

Discovery of simple variant selection effect during stress-driven martensitic transformation

Martensitic transformations (MTs) have been found in various material systems induced by either temperature or pressure/stress, and are the basic principle for shape memory and superelastic effects. The most well-known MTs are those of Fe and its alloys: the fcc (face-centered cubic) to bcc (bodycentered cubic) transition during cooling and the bcc to hcp (hexagonal close packed) transition under pressure [1]. The perovskite to post-perovskite (pPv) transition of MgSiO₃ in the D" layer of the Earth's deep mantle is also inferred to be martensitic and shows strong inheritance of texture [2].

In martensitic transformations, the development of transformation textures is correlated with the original orientation of the parent phase. These relationships are usually expressed by the parallelism of certain planes and directions of the parent and transformed structures. One example is the Burgers' orientation relationship in the temperature-induced $\alpha \rightarrow \beta$ transition of Ti and Zr: (0001)_{α} // {110}_{β} where 12 variants are involved [3]. However, sometimes, some particular variants are favored more than others during the transition owing to the presence of external stress or strain. For the temperature-induced martensitic phase transition of alloys, the variant selection phenomenon has been extensively studied. In contrast, the variant selection effect in stress- and pressure-driven MTs is still much less understood because of the major technical challenge. Hence, it is of great interest to study the variant selection effect in pressure/stress-driven MTs, which are important in both multifunctional material design and geodynamics.

Using radial synchrotron X-ray diffraction at SPring-8 **BL10XU**, we study the *in situ* variant selection during the cubic-to-orthorhombic martensitic transformation of Mn_2O_3 at pressure up to 51.5 GPa and stress up to 5.5 GPa [4]. Mn_2O_3 crystallizes into a cubic structure under ambient conditions and transfers to the orthorhombic pPv structure under pressure (Fig. 1) [5]. The transition from a highly



Fig. 1. Crystal structures of Mn₂O₃.

symmetric cubic structure to a less symmetric orthorhombic structure makes it a perfect sample for the investigation of variant selection under pressure and stress.

Figure 2 shows unrolled diffraction images of Mn_2O_3 at various pressures. The systematic intensity variation on each pattern represents the preferred orientation of the lattice (texture). At low pressure it is a pure cubic phase and strong texture appears at 10.3 GPa (Fig. 2(a)). Phase transition starts at 24.1 GPa, as proved by the appearance of new peak lines indicated by red arrows (Fig. 2(b)). No further phase transition can be observed up to 51.5 GPa (Fig. 2(c)). The quenched sample went back to the cubic phase with the same original preferred lattice orientation (Fig. 2(d)), indicating that this phase transformation is reversible.

Inverse pole figures (IPFs) were obtained for both phases of Mn₂O₃, and partial IPFs represent complete texture information in accordance with cubic and orthorhombic crystal symmetry (Figs. 3(a) and3(b)). The low-pressure cubic phase displayed a 110 texture, while the intensity increased with pressure and reached its highest value of 3.24 m.r.d. at ~20.2 GPa $(t \approx 3.5 \text{ GPa})$ (Fig. 3(a)). Above the phase transition point, the high-pressure phase developed a very strong 100 texture with an intensity of 11.3 m.r.d. (Fig.3(b)). The texture change during the phase transition suggests a relationship of $(110)_c//(100)_o$, where $(110)_c$ is the lattice plane perpendicular to the stress direction. The much higher texture intensity of the high-pressure phase indicates that variant selection might occur during the phase transition. This can be more clearly presented in the pole figures (PFs) projected along the compression direction (Figs. 3(c) and 3(d)). They have axial symmetry, conforming to the geometry of the deformation experiment. For the cubic phase, it is clear that one {110} plane is in the center of the 110 PF, while four planes are at around 30° and one at 90° (Fig.3(c)). This means that only one of the six {110} planes of cubic phase, the (110) plane, is aligned perpendicular to the compression direction. For the orthorhombic phase, there is only one maximum at the center of the 100 PF, indicating that (100)_o lattice planes are preferentially oriented perpendicular to the compression direction (Fig.3(d)). Because of the orientation relationship $\{110\}_c // (100)_o$, all $\{110\}_c$ planes have a chance to became $(100)_o$. However, with stress there is obviously variant selection and the orthorhombic phase selects one of the cubic



Fig. 2. Unrolled diffraction patterns of Mn₂O₃ under pressure: (a) cubic; (b) two-phase mixture; (c) orthorhombic; (d) two-phase mixture during decompression.

{110} planes that is closest to perpendicular to the compression direction.

Our study provides an example of almost perfect variant selection during a phase transition under stress. For Mn₂O₃, similarities in atomic arrangements of the cubic {110} and orthorhombic (100) lattice planes can explain the texture transfer of $(110)_c$ to

 $(100)_o$ during the phase transition. In addition, the axial stress applied in our experiments will lead to stronger strain of lattice planes perpendicular to the compression direction than in other directions. Thus, these planes will more easily transfer to the highpressure phase and consequently result in the variant selection during the phase transition.



Fig. 3. Orientation relationship and variant selection during phase transition of Mn₂O₃. Inverse pole figures of (a) cubic and (b) orthorhombic phases. Pole figures of (c) cubic and (d) orthorhombic phases. Pressure is 24.1 GPa. An equal area projection is shown.

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