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Deformation twinning in Ni_2MnGa

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Abstract

Deformation twinning is investigated in the martensitic phase of a $Ni_{46.75}Mn_{34}Ga_{19.25}$ (at.%) alloy. X-ray and electron diffraction are used to establish the crystallography of the non-modulated tetragonal martensite, and transmission electron microscopy is employed to deduce the twinning parameters. It is convenient to define the twinning parameters with respect to a "monoclinic" unit cell, designated 2M: then K_1, η_1, K_2, and η_2 are (001), [100], (100), and [001] respectively. The Burgers vector of the active twinning disconnections is close to 1/6[100] and the disconnections are associated with steps of height $d_{(002)}$. These defects are expected to be highly mobile since their motion does not require atomic shuffling. It is shown that periodic arrangements of two layer twins produce modulated crystal structures, such as 14M.

Keywords: Transmission electron microscopy; Heusler phases; Deformation structure; Twinning; Dislocations

1. Introduction

Alloys with compositions near Ni_2MnGa (hereafter NMG) are ferromagnetic shape memory alloys (FSMAs) suitable for device applications [1–4]. For example, in the martensitic state, strains of up to 10% can be induced reversibly by an external magnetic field [5,6]. To exploit the potential of this material, it is important to elucidate the microstructural processes underpinning its useful properties.

NMG transforms from the cubic $L2_1$ ordered Heusler phase [7] to one of several known martensite structures. The ground state of the martensitic phase is thought to be tetragonal [8], however, several studies have reported more complex forms wherein tetragonal or orthorhombic regions are modulated by thin lamellae of twinned material arranged more or less periodically [9–11]. The objective of the present work is to characterise these twinned regions using transmission electron microscopy (TEM) and to deduce their mechanism of formation. In Section 2 we review the crystallography of NMG phases, and outline the principles of deformation twinning in Section 3. Our experimental observations are set out in Section 4, and interpreted in Section 5. Section 6 is a discussion of the results, and Section 7 is a summary of our conclusions.

2. Crystal structures

A unit cell of cubic NMG is depicted in Fig. 1a. This phase is denoted C with lattice parameter a_c and spacegroup $Fm\bar{3}m$ [7]. At lower temperatures a tetragonal form T arises [9] (Fig. 1b), with lattice parameters a_T and c_T, and spacegroup $F\frac{4}{m}mm$. Both of these unit cells comprise 16 atoms: 4 lattice sites, each decorated by a Ni_2MnGa motif in the stoichiometric compound. In the present context it is convenient to use an alternative description of the tetragonal form in terms of a "monoclinic" unit cell exhibiting 8 atoms Fig. 1c [12]. This body-centred cell is designated 2M, and has lattice parameters a_{2M}, b_{2M}, c_{2M}, and β_{2M}, where $a_{2M} = c_{2M}$, $b_{2M} = b_T$, $c_{2M} = 1/2\sqrt{(c_T^2 + a_T^2)}$, and $\beta_{2M} = 2\tan^{-1} c_T/a_T$. All three unit cells depicted in Fig. 1

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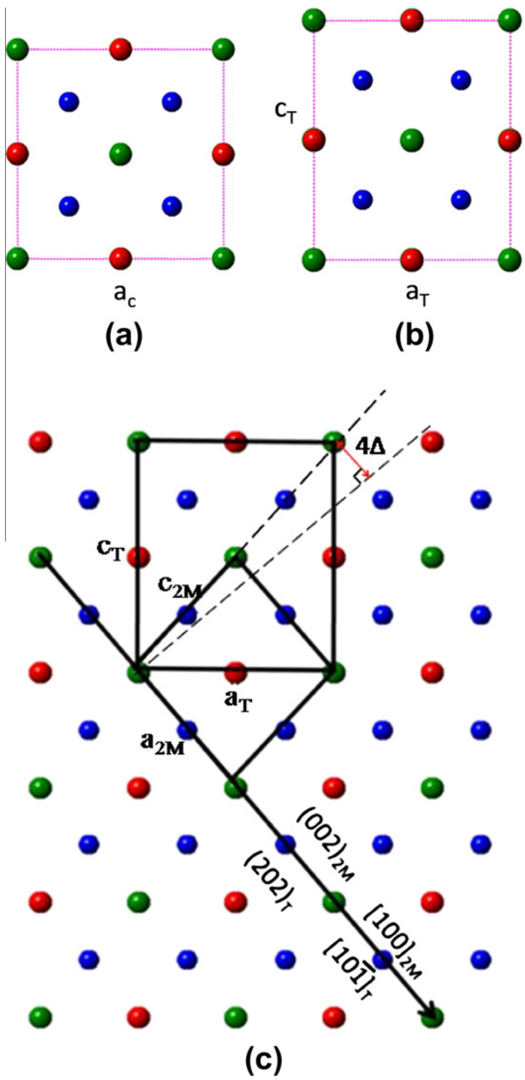

