Memo 13-D: $BaTiO_3$ (X22A 5/15-20)

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X-ray scattering experiments were carried out at the National Synchrotron Light Source beam line X22A. A single crystal sample from Fujikura, Ltd., cut along the [111] surface (#F-1) was used for the measurements. The sample dimension is $3.142 \times 2.991 \times 0.693$ mm^3, and the sample mosaicity is typically $\sim 0.03°$ HWHM. The sample was placed on a sample holder made with plexiglas, after electrodes had been attached with silver paste. Incident x-ray energy of 32 keV was used to operate in transmission geometry. At this energy the attenuation length of $BaTiO_3$ is about ~ 0.3 mm, and our sample is thin enough for the transmission experiment. The (111) reflection of Si analyzer was used to obtain a very good Q-resolution (~ 0.001 Å^{-1}). Throughout this memo, we note Q in units of $(2\pi/a,\ 2\pi/a,\ 2\pi/c)$, where $a = 3.992\mathring{A}$ and $c = 4.036$ Å.

In Fig. 1, HHL mesh scans at zero field and at E=17 kV/cm are shown for the (110) peak and the (002) peak. The main feature consists of two dominant peaks corresponding to tetragonal twins. For example, the (110) peak and the (101) peak are shown in the left panels, and the (002) and (020) peaks are shown in the right panels. The only notable difference between the zero field data and E=17 kV/cm data is the appearance of a third peak around (0.985 0.985 0) at high field. It is tempting to associate this with a third lattice constant arising from transition to an orthorhombic or a monoclinic phase. However, no apparent change in the profile of the (002) peak makes this association difficult. In fact, it is impossible to consistently describe the E=17 kV/cm data with either orthorhombic or monoclinic phase.

In Fig. 2, we plot integrated intensity along the longitudinal direction at each Q position. This plot is obtained by integrating over intensities along the transverse direction shown in Fig. 2. As one can see from the figure, the third lattice constant has a very little

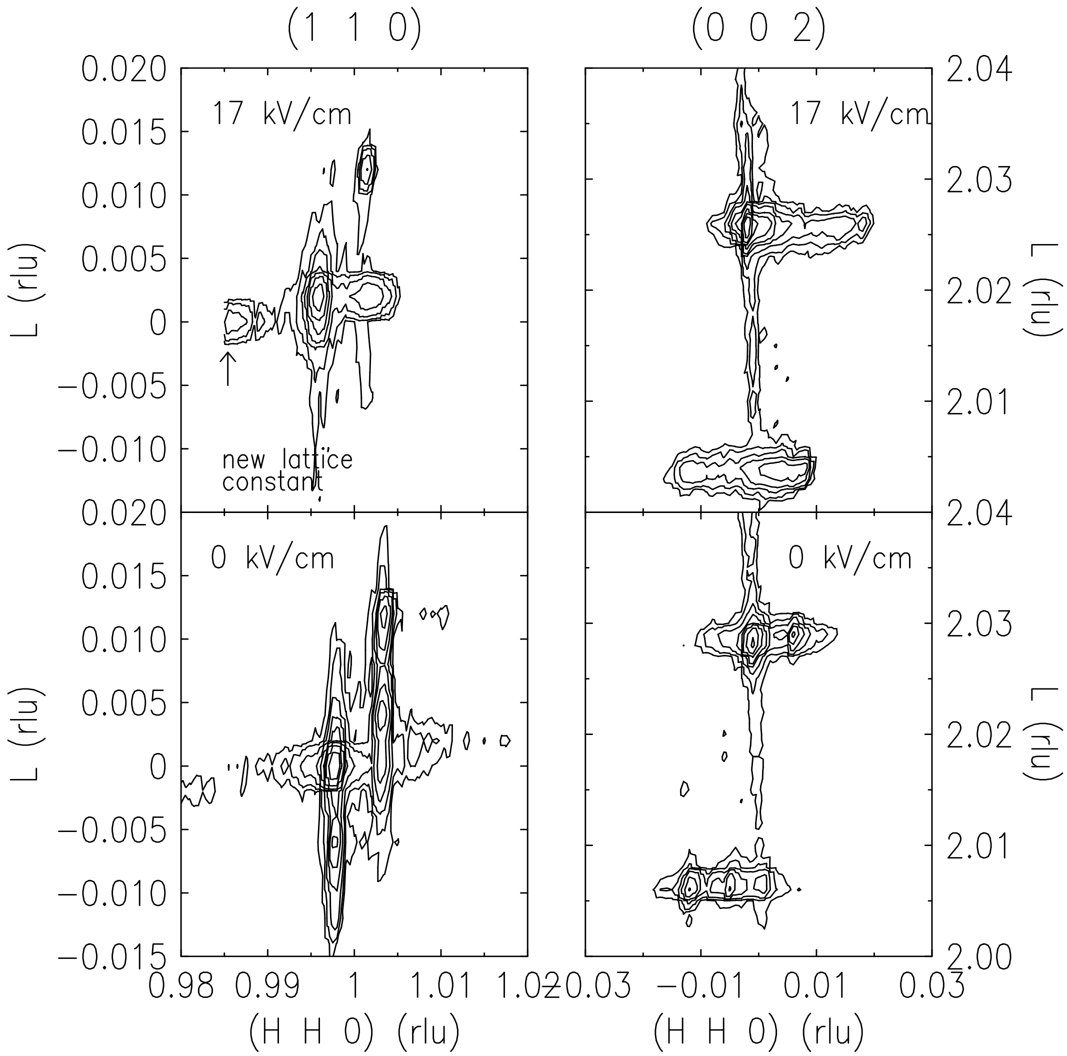

FIG. 1: HHL mesh scans at (110) and (002) with the static electric field applied along the [111] direction.

intensity contribution. Therefore, it is presumably coming from a minority phase in our measurements, and all our measurements can be explained by dominant tetragonal phase. One interesting aspect to notice in Fig. 2 is that the change in the domain distribution between zero and high field. For example, intensity of the peaks from (110) and (002) domain becomes smaller at high fields, while that of (101) and (020) domain remains almost constant.

