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Surface Layer of $BaTiO_3$ a-plate

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The existence of surface layer in $BaTiO_3$ crystal was first suggested by Känzig,[1] and later works were reviewed by Jona and Shirane.[2] But the detail has not been made clear yet. The anomalous lattice strain in a-plate was previously detected by X-ray topography at room temperature.[3] In the present work, it was found from the careful study of the contrast on X-ray topographs of (100) plates ($50\sim200$ μm thick) that such an anomalous strain was due to the following shear-distorted surface layer of an order of 1 μm thick. It exists on (100) surface without applying any external field. The component of the distortion is ε_{xz} whose value is $\sim0.5\times10^{-4}$. The surface layer is shown in Fig. 1(a) as the shaded region. The (001) lattice planes with and without shear strain ε_{xz} are drawn by solid and dotted lines respectively. The sense of the strain depends uniquely on the directions of the spontaneous polarization $\boldsymbol{P}_s$ and the surface normal. When the two anti-parallel domains coexist (Fig. 1(b)), the senses of the strain in these domains were opposite to each other. The existence of the layer was also confirmed by the other experiment shown in Fig. 2(a), using a large plate distance $\sim$100 mm to detect the angular spread of the diffracted beam produced by the shear strain. As the beam divergence is large enough to excite the Bragg reflection from the unstrained and also the strained surface layer, the intensity profile is expected to have a tail at lower or higher angle side depending on the direction of $\boldsymbol{P}_s$. It was really observed (Fig. 2(b)) using the crystal with the domain configuration as shown in Fig. 2(c) which is an ordinary surface reflection. The observed profile of Fig. 2(b) was fitted with the calculated one by considering the beam divergence, spectral width, experimental geometry and by assuming an exponentially damped lattice strain $\varepsilon_{xz}(x)=\varepsilon_0\cdot\exp(-k\cdot x)$. The good fitting was obtained for the damping factor $k=6.5$ (μm^{-1}) and the maximum shear strain $\varepsilon_0=1.5\times10^{-4}$. The thickness of the layer corresponds roughly to $1/k$ ($\sim$0.15 μm). When an weak electric field was applied perpendicular to $\boldsymbol{P}_s$ (Fig. 2(a)), the shear strain became smaller at the positive side and larger at the negative side of electrodes respectively as expected from the piezo-electric effect. The field effect was remarkable at the negative side. Figure 2(d), 2(e) and 2(f) are at the field of -1, -4 and $+4$ Volt per 220 μm respectively. This fact suggests that the externally applied potential is largely dropped only near the negative side of electrodes as suggested by Motegi.[4]

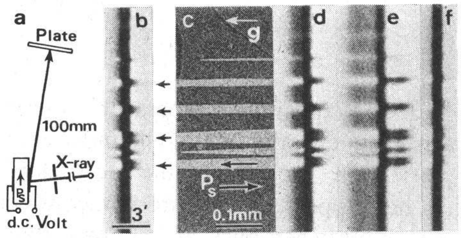

Fig. 2. (a) Experimental configuration. (b) Observed pattern at a free surface, CuKα (303). (c) Ordinary surface reflection, CuKα (30$\bar{3}$). (d) At applying an electric field of -1 V/220 μm. (e) -4 V/220 μm. (f) $+4$ V/220 μm.

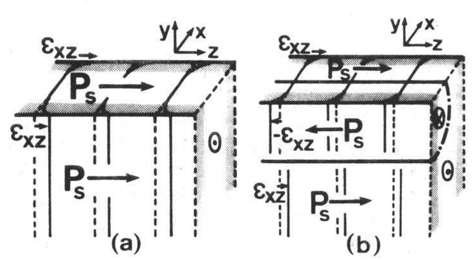

Fig. 1. Lattice strain of the surface layer (a) at single *a*-domain, and (b) at two anti-parallel domains.

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