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Direction of modulation during twin boundary motion

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To study the change of modulation direction during deformation, two NiMnGa single crystals, one with a five-layered modulated tetragonal structure (5 M) and the other with a seven-layered modulated orthorhombic structure (7 M), were chosen. Synchrotron diffraction experiments show that the modulation takes place on the {1 1 0) plane along the ⟨1 1 0] directions. During deformation the *c*-axis orientation changes by twinning, and with this the direction of modulation obeying the twin relation also changes.

Keywords: Synchrotron radiation; Diffraction; Martensitic phase transformation; Twinning; Modulation

NiMnGa alloys close to the stoichiometric composition Ni_2MnGa belong to the quite new family of ferromagnetic shape memory alloys. These alloys are characterized by magnetic field-induced strain (MFIS) [1,2]. MFIS in NiMnGa alloys is based on the comparatively easy motion of twin boundaries under a magnetic field, which is especially promising from the point of view of application as actuators and sensors. Depending on the chemical composition and the heat treatment used, at least three martensitic structures can be distinguished in the NiMnGa system. However, the effect mentioned above only exists in two different modulated structures: the five-layered modulated tetragonal (5 M) and seven-layered modulated orthorhombic (7 M) structures. The modulation consists of periodic shuffling along the ⟨1 1 0] directions [3,4], and in diffraction patterns is observed as extra spots along this direction. The nature, stability and role of the modulation are described in [5–7]. The twinning stress of the third, non-modulated (NM), martensitic phase is much higher than those measured for the modulated structures [8]. Therefore, and because of the absence of a uniaxial magnetic anisotropy [9], MFIS does not exist in the NM structure. Thus, in order to understand the easy motion of twin boundaries in modulated NiMnGa structures, it is the aim of this work to study the behaviour of modulation during twin boundary motion.

To study the effect of twin boundary motion on modulation, two oriented NiMnGa single crystals, one with 5 M and the other with 7 M martensitic structure at room temperature, were chosen. The single crystals, prepared by the Bridgman method, were supplied by company Adaptamat. After slight deformation, the orientation of the single crystals was determined by means of Laue patterns in undeformed and deformed areas representing two martensitic variants related by twin relationship. The change of the direction of modulation was measured by diffraction of high-energy synchrotron radiation (100 keV) using beam line HARWI-II at DESY in Hamburg, Germany. To do this, before and after deformation the single crystals were transmitted by X-rays at two specific places. Since the modulation is only visible when the beam direction is parallel to the *c*-axis, the samples were X-rayed along directions parallel to the main tetragonal and orthorhombic axes (possible *c*-axis localization) to find optimal diffraction parameters. The modulation in the 5 M and 7 M structures is visible by the presence of four and six extra spots along the ⟨1 1 0] direction between the main reflections, respectively.

All the planes and directions mentioned in this paper are given in a cubic coordinate system that is expressed with respect to cubic axes of the parent $L2_1$ phase. The tetragonal and orthorhombic unit cell dimensions are given in the orders $a > c$ and $a > b > c$, respectively.

Synchrotron diffraction in transmission of a sample volume of 3 mm × 3 mm × 0.5 mm in different directions shows that the structure modulation takes place along ⟨1 1 0] directions. Modulation along the ⟨1 1 0]

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directions has already been shown by Ge et al. [10] with high-resolution transmission electron microscopy. The different modulation directions belong to different areas in the single crystal and are separated by a faceted interface [10]. During twin boundary motion the *c*-axis orientation changes, and with this the direction of modulation with respect to the initial single crystal reference system also changes (Figs. 1–3). A schematic sketch of this process is shown in Figure 4 for the 7 M structure. The modulation is only visible when the beam direction is parallel to the *c*-axis. If the beam direction is along the *a*-axis (or the *b*-axis in the orthorhombic case), the characteristic diffraction features of modulation are absent. Figures 1 and 3 each present a diagram with the directions of modulation of a different variant. Initially the modulation is on the {1 1 0) plane in one variant while after deformation it is on the crystallographically equivalent plane in the variant generated by twinning. The modulation direction obeys the twinning relation. Additionally, in Figure 2 the upper diffraction pattern shows additional spots due to twinning. The non-split spots belong to the common ($\bar{2}$02) plane. The results clearly demonstrate that the direction of modulation in the 5 M and 7 M structures is crystallographically fixed normal to the *c*-axis. Thus, during twin boundary motion, different atom movements take place in modulated structures compared to non-modulated ones. In addition to ⟨1 0 1] movements, these are movements normal to the *a*–*c* plane. This may be the reason for the much lower stresses observed for twin boundary motion in modulated structures, as they have a more “flexible” lattice.

