Surface acoustic wave propagation properties in 0.67Pb($Mg_{1/3}Nb_{2/3}$)O_3-0.33PbTiO$_3$ single crystal poled along $[111]_c$

Xiuming Li,[1,2] Rui Zhang,[1,2,a)] Naixing Huang,[1] Tianquan Lü,[1] and Wenwu Cao[1,3]
[1]*Department of Physics, Harbin Institute of Technology, Harbin, Heilongjiang 150080, People's Republic of China*
[2]*Department of Physics, Daqing Normal University, Daqing, Heilongjiang 163712, People's Republic of China*
[3]*Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania 16802, USA*

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Surface acoustic wave (SAW) propagation properties in relaxor-based 0.67Pb($Mg_{1/3}Nb_{2/3}$)O_3-0.33PbTiO$_3$ (PMN-33%PT) ferroelectric single crystals poled along $[111]_c$ has been analyzed theoretically. We found that the *X*-cut PMN-33%PT has lower phase velocity and higher electromechanical coupling coefficient compared to traditional piezoelectric materials. The power flow angle (PFA) can be zero in specific directions, which could drastically improve the performance of SAW devices. Our theoretical results indicate that the direction about 5° canted from $[111]_c$ is the optimum direction for the *X*-cut $[111]_c$ poled crystals in SAW device applications. Characteristic curves were also obtained for the phase velocity, electromechanical coupling coefficient, and PFA in *Z*-cut single-domain PMN-33%PT single crystals. © *2009 American Institute of Physics*. [doi:10.1063/1.3271775]

Relaxor-based ferroelectric single crystals 0.67Pb($Mn_{1/3}Nb_{2/3}$)O_3-0.33PbTiO$_3$ (PMN-33%PT) have attracted considerable attention in the past several years due to its large electromechanical coupling coefficients, high piezoelectric coefficients, high dielectric constants, and low dielectric losses.[1–3] When the crystal is poled along $[001]_c$, its electromechanical coupling coefficient k_{33} and piezoelectric coefficient d_{33} can reach 90% and 2500 pC/N, respectively. Such values are four times more than that of the best modified Pb(Zr_xTi_{1-x})O_3(PZT) ceramics. PMN-33%PT crystals are now commercially available in United States, China, Korea, and Singapore.[1,4] Hence, these crystals are favored in the next generation electromechanical devices, actuators, ultrasonic motors, wideband medical ultrasonic transducers, etc.[5]

Surface acoustic wave (SAW) devices made of piezoelectric materials are widely used as radio frequency filters, delay line oscillators, resonators in communication systems, and sensors in chemical and biological industries. Recently, $[001]_c$ poled PMN-33%PT single crystals has shown great potential for making miniaturized SAW devices with wide frequency band and high sensitivity.[6] While, based on property characterization, it has been recognized that more than 80% of the superior electromechanical properties of the PMN-33%PT come from orientation effect, i.e., from crystal anisotropy, and the large shear piezoelectric coefficient d_{15} in the single-domain state.[7]

In this letter, we report a theoretical study on the SAW propagation characteristics in *X*-cut and *Z*-cut single-domain PMN-33%PT crystals poled along $[111]_c$, which could provide useful information for designing future SAW devices.

The SAW propagation in a piezoelectric single crystal is governed by the Christoffel equation with semi-infinite boundary conditions.[8,9] The coordinate system under investigation is illustrated in Fig. 1. Using the measured material parameters of $[111]_c$ polarized PMN-33%PT,[10] the SAW propagation characteristics in this single crystal can be calculated. We found that the calculated result of SAW phase velocity in the *Z*-cut PMN-33%PT single domain crystal poled along $[001]_c$ agrees well with the measured data.[11] When the propagation angle θ changes in the range of 0°–180°, the variations of phase velocity v, the electromechanical coupling coefficient k, and power flow angle (PFA) φ for *X*-cut and *Z*-cut are shown in Figs. 2–4, respectively.

As shown in Fig. 2 the SAW phase velocities in the *Z*-cut single domain PMN-33%PT single crystal poled along $[111]_c$ are fairly low, ranging from 583–1018 m/s. While for the *X*-cut crystals, the minimum SAW phase velocity could be as low as 470 m/s, which occurs in the directions of 56.41° and 108°, respectively. Obviously, the SAW phase velocity is much lower than that of traditional piezoelectric materials, such as quartz and LiNbO$_3$ crystals, which are around 3500 and 3600 m/s, respectively.[12,13] Moreover, the SAW phase velocities of PMN-33%PT single crystal poled along $[111]_c$ are lower than that of crystal poled along $[001]_c$ in most directions.[6,14] Generally speaking, the decrease in

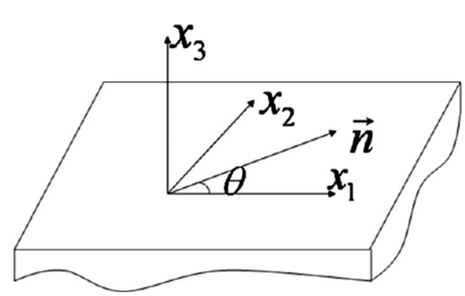

FIG. 1. Coordinate system used in this work.

a)Electronic mail: ruizhang@hit.edu.cn.

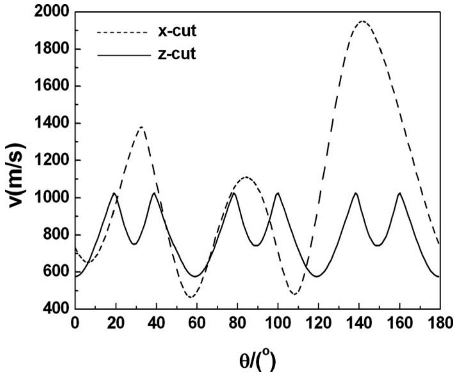

FIG. 2. The SAW phase velocity of PMN-33%PT single crystals poled along $[111]_c$.

SAW phase velocities will reduce the device size. Therefore, the $[111]_c$ poled PMN-33%PT single crystals are excellent candidates for further generation miniaturized SAW devices.

As shown in Fig. 3, the SAW electromechanical coupling coefficients k of PMN-33%PT single crystal poled along $[111]_c$ for the X-cut and Z-cut situations are strongly dependent on wave propagation directions. It can be noticed