Quantitative evaluation of elastic properties of LiTaO3 crystals by line-focus-beam acoustic microscopy

doi: 10.1063/1.105217

Quantitative evaluation of elastic properties of $LiTaO_3$ crystals by line-focus-beam acoustic microscopy

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(Received 31 October 1990; accepted for publication 18 December 1990)

The line-focus-beam acoustic microscope system is applied to investigate the elastic properties of $LiTaO_3$. Elastic inhomogeneities are detected quantitatively as a significant variation of leaky surface acoustic wave (LSAW) velocities in X-112.2°Y $LiTaO_3$ wafers. Large changes, about 2.5%, in LSAW velocities are observed in some wafers, which correspond to a difference between the velocities for single and multidomains. One of the causes is found to be in the poling process during wafer fabrication.

Lithium tantalate ($LiTaO_3$) is one of the more important ferroelectric materials for surface acoustic wave (SAW) devices, as well as for integrated optoelectronic devices, because of its favorable piezoelectric, electro-optic, and nonlinear optical properties. In particular, X-cut 112.2° rotated Y-propagating (X-112.2°Y) $LiTaO_3$ wafers have been found to be one of the most suitable substrates for SAW devices.[1] Development of large diameter single crystals has been of great interest for mass production by industry to supply high quality wafers of homogeneous SAW properties. Pulled crystals are processed into wafers through various fabrication processes including annealing, poling, grinding, slicing, and polishing.[2] Serious elastic inhomogeneities in wafers, as well as mechanical damage to the wafer surface, can result from problems originating with crystal growth and wafer fabrication. Elastic inhomogeneities related to variation in chemical composition and residual stresses are more important and should be avoidable in device fabrication by establishing optimum conditions of crystal growth. From the point of view of mass production of SAW devices, it is desirable for the wafers to have less variation in the SAW velocity, not only on a wafer, but also among wafers. In general, the variation should be within ±0.1% for filters and within ±0.04% for resonators.[2]

A serious problem has occurred regarding the elastic properties of X-112.2°Y $LiTaO_3$ wafers during industrial preparation, which could not be understood from data obtained by conventional x-ray methods, such as diffractometer and topographic techniques, to analyze lattice deformation from imperfections in crystals and optical methods using photoelasticity to evaluate the residual stress distribution.

This letter reports quantitative characterization of elastic inhomogeneities in X-112.2°Y $LiTaO_3$ wafers observed with line-focus-beam (LFB) acoustic microscopy.[3–5] The effects of multidomains and chemical composition changes on elastic properties of the wafers are discussed. The LFB acoustic microscope system was operated at 225 MHz for velocity measurements of leaky surface acoustic waves (LSAWs) excited on the water-loaded wafer surface. The relative accuracy of the LSAW velocity measurements is estimated to be better than ±0.005% at a chosen point and ±0.02% over a scanning area of 75 mm×75 mm.[5] Such accuracy enables us to make two-dimensional nondestructive and noncontacting evaluation of the elastic properties of a wafer.

LSAW velocity distributions for a number of 3-in.-diam X-cut $LiTaO_3$ wafers, selected from different crystal lots obtained at the developmental stage, were examined by the $V(z)$ curve analysis method.[3] Different types of velocity variations were observed depending upon the elastic property of the wafer specimen. Figure 1 shows a typical velocity distribution observed on a wafer, where the area was segmented into 7 mm×7 mm sections and the LSAW velocities propagating in the 112.2°Y direction parallel to the orientation flat were measured at the center of the squares. Large velocity changes are observed clearly at the wafer edges along the crystallographic Z axis. The velocities at the left sections along the Z axis are about 77 m/s larger than those at the other regions. With reference to the LSAW velocity of 3290 m/s calculated using the physical constants reported by Warner *et al.*,[6] it can be deduced that the elastic properties of the higher velocity region are abnormal and those of the lower velocity region are normal. Figure 2 shows the velocity variation determined along the scan line diameter of Fig. 1 over a distance of 70 mm. For comparison, the a-axis lattice constants were also measured by x-ray analysis, using the Bond method, along the same diameter direction, with resolution of 0.00002 Å shown in Fig. 3. It is seen in Fig. 2 that the velocities

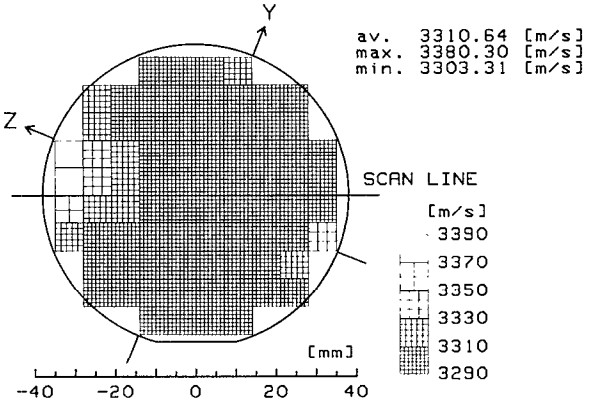

FIG. 1. Typical distribution of LSAW velocities measured on an X-112.2°Y $LiTaO_3$ wafer.