Fig. 1. Crystal structures: (a) cubic, C; (b) tetragonal, T; (c) monoclinic, 2M. Mn, Ga and Ni are represented by green, red and blue symbols, respectively. All structures are viewed along their [0 1 0] directions.

are viewed along their [0 1 0] direction. As shown in Fig. 1c, successive $(0\,0\,2)_{2M}/(2\,0\,2)_T$ planes are relatively sheared with displacement Δ in the direction $[\bar{1}\,0\,0]_{2M}/[\bar{1}\,0\,1]_T$ [12,13]. We subsequently show that the Burgers vectors of twinning disconnections are equal to $2\Delta[1\,0\,0]$. The coordinate transformations **P** inter-relating the C, T and 2M crystal structures are set out in Appendix A.

3. Deformation twinning

The mechanism of deformation twinning in various crystal structures has been reviewed by Christian and Mahajan [14]. It proceeds by the motion of twinning dislocations, referred to here as disconnections, since these defects exhibit both dislocation and a step character [15]. In simple cases the Burgers vectors **b** of such disconnections are parallel to η_1, and their step heights h, are equal to the interplanar spacing of the K_1 planes. Motion of a disconnection across each sequential K_1 plane produces

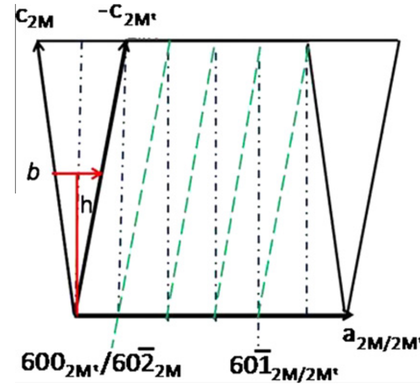

Fig. 2. Schematic illustration of twinned unit cells 2M and 2M^t projected along [0 1 0]. The twinning parameters K_1, η_1, K_2, and η_2 are (0 0 1), [1 0 0], (1 0 0), and [0 0 1], respectively, and the elementary twinning disconnection has $\mathbf{b} = 2\Delta[1\,0\,0]$ and $h = d_{(002)}$. The diagram is constructed for a nominal value of Δ of 1/12.

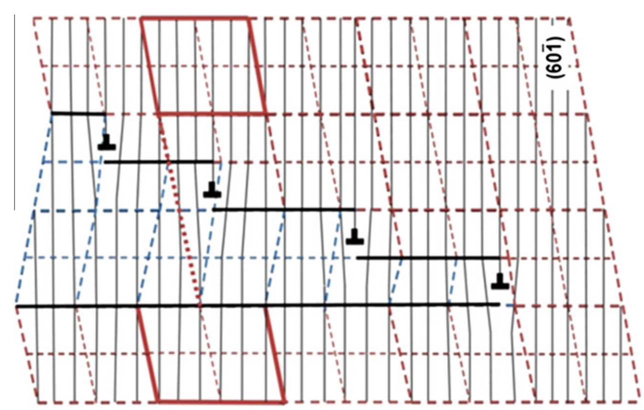

Fig. 3. Schematic view along [0 1 0] of the tip of a four layer deformation twin in a 2M crystal. The dislocation symbols mark the disconnections. A half plane of type $(6\,0\,\bar{1})_{2M}$ ends at each disconnection. The offsets of the 200 matrix (red) planes across the twin (blue) changes from one disconnection to the next by +1/3, −1/3, and 0. The offset of 0 after three disconnections is highlighted with a red dotted line. The diagram is constructed for a nominal value of Δ of 1/12. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the twin. The twinned form of 2M crystals, designated 2M^t, is depicted in Fig. 2. We take the twinning operation inter-relating 2M and 2M^t to be a mirror reflection across the K_1 plane, as defined in Appendix A. In this case the twin is compound, since K_1, η_1, K_2, and η_2 are all rational, as depicted in Fig. 2. For simplicity the nominal value of Δ is taken to be the rational value 1/12, in this work, unless stated otherwise.

The $(\mathbf{b}, h)$ parameters for twinning disconnections can be obtained from the theory of interfacial defects [16]: for the elementary disconnection we have $\mathbf{b} = 1/2[1\,1\,\bar{1}]_{2M^t} - 1/2[1\,1\,1]_{2M}$, which can be expressed as $\mathbf{b} = 2\Delta[1\,0\,0]$, and $h = d_{(002)}$ (indexing relates to 2M unless otherwise stated). Motion of this disconnection is expected to occur at low stresses, since all atoms would be sheared into the correct positions without additional shuffling [14]. Deformation