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A neutron diffraction, of the populations and orientation relationships between the twin domains formed in the martensitic phase transition in Ni₂MnGa has suggested a possible origin for its shape memory properties. It was found that small amounts of uniaxial stress or magnetic field can switch domains with c-axes perpendicular the constraint to ones in which they are parallel to it. The results suggest that plastic deformation in the martensitic phase takes place by twinning (change of domain), rather than by slip and that the shape memory property arises from the fixed orientation relationship between the

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martensitic twins and the high temperature cubic cell.

Ni, MnGa is one of the very few shape memory alloys which are also ferromagnetic. Materials exhibiting the shape memory effect can be formed at one temperature $T_{F'}$ then cooled to a lower temperature T_{p} and plastically deformed; on reheating to T_E they will regain their original shape. The origin of this effect is a structural phase transition which must occur at a temperature T_{M} intermediate between T_{E} and $T_{\rm D}$. In Ni₂MnGa $T_{\rm M}$ is 200 K, and the phase transition is from the cubic L2, Heusler structure to a pseudo-tetragonal structure with c/a ≈ 0.95 whose true structure is orthorhombic

Ni, MnGa

 $(a_{orth} = a_{tet} / \sqrt{2}, b_{orth} = 7a_{tet} / \sqrt{2}, c_{orth} = c_{tet})$ [1]. Although, up to now, the exact mechanism which allows shape recovery is not well understood, the shape memory property has already been exploited in devices used in fields as wide ranging as communications and medicine [2]. Its utility is further enhanced when it is combined with, ferromagnetism [3]. In an attempt to clarify the mesoscopic origin of shape memory we have used neutron diffraction with a multi-detec-

tor to follow the distribution and orientation of the twin domains which form in single crystals of Ni, MnGa during the martensitic transformation [5]. Experiments have been made on annealed and on pre-stressed crystals and also on crystals subject to in-situ stress and applied magnetic field. Neutron diffraction is a particularly appropriate tool for such a study because the martensitic distortion is big enough for the reflections from different domains to be easily resolved and the low neutron absorption of the alloy allows a relatively large (≈ 50 mm³) volume to be sampled. Scans through the positions of the fundamental reflections were made at small temperature intervals in the range 220 to 174 K both heating and cooling. The contour plot in figure 1 shows the evolution of the 400 and 040 reflections from an annealed sample above, during and below the transition.

The number and orientation of the martensite twins observed in the transformed phase is different for each sam-

ple and evolves during thermal cycling. But, at temperatures above 206 K in each cycle, all the samples resume their original form and orientation. The orientations of the martensitic twins relative to the cubic crystal are consistent with a transformation resulting from successive shears in <110> directions on two {110} planes at 120° [4]. A pseudotetragonal cell (c/a < 1) is obtained either by equal shears, or by reversing and doubling the magnitude of one of them. In the former case the tetragonal c-axis is the axis common to the two shear planes, and in the latter it is the cube axis perpendicular to the plane of the smaller shear. Twins with orientations corresponding to both types of shear were identified.

Figure 2 shows the effect of a very small uniaxial stress on the twin populations. The domains whose c-axes are parallel to the stress are favoured, whilst those with perpendicular c-axes, disappear. A very similar behaviour is observed on applying a magnetic field; 0.03 T was sufficient to convert all twins whose c-axes were perpendicular to the field direction to ones with parallel c-axes. This change is probably due to magnetostrictive strain rather than magneto-crystalline anisotropy since the domains can change identity by simple reversal of the unfavourable shears. For example a [010] domain formed by type 1 shears on 101 and 011



Figure 1: Contour plots of the counts summed over the vertical pixels 7 to 25 of the detector as a function of the scattering angle (vertical axis) and the scan step (horizontal-axis) for scans through the 040 and 400 reflections of an annealed crystal. Higher values of X correspond to smaller scattering angles. At 220 K (a) the sample is in the cubic phase, at 196 K (b) it is transforming, and at 174 K (c) it is in the pseudo-tetragonal phase.

will change to an [001] domain of type 2 if the shear on 011 is reversed and doubled.

