Domain Structures of Antiferroelectric $Pb(Yb_{1/2}Nb_{1/2})O_3$

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The domain structure of antiferroelectric $Pb(Yb_{1/2}Nb_{1/2})O_3$ with ordered complex perovskite structure was investigated by the theoretical approach and experimental observation. $Pb(Yb_{1/2}Nb_{1/2})O_3$ undergoes a first-order structural phase transition from the paraelectric cubic to antiferroelectric phase near 300°C. During the transition, the prototype cubic cell is monoclinically distorted. By previous report, we revealed that antiferroelectric $Pb(Yb_{1/2}Nb_{1/2})O_3$ has a point group of mmm from the CBED analysis. The breaking of reflection symmetry during transition occurred at (1 0 0), (0 1 0), (0 1 1), (0 $\bar{1}$ 1), ($\bar{1}$0 1) and (1 0 1) planes of the cubic prototype.

The domain-wall orientations of $Pb(Yb_{1/2}Nb_{1/2})O_3$ were investigated by spontaneous strain method based on the point group determined by CBED analysis. Antiferroelectric $Pb(Yb_{1/2}Nb_{1/2})O_3$ has two types of domain walls, the W and W'-walls, which are formed at the ferroelastic phase transition. In the monoclinic lattice frame, the orientations of the W-walls were calculated to be $(1\ 0\ 0)_m$, $(0\ 1\ 0)_m$, $(0\ 1\ 1)_m$, $(0\ \bar{1}\ 1)_m$, $(\bar{1}0\ 1)_m$ and $(1\ 0\ 1)_m$ planes. As the W-wall is characterized by the mirror planes lost on ferroelastic transition, these planes correspond to the CBED results. Taking into account of the modulation vector in each domain, the $(1\ 0\ 0)_m$ and $(0\ 1\ 0)_m$ planes are the 90° domain-boundaries and the others are 60° ones. These two kinds of W-wall were determined to be 'reflection twins' with common lattice plane on boundary by the zone axis pattern analysis. The analysis of the fringe contrast at the boundaries represents that the 90° and 60° boundaries have different boundary nature. The 90° domain-boundary has α-character

showing a displacement along the boundary while the 60° domain-boundary are δ-boundary having only twinning component. The orientations of W'-walls calculated from the strain components were approximately $(\bar{2}\ 3\ 3)_m$, $(2\ \bar{3}\ 3)_m$, $(\bar{3}\ 2\ 3)_m$ and $(3\ \bar{2}\ 3)_m$ planes at room temperature. On approaching the transition these W'-walls tend to orient themselves toward the direction of 60° W-walls because of the variation of spontaneous strain component. The W'-walls correspond to 120° domain-boundaries perpendicular to the W-walls and 'parallel rotation twin' having a common lattice row along the rotation axes, i.e. two-fold axes disappeared during the transition. However, bright field images and diffraction patterns show that the W'-wall at room temperature is classified into the eight indices, $(2\ \bar{3}\ 3)_m$, $(\bar{2}\ 3\ 3)_m$, $(\bar{3}\ 2\ 3)_m$, $(3\ \bar{2}\ 3)_m$, $(2\ 3\ \bar{3})_m$, $(2\ 3\ 3)_m$, $(3\ 2\ \bar{3})_m$ and $(3\ 2\ 3)_m$. The last four planes of the W'-wall orientations do not correspond to the previous results expected from spontaneous strain method on the basis of the crystal structure having an orthorhombic symmetry. It is thought that, macroscopically, antiferroelectric $Pb(Yb_{1/2}Nb_{1/2})O_3$ belongs to the point group mmm. However, its local structure on a nanoscale may be lower symmetry than mmm. The images of high resolution electron microscopy show that the W-wall has not well-defined boundary. The 90° W-walls have zigzag morphology in subcell unit and some steps. The 60° W-walls are also rough boundaries on a nanoscale.

