Al. In Fe–22.0–25.0at.%Al single crystals, the NNAPB pulled back the superpartials to decrease its energy during unloading, resulting in the giant pseudoelasticity. In contrast, the surface tension of the NNNAPB was lower than that of the NNAPB, leading to the small strain recovery in Fe–28.0at.%Al.

Keywords: Iron aluminides; Transmission electron microscopy; Order–disorder phenomena; Shape memory alloys; Dislocation

1. Introduction

Shape memory materials that show giant pseudoelasticity, such as Ti–Ni and Cu–Al–Ni alloys, have been widely used for eyeglass frames, cellular phone antennas and catheters, due to their large recoverable strain [1]. The pseudoelasticity of Ti–Ni and Cu–Al–Ni alloys is known to result from a thermoelastic martensitic transformation: a stress-induced transformation during loading and the reverse transformation during unloading. Unfortunately, the thermoelastic martensitic transformation seldom occurs in ferrous alloys, although Fe–Pd and Fe–Pt alloys exhibit the transformation [1]. Hence, there are few ferrous alloys showing giant pseudoelasticity caused by the thermoelastic martensitic transformation. In contrast, Fe_3Al single crystals with the $D0_3$ structure were found to demonstrate giant pseudoelasticity regardless of the martensitic transformation [2–13]. Recently, we successfully improved the pseudoelasticity of Fe_3Al single crystals; a recoverable strain of 5.0% was realized at 23.0at.%Al [8–12]. When pseudoelasticity appeared in the $D0_3$-ordered crystals, a superpartial dislocation with Burgers vector (b) of 1/4[1 1 1] moved individually dragging the nearest-neighbour antiphase boundary (NNAPB) during loading [4–12], although a fourfold dissociation of $b = [1\,1\,1]$ occurred in Fe–28.0at.%Al [9,14,15]. During unloading, the superpartials moved back due to the surface tension of the NNAPB, resulting in the pseudoelasticity. It should be noted that the intersection between a specific type of ordered domain boundaries and the superpartials was considered to induce the individual motion of the superpartials and to assist the strain recovery [8,9]. Thus, the fine ordered domain structure in Fe–23.0at.%Al single crystals was favourable for the appearance of perfect pseudoelasticity.

In the last two decades, the Fe–Al phase diagram near 25.0at.%Al has been extensively examined since the process of ordering and phase separation is quite unique. Fig. 1

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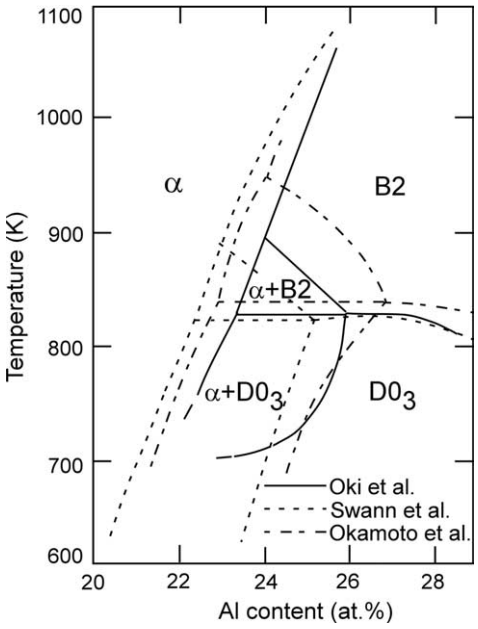

Fig. 1. Phase diagrams of Fe–Al binary systems near 25.0at.%Al [16–18].

shows the phase diagrams proposed by many authors [16–19]. The phase diagrams basically have a common feature, although the chemical compositions of the phase boundaries slightly differ. In the phase diagrams, a tricritical point exists at the end of α/B2 phase boundary; the $(\alpha + B2)$ and $(\alpha + D0_3)$ phase fields are present at lower temperatures. Furthermore, the $D0_3$ single-phase region extends over a wide Al concentration range (C_{Al}). Therefore, the pseudoelastic behaviour of Fe_3Al single crystals may strongly depend on the Al concentration. In this paper, we report the effect of Al concentration on pseudoelasticity in Fe_3Al single crystals with an emphasis on the dislocation configuration and the ordered domain structure.