These experiments show that small stresses applied in the martensitic phase can make inelastic changes in the martensitic domain populations. It is suggested that such stress induced twinning substitutes for normal slip, in the plastic deformation of Ni₂MnGa. Under stress the martensitic twin domains transform into one another; those whose c-axes are parallel to the axis of stress being favoured. However all the domains which can form have fixed relationships to the parent cubic crystal determined by the orientation of the relevant {110} shear planes. When the reverse shears occur on warming, they all give the original cubic crystal orientation. The same process in a polycrystalline sample leads to shape memory since all twins formed from a single cubic crystallite always transform back to their original cubic orientation regardless of how their populations may have been changed by stresses applied in the martensitic phase.



Figure 2: Intensity recorded at 172 K in scans through the position of the cubic 400 reflection plotted against the scattering angle (2θ) . (a) After cooling with no applied stress, (b) is (a) with 30 MPa applied at 172 K || [001]; (c) is (b) with the 30 MPa removed and (d) is after heating to 250 K and recooling with no stress applied. The higher angle peak in the scans is due to domains with the pseudo-tetragonal c-axis parallel to $[100]_{cubic}$ they are suppressed by applying the stress.

References: [1] P.J. Brown, J. Crangle, T. Kanomata, M. Matsumoto, K.U. Neumann, B. Ouladdiaf and K.R.A. Ziebeck, J. Phys. Condens. Matter, 14 (2002) 10159
[2] R.C. O'Handley, J. App. Phys., 83 (1998) 3263
[3] S.J. Murray, M. Farinelli, C. Kantner, J.K. Huang, S.M. Allen and R.C. O'Handley, J. App. Phys., 83 (1998) 7297
[3] S.J. Murray, M. Farinelli, C. Kantner, J.K. Huang, S.M. Allen and R.C. O'Handley, J. App. Phys., 83 (1998) 7297
[4] B.W. Batterman and C.S. Barret, Phys. Rev. Letters, 13 (1964) 390
[5] P.J. Brown, B. Dennis, J. Crangle, T. Kanomata, M. Matsumoto, K.-U. Neumann, L.M. Justham and K.R.A. Ziebeck, J. Phys. [5] P.J. Brown, B. Dennis, J. Crangle, T. Kanomata, M. Matsumoto, K.-U. Neumann, L.M. Justham and K.R.A. Ziebeck, J. Phys. [5] P.J. Brown, B. Dennis, J. Crangle, T. Kanomata, M. Matsumoto, K.-U. Neumann, L.M. Justham and K.R.A. Ziebeck, J. Phys. [5] P.J. Brown, B. Dennis, J. Crangle, T. Kanomata, M. Matsumoto, K.-U. Neumann, L.M. Justham and K.R.A. Ziebeck, J. Phys. [5] P.J. Brown, B. Dennis, J. Crangle, T. Kanomata, M. Matsumoto, K.-U. Neumann, L.M. Justham and K.R.A. Ziebeck, J. Phys. [5] P.J. Brown, B. Dennis, J. Crangle, T. Kanomata, M. Matsumoto, K.-U. Neumann, L.M. Justham and K.R.A. Ziebeck, J. Phys. [5] P.J. Brown, B. Dennis, J. Crangle, T. Kanomata, M. Matsumoto, K.-U. Neumann, L.M. Justham and K.R.A. Ziebeck, J. Phys. [5] P.J. Brown, B. Dennis, J. Crangle, T. Kanomata, M. Matsumoto, K.-U. Neumann, L.M. Justham and K.R.A. Ziebeck, J. Phys. [5] P.J. Brown, B. Dennis, J. Crangle, T. Kanomata, M. Matsumoto, K.-U. Neumann, L.M. Justham and K.R.A. Ziebeck, J. Phys. [5] P.J. Brown, B. Dennis, J. Crangle, T. Kanomata, M. Matsumoto, K.-U. Neumann, L.M. Justham and K.R.A. Ziebeck, J. Phys. [6] Phys. Rev. Letters, Barter, Barte