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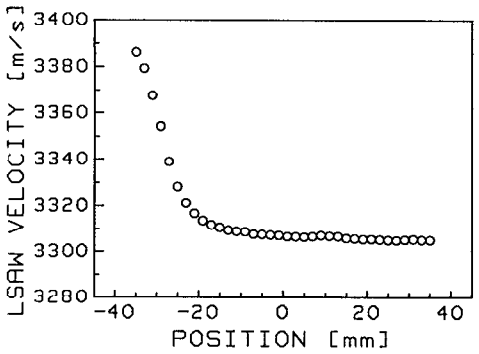

FIG. 2. Velocity variation along diameter direction in Fig. 1 for an X-112.2°Y $LiTaO_3$ wafer.

change drastically from 3386 m/s, at the edge of the wafer, to about 3313 m/s, around the position of -20 mm, and then exhibit a slight variation to 3305 m/s. The maximum difference in the velocities is 81.2 m/s (2.46%). On the other hand, Fig. 3 shows that the lattice constants vary slightly and randomly within ± 0.0001 Å in the left region, where the large variations of the LSAW velocities were observed, and with the average lattice constant value of 5.15356 Å at the normal part. This suggests lattice deformation, although this variation cannot explain that of the elastic properties shown in Fig. 2. In addition, it was barely observable from the slight color change of the photoelastic method that the corresponding regions were under elastic deformation, as shown in Fig. 4. But the information in Fig. 4 is only qualitative. It was supposed, from these results, that the observed variation might be the result of the nonuniform distribution of electric fields during the poling process.

In order to clarify this issue, we obtained two commercially available X-cut wafers. One wafer was heated to about 700 °C and cooled without applying voltage. This was a depoled sample with multidomains, and with no piezoelectric properties. Velocity measurements were made as a function of the wave propagation direction for both samples. Figure 5 shows the measured LSAW velocities, where the propagation direction of 0° corresponds to the crystallographic Y axis. The open and closed circles identify the measured LSAW velocities for the single and multidomain samples, respectively, and the solid lines are for the theoretical LSAW and leaky pseudosurface acoustic wave (LPSAW) velocities calculated for a single-domain X-cut $LiTaO_3$ sample. In Fig. 5, in the range from 120° to 140°, curious velocity variations occur for both samples due to a processing problem of the $V(z)$ curves for two closed modes of LSAWs and LPSAWs. This is not responsible for the physical properties of the single/multidomains. As a whole, the velocities for the multidomain sample are greater than those for the single-domain sample. In the range from 20° to 30°, the differences between the velocities for both samples are less significant. This stands for less contribution of piezoelectricity to the wave propagation directions in the single-domain sample. The velocities along the 112.2°Y propagation direction are 3294.6 m/s for the single-domain sample and 3382.2 m/s for the multidomain sample. The difference of 87.6 m/s is

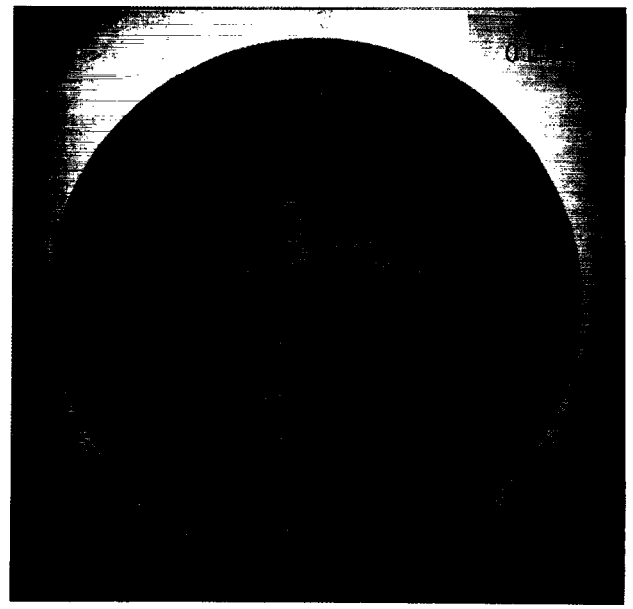

FIG. 4. Photograph showing residual stress distribution for the wafer in Figs. 1 and 2 taken by photoelastic method.