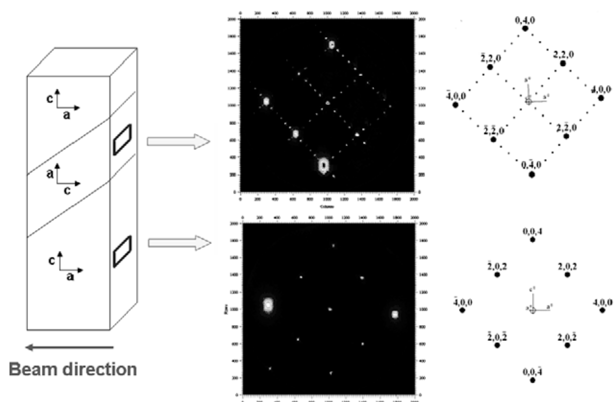

Figure 1. X-ray diffraction of a 5 M single crystal with a twin band (*c*-axis differently oriented). The modulation is only visible when the beam is parallel to the *c*-axis.

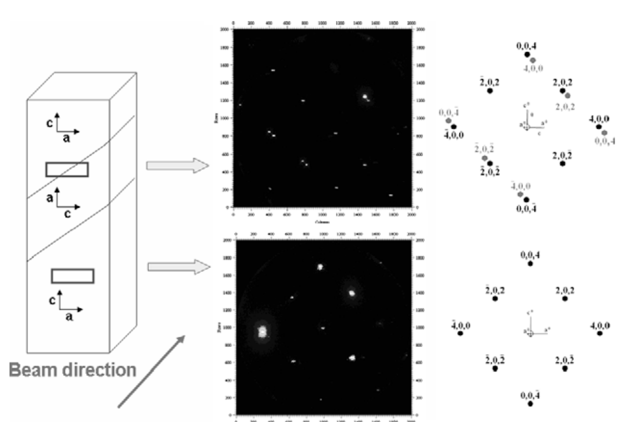

Figure 2. X-ray diffraction of a 5 M single crystal with a twin band (*c*-axis differently oriented). The upper diffraction pattern shows a twin relation.

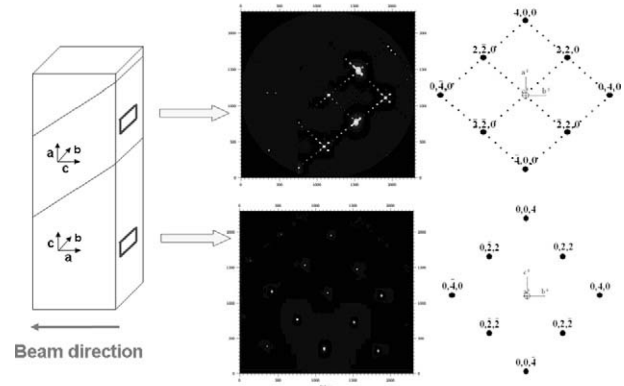

Figure 3. X-ray diffraction of a 7 M single crystal with a twin band (*c*-axis differently oriented). The modulation is only visible when the beam is parallel to the *c*-axis.

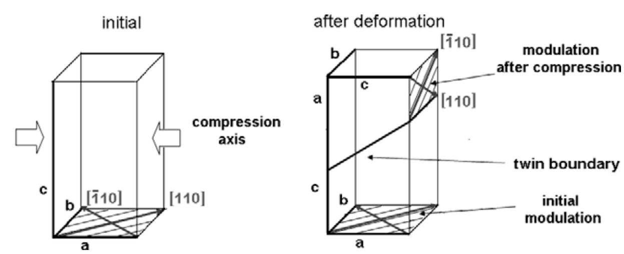

Figure 4. Change of direction of modulation in a 7 M structure during twin boundary motion induced by compression in the *a*-direction.

Note that in the 7 M structure there also occurs another type of twinning system on {1 1 0) planes. However, motion of these twins only switches the *a*- and *b*-axes, leaving the *c*-axis unchanged. In other words, the direction of modulation does not change.

In summary, it is concluded that:

(1) Modulation takes place on {1 1 0) along ⟨1 1 0].
(2) The *c*-axis orientation changes during twin boundary motion, and with this the direction of modulation in the sample coordinate system also changes.

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