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Origin of pseudoelasticity by twinning in $D0_3$-type Fe_3Ga

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ABSTRACT

We investigated the process of twin boundary migration to clarify the origin of pseudoelasticity by twinning in $D0_3$-type Fe_3Ga using first-principles calculations. We calculated the energy profile of twin boundary migration and found that although energy barriers appear during twin boundary migration in bcc Fe and bcc Mo, there was no energy barrier for twin boundary migration in $D0_3$-type Fe_3Ga. Analysis of the shear strain at each twin layer revealed that twin boundary migration in $D0_3$-type Fe_3Ga proceeded not in a layer-by-layer fashion but by the sliding of more than two layers that include the twin boundary, which led to the flat energy profile in $D0_3$-type Fe_3Ga. This sliding mechanism originated from shear strain introduced near the twin boundary to accommodate the lattice distortion induced by the difference in the atomic arrangement between the $D0_3$ matrix and the pseudo twin layers.

1. Introduction

Pseudoelastic behavior, which appears in shape memory alloys, is due to stress-induced martensitic transformation: the applied stress is recovered by reverse transformation of the martensites during unloading without heating. However, in addition to stress-induced martensitic transformation, Fe_3Ga single crystals with $D0_3$ structure were found to exhibit pseudoelasticity based on reversible dislocation motion, and twinning and untwinning [1]. The twinning pseudoelasticity becomes more dominant with decreasing deformation temperature in ordered Fe_3Ga single crystals [2]. In ordered alloys, there are cases in which the mirror symmetry at the twin boundary disappears because of the change in the atomic arrangement in the twin region caused by introducing twin shear. The shape of the unit cell is also deformed in the twin region. In the case of the $D0_3$-type structure, the unit cell of the twin region changes to an orthorhombic structure. Thus, the twinning deformation can be regarded as a type of displacive transformation. The energy difference between the matrix and pseudotwin phase is crucial for twinning pseudoelasticity. This energy difference is considered to be the driving force for the recovery of the twin strain upon unloading. On the other hand, a higher energy difference suppresses the formation of pseudotwins. In our previous study [3], we investigated the stability of pseudotwins in $D0_3$-type Fe_3Ga, Fe_3Al, Fe_3Ge and Fe_3Si using first-principles calculations and found that the energy difference between the matrix and the pseudotwin phase is lowest in Fe_3Ga. The calculated energy difference of 1.23×10^8 J/m^3 in Fe_3Ga is in good agreement with the experimental value of 1.56×10^8 J/m^3 obtained from the stress-strain curves of Fe–24.4 at.%Ga single crystals by Yasuda et al. [4]. However, for twinning pseudoelasticity, not only a low formation energy of the pseudotwin phase but also a low migration energy of the twin boundary is required.

The migration energy of twin boundaries has been calculated based on the generalized planar fault energy (GPFE) with respect to the shear displacement for body-centered cubic (bcc) [5–8] and face-centered cubic (fcc) metals [5,9]. Wang and Sehitoglu [10] calculated the GPFE curve of pseudowinning in $D0_3$-type Fe_3Ga and found that the energy barrier of pseudotwin migration is 50 mJ/m^2, which is lower than that in fcc metals but comparable to that in bcc Mo [5] and bcc Fe [7]. Ojha et al. [11] evaluated the effect of interstitial B on the GPFE curve of pseudowinning in $D0_3$-type Fe_3Ga. These calculated results were obtained under the assumption that the migration of the twin boundary proceeds in a layer-by-layer fashion, i.e., twin shear is introduced layer by layer. In our previous study [3], to avoid this assumption, twin shear was introduced on half of the layers in the supercell and the shear strain of the supercell, which was introduced with the twin shear, was gradually reduced to allow the twin boundary to migrate by structural relaxation. No energy barrier was found in the energy profile of the twin boundary migration. Analysis of the densities of states (DOS) suggested that the minority-spin DOS around the Fermi level in the $D0_3$ layers contributed to the

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stability of the pseudotwin phase. However, the question remains as to how the twin boundary migrates with no energy barrier in $D0_3$-type Fe_3Ga. Comparisons with bcc metals, which have the same atomic coordinates as $D0_3$-type alloys, can provide information about the mechanism of twin boundary migration in $D0_3$-type Fe_3Ga.

In the present study, to clarify the origin of the flat energy profile of twin boundary migration in $D0_3$-type Fe_3Ga, we calculated the energy profile of twin boundary migration in $D0_3$-type Fe_3Ga, bcc Fe and bcc Mo. The changes in shear strain at each twin layer during twin boundary migration were examined to clarify the migration process of the twin boundary. We also discuss the validity of the model of twin boundary migration in a layer-by-layer fashion.

