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Formation process of the incompatible martensite microstructure in a beta-titanium shape memory alloy

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ABSTRACT

The formation modes of habit plane variant (HV) clusters (HVCs) in a Ti-23Nb-3Al (mol%) shape memory alloy were investigated by *in situ* optical microscopy with high-speed digital video camera. In addition to the kinematic compatibility condition, the nucleation mode and the interfacial energy between martensites were clearly shown to have critical roles. The V_I cluster, which is formed by two HVs connected by a {111} type I twin, predominated in the early stage of the martensitic transformation, and had a lower energy barrier to nucleation and growth than did the V_{II} cluster, which is formed by two HVs connected by a <211> type II twin. Eighty percent of the V_I clusters were observed to form by paired nucleation or branching, in which the junction plane corresponds to the nucleation site of the relevant HV(s). In contrast, V_{II} clusters formed as a result of collisions of HVs. Neither paired nucleation nor branching was observed for V_{II}. V_I nuclei rather than V_{II} nuclei had a strong tendency to form, and this difference was not fully explained by the kinematic compatibility (KC) conditions. The junction planes formed by the collision of growing HVs should have larger deviation from the KC condition. The compatibility of the junction plane between HVs depends on the formation modes.

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1. Introduction

The martensite plate in most shape memory alloys (SMAs) has a habit plane that is an invariant plane as described by the phenomenological theory of martensite crystallography [1–3]. Such a martensite plate is conventionally called a “habit plane variant (HV)”. The martensite microstructure consists of clustering HVs that reduce the net strain of the martensitic transformation in general [4]. A cluster of HVs is termed an “HV cluster (HVC)” in this study. The concept of self-accommodation or that of the plate group well explain the nature of the martensite microstructure [4]. However, understanding the connection between HVs is necessary for completely understanding the martensite microstructure and the thermomechanical properties of SMAs. Recent studies have shown that understanding the kinematic compatibility (KC) [5] between HVs is a key to understanding the martensite microstructure [6–17] and to controlling the properties of SMAs [18–21].

The continuity of a deformation at the interface between domain Ω_A and Ω_B with constant deformation gradients **A** and **B**, respectively, can be maintained if Eq. (1) has a solution for **Q**, **n**, and **a** [22].

$$\mathbf{QA} - \mathbf{B} = \mathbf{a} \otimes \mathbf{n} \tag{1}$$

In Eq. (1), **Q** is a rigid body rotation, and **a** and **n** are vectors, with the vector **n** being that normal to the plane of the interface between Ω_A and Ω_B. Eq. (1) corresponds to the KC condition for the HVC if Ω_A and Ω_B are HVs. The invariant plane condition at the habit plane is expressed by Eq. (1) assuming that **QA** is the deformation gradient of an HV and $\mathbf{B} = \mathbf{I}$, where **I** is the identity matrix representing the parent phase. For an HVC, A and B are the deformation gradients of

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the HVs and the rotation **Q** is the index of incompatibility of the connection between HVs. In general, SMAs, $\mathbf{Q} \neq \mathbf{I}$ and the junction plane between HVs maintains the KC condition when an HV is rotated by **Q**; the rotation **Q** breaks the KC condition at the habit plane of the HV. Therefore, the incompatibility remains somewhere in the HVC for the case of $\mathbf{Q} \neq \mathbf{I}$ in general. Though the existence of the incompatibility is obvious, its location is not clear from geometrical considerations alone. Determining the location of the incompatibility is essential for understanding the nature of the martensite microstructure and the generation of lattice defects during cyclic actuation of SMAs.

In our previous work [9], the relationship between the frequency of formation of HVC and **Q** was investigated for a Ti-23Nb-3Al (mol%) SMA using transmission electron microscopy (TEM). Fig. 1 shows the typical morphologies and KC conditions of the HVCs of this alloy, which undergoes a β (bcc) − α″ (orthorhombic) martensitic transformation [23]. There is no lattice invariant deformation in the alloy because the middle eigenvalue of the lattice deformation is unity as reported in $Ti_{50}Ni_{39}Pd_{11}$ alloy [21]. There are 10 types of HVCs in combination logic and only two HVCs that have very small **Q** are dominant in the alloy. The first type is termed a "V_I cluster" and is formed by two HVs with the junction plane corresponding to the K_1 plane of the $\{111\}_o$ type I twin. The subscript "o" denotes α″-martensite. The second type is termed a "V_{II} cluster" with the junction plane corresponding to the K_1 plane of the $<211>_o$ type II twin. A theoretical analysis based on Eq. (1) showed the KC condition at the habit plane and junction plane to be conflicting each other in this alloy because $\mathbf{Q} \neq \mathbf{I}$; the rotation angle of **Q** was calculated to be 0.69° and 0.57° for V_I and V_{II} clusters, respectively. The KC condition at the junction plane is satisfied when **Q** is applied to one HV and then the exact $\{111\}_o$ type I twin orientation relationship (OR) and $<211>_o$ type II twin OR appears across the junction plane for V_I and V_{II}, respectively. Interestingly the location of the incompatibility was found to depend on the type of HVC in our previous study using precise Kikuchi line analysis [9]. For the V_I cluster, 80% of the junction planes had a $\{111\}_o$ type I twin OR with angular deviation less than 0.1° (less than the error of the orientation analysis by Kikuchi line). Here, the rotation **Q** acts and the KC at the junction plane is maintained at the expense of the KC at the habit plane. However, for the V_{II} cluster, 70% of the junction planes showed angular deviations greater than 0.4° from the exact $<211>_o$ type II twin OR. Here, most of the junction planes were incompatible with maintaining the KC condition at the habit plane. Note that a microscopic observation of the fully developed microstructure did not seem to be able to explain the relatively high degree of maintaining KC at the junction plane of the V_I cluster. Diversity of the microstructure in the vicinity of the junction plane has been considered to depend not only on the KC condition but also on the dynamic features of the formation of the microstructure [8]. Information obtained from a static observation of the fully transformed microstructure is, however, limited to the former factor.