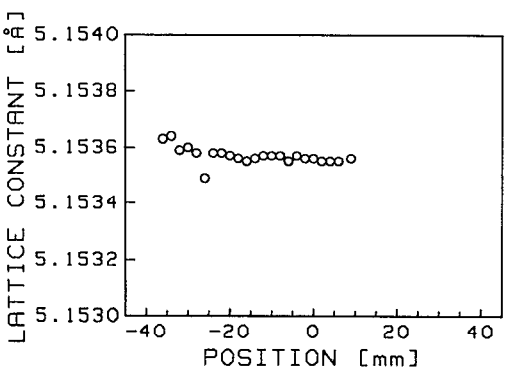

FIG. 3. Variation of a-axis lattice constant along diameter direction in Fig. 1 for an X-112.2°Y $LiTaO_3$ wafer.

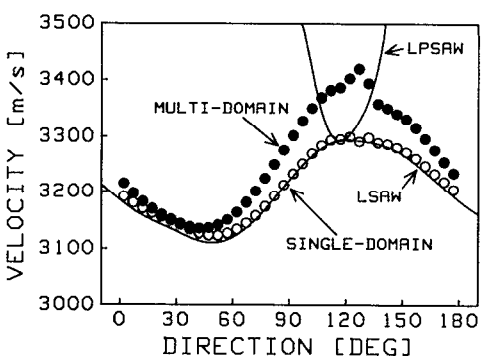

FIG. 5. LSAW velocities for two samples of X-cut $LiTaO_3$ with single and multidomains, and calculated LSAW and LPSAW velocities for the single-domain sample.

in good agreement with the maximum velocity difference shown in Figs. 1 and 2. It can be seen that one of the causes in the velocity variations is associated with the poling process. The remarkable variation in the LSAW velocities observed in Figs. 1 and 2 can be considered to correspond to the distribution of unpoled domains, which reduces the magnitude of the piezoelectric constants.[7] Further investigation should be carried out to confirm this.

The velocity value of about 3305 m/s along the 1 12.2°Y direction at the normal parts of the wafer, as shown in Figs. 1 and 2, is about 10 m/s larger than the 3294.6 m/s of the commercial wafer. With knowledge of the relations between LSAW velocities and chemical compositions,[8] it can be presumed that the crystal was grown with a Li-richer chemical melting composition than the congruent composition of $LiTaO_3$.[2,9–12]

From the above discussion of Fig. 5, it is easy to understand that for LSAW propagation along the 20°–30° directions, a nearly uniform distribution of LSAW velocities, on the same wafer, can be obtained as compared with the large elastic inhomogeneity detected for the 112.2°*Y* propagation, given in Figs. 1 and 2. This has been confirmed by experiments.[13] The greatest advantage of the LFB acoustic microscope system is that the LSAW propagation direction suitable for material analyses can be chosen propitiously, and this is the reason an acoustic microscope, with an LFB acoustic device, is superior in providing quantitative measurements to the microscope with a point-focus-beam (PFB) acoustic device. Other types of elastic inhomogeneities and further discussions will be reported elsewhere.[13]

It has been demonstrated successfully in this study that the LFB acoustic microscope system is a powerful tool to resolve scientific and industrial problems associated with SAW device materials; one of the most promising applications. Further developments of the applications will be made for quantitative analyses, not only of SAW material problems such as the mechanical damages of the wafer surface[2] and the Rh impurity in $LiTaO_3$,[12] but also of optical material problems such as the MgO-doped $LiNbO_3$ crystals[14,15] and the Ti-diffused and proton-exchanged layers in integrated optical waveguides,[16,17] and of local domain inversion problems of $LiNbO_3$ and $LiTaO_3$.[7]

The authors are very grateful to T. Sannomiya, H. Kobayashi, and S. Watanabe for helpful discussions, and to I. Sahashi and T. Sasamata of the Yamaju Ceramics Co. for preparing a depoled sample of *X*-cut $LiTaO_3$ wafer. This work was supported in part by Research Grant-in-Aids from the Japan Ministry of Education, Science & Culture.

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