However, There are a couple of points to consider before concluding that $BaTiO_3$ remains tetragonal up to 17 kV/cm. First, the x-ray beam size in this case is roughly 0.3×0.3 mm^2, and therefore it is possible that we are only probing regions where tetragonal-monoclinic transition has not occurred. Second, the skin effect is probably not important, since we are using a hard x-ray in the transmission geometry. It is quite obvious that we need to apply higher field to fully understand the phase behavior. (The sample did not break up to 22 kV/cm.) In addition, studying a larger sample area, either by increasing the beam size or by scanning the sample, is probably necessary.

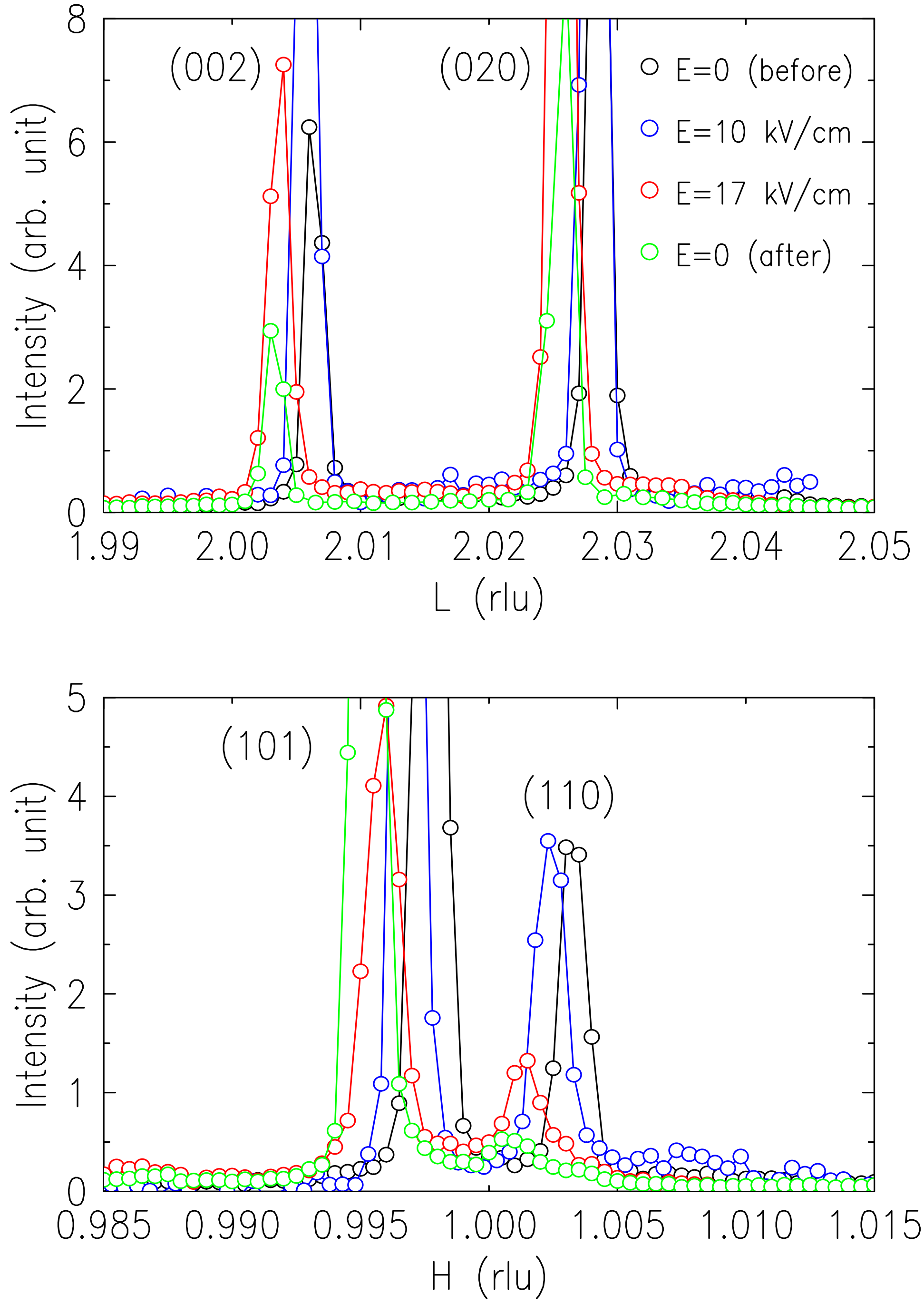

FIG. 2: Integrated intensity along the Q direction at various stage of static applied field.