Against this background, we focused on the dynamic process by which the martensite microstructure forms. The purpose of this study was to reveal this process and the origin of the location of incompatibility by *in situ* observation of the process of the martensitic transformation. According to these *in situ* observations, the V_I and V_{II} clusters showed distinct differences in formation modes, and these differences were related to the differences in their locations of incompatibility.

2. Experimental procedures

2.1. Alloy

Following our previous study [9], Ti-23 mol%Nb-3mol%Al was selected for this study. An ingot with a mass of about 10 g was fabricated from high-purity starting elements of Ti (99.99%), Nb (99.9%), and Al (99.99%) by Ar arc-melting with a non-consumable W-electrode in an Ar-1%H_2 reducing atmosphere. Each ingot was arc-melted and then flipped. This set of melting procedures was repeated five times to ensure homogeneity of the product. The change in weight caused by arc-melting was less than 0.16 wt % and was judged to be negligible, hence requiring no chemical analysis. The oxygen content of the ingots previously fabricated by this method was less than 400 ppm by weight; thus, we assumed that the oxygen content of the current ingot was similar. The ingot was wrapped in a Ti foil, encapsulated in a quartz tube filled with an Ar atmosphere, homogenized at 1273 K for 7.2 ks, and then quenched by breaking the quartz tube in iced water. The martensitic transformation temperatures of the ingot were determined by preliminary differential scanning calorimetry to be M_s = 291 K, M_f = 249 K, A_s = 277 K and A_f = 319 K. The hysteresis, $(A_f + A_s - M_f - M_s)/2$, was 28 K and seemed to be high, comparing with that of Ti-Ni-Pd with middle eigenvalue of unity [19]. However, according to that Ti-24 mol%Nb-3mol%Al alloy has hysteresis of about 60 K and the middle eigenvalue is 0.999 [24], the hysteresis seems to be lowered in the present alloy by the middle eigenvalue of 1.0003 as described in the following.

Owing to that $A_s < RT < A_f$, the lattice parameters of both phases were able to be determined directly at room temperature (RT, 298 K) by a preliminary X-ray diffraction as $a_b = 328.0 \pm 0.5$ pm, $a_o = 317.5 \pm 0.7$ pm, $b_o = 479.0 \pm 0.1$ pm, and $c_o = 464.0 \pm 0.1$ pm, where the subscript b indicates the parent (bcc) phase. The eigenvalues of the lattice deformation with Au-Cd type lattice correspondence [25] were 0.9680, 1.0003 and 1.0326, with the middle eigenvalue being very close to unity at RT; no lattice-invariant deformation was observed by TEM [19,23]. **Q** of V_I and V_{II} clusters

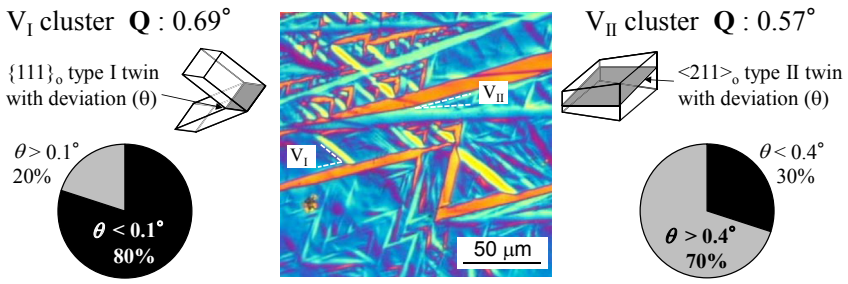

Fig. 1. Typical morphologies and the KC conditions of the HVCs in Ti-23Nb-3Al. "V_I cluster" and "V_{II} cluster" are formed with the junction plane corresponding to the K_1 plane of the $\{111\}_o$ type I twin and the $<211>_o$ type II twin, respectively. The rotation angles for KC condition at junction plane (**Q**) are 0.69° and 0.57° for V_I and V_{II} clusters, respectively. Our previous study showed that rotation **Q** acted only in V_I cluster and the junction plane of V_{II} is incompatible [9].

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