2. Structure and migration process of twin boundary

We begin by considering the structure and migration process of twin boundaries in bcc metals. As compared to $\{1\,1\,1\}\langle 1\,1\,2\rangle$ twins in fcc metals, the general trend is that $\{1\,1\,2\}\langle 1\,1\,1\rangle$ twin boundaries in bcc metals exhibit higher formation energy and lower migration energy [5–9]. To the best of our knowledge, the reason for this trend has not been clearly explained. However, one possible reason for this trend may be differences in the atomic arrangement near the twin boundary. Fig. 1 shows the atomic arrangement of a bcc metal in which $\{1\,1\,2\}\langle 1\,1\,1\rangle$ twin shears are introduced on half of the layers. The stacking sequence along the $\langle 1\,1\,0\rangle$ direction is AB stacking. The displacement vector of the stacking, $1/2\,\langle 1\,0\,0\rangle$, is not parallel to the twin shear,

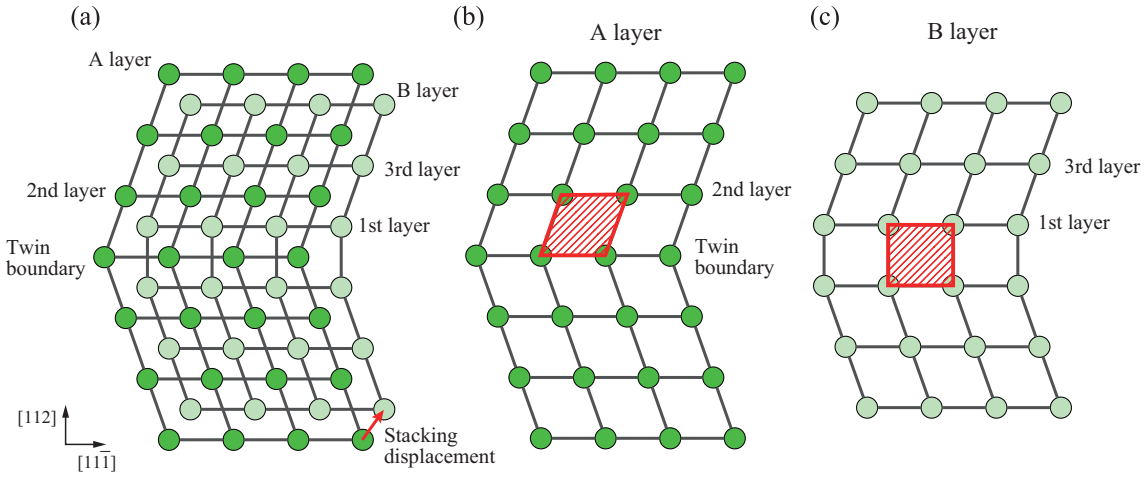

Fig. 1. Atomic arrangement of $\{1\,1\,2\}\langle 1\,1\,1\rangle$ twin in bcc metals. (a) A and B layers. (b) A layer, and (c) B layer.

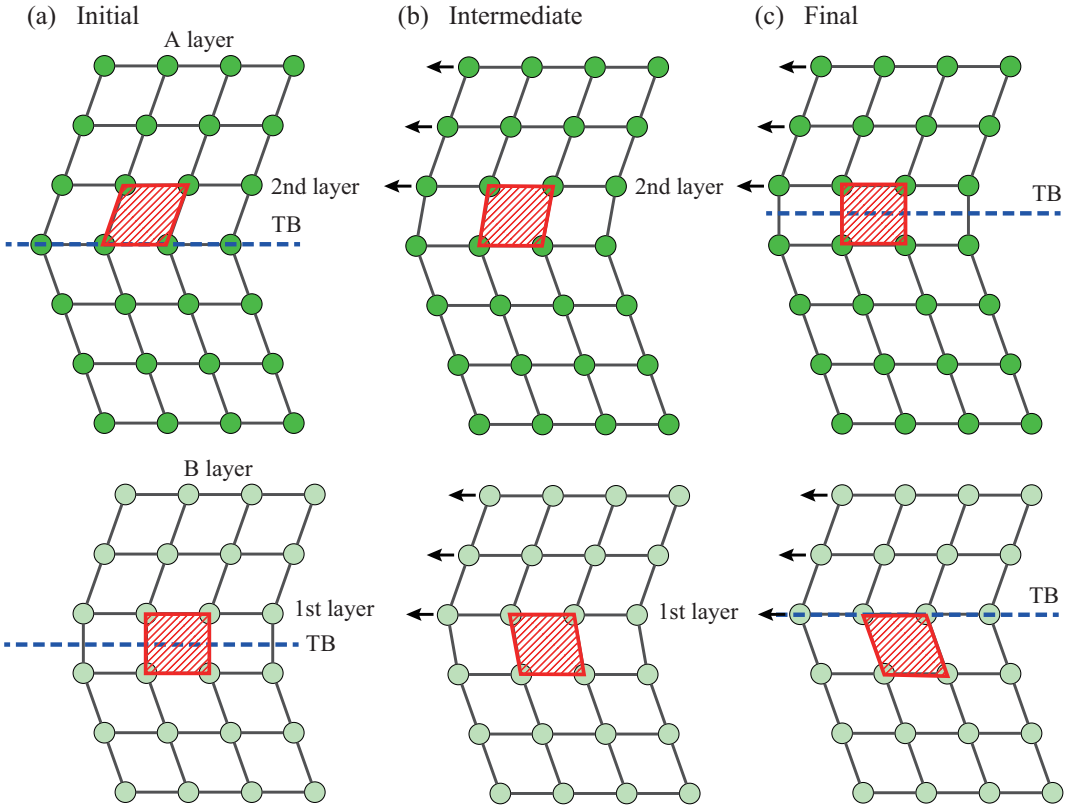

Fig. 2. Changes in the atomic arrangement of A and B layers during the twin boundary migration in bcc metals: (a) Initial state, (b) intermediate state, and (c) final state.