2. Proposed model for pseudoelasticity in Fe_3Al

In Fe–23.0at.%Al single crystals with the $D0_3$ structure, superpartial dislocations with $b = 1/4\langle 1\,1\,1\rangle$ independently glided, trailing the NNAPB during loading. During unloading, the superpartials were pulled back by the surface tension of the NNAPB, which caused the pseudoelasticity. Kubin et al. [4] and Langmaack et al. [7] performed in situ observations of the deformation microstructure using a transmission electron microscope (TEM) and observed the to-and-fro motion of the superpartials during loading and unloading. A typical stress–strain curve of a Fe_3Al single crystal is shown in Fig. 2. In the figure, the Fe_3Al crystal yields at a critical resolved shear stress, τ_y, during loading, while the recovery of the plastic strain begins at a shear stress, τ_r, during unloading. When pseudoelasticity appears in Fe_3Al single crystals, the following equations hold true during loading and unloading [4–12]

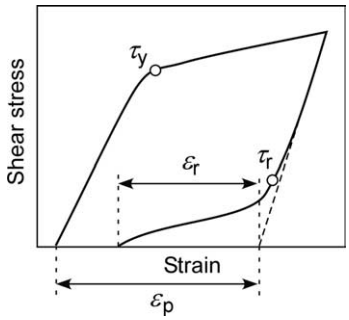

Fig. 2. Schematic illustration of a stress–strain curve of a Fe_3Al single crystal.

$$\tau_y = \tau_0 + \tau_b, \tag{1}$$

$$\tau_r = \tau_b - \tau_0, \tag{2}$$

where τ_0 is the frictional stress (Peierls stress) of $1/4\langle 1\,1\,1\rangle$ superpartials and τ_b is the backward stress acting on the superpartials. Both τ_0 and τ_b can be deduced by solving the simultaneous Eqs. (1) and (2). It is noteworthy that τ_0 of Fe_3Al is almost identical to that of the body-centred cubic metals. On the other hand, τ_b is mainly caused by the surface tension of the NNAPB (τ_{NN}) following $1/4\langle 1\,1\,1\rangle$ superpartials, given by [20]

$$\tau_{NN} = \frac{2\sqrt{2}}{ba_0^2}\left\{4V_1S_1^2 + V_2\left(S_2^2 - 4S_1^2\right)\right\}, \tag{3}$$

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. However, τ_b measured at $C_{Al} = 23.0$at.% is higher than τ_{NN} by 10–20 MPa [9]. Hence, there are other factors when considering τ_b. Considering the dislocation configuration in Fe_3Al, a fourfold dissociation of $\langle 1\,1\,1\rangle$ superdislocations generally occurs, especially at higher C_{Al} [14,15]. In this case, the yield stress of Fe_3Al is extremely low since no APB is left behind the superpartials (i.e., $\tau_y = \tau_0$). However, when giant pseudoelasticity takes place in Fe_3Al, $1/4\langle 1\,1\,1\rangle$ superpartials move individually dragging the NNAPB resulting in higher yield stress. During unloading, the NNAPB pulls back the superpartials resulting in the pseudoelasticity. One can say that a decrease in the NNAPB energy leads to the individual motion of the superpartials. However, if the energy of the NNAPB decreases, the backward stress, τ_b in Eqs. (1) and (2) is also reduced. Thus, pseudoelasticity is unlikely to occur. In order to solve this inconsistency, the effect of the ordered domain structure in Fe_3Al on the pseudoelasticity was considered [9].

In the $D0_3$ structure, there are three types of ordered domain boundaries: B2(I)-, B2(II)- and $D0_3$-types [21,22]. The displacement vector (R) of B2(I)- and B2(II)-type boundaries (hereafter, both are designated as B2-type) is $1/4\langle 1\,1\,1\rangle$, while $R = 1/2\langle 1\,1\,1\rangle$ at $D0_3$-type boundaries. If the leading superpartials with $b = 1/4[1\,1\,1]$ glide independently leaving the NNAPB and pass through the domain