References

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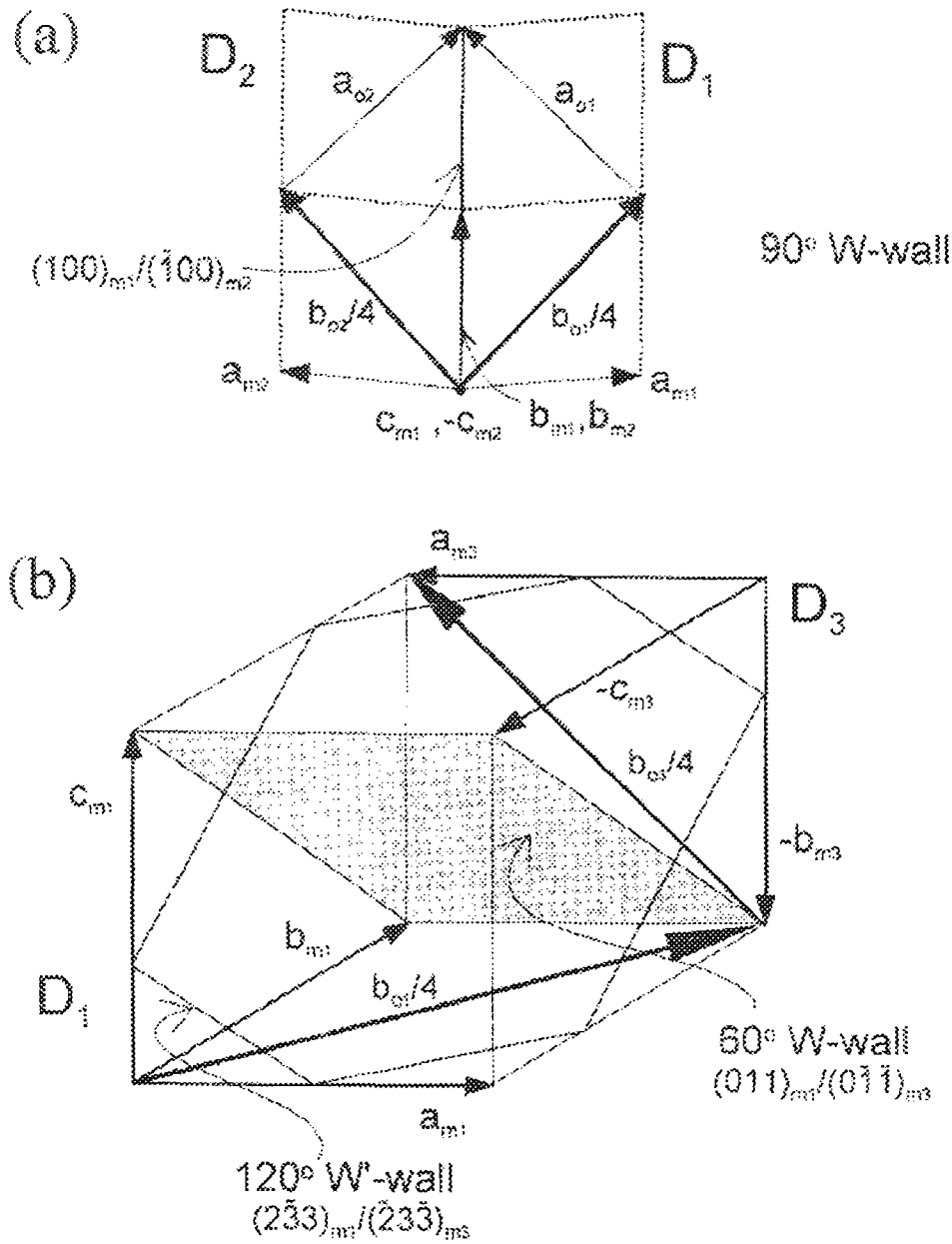

Schematic representation of (a)90°, (b)60° and 120° walls in $Pb(Yb_{1/2}Nb_{1/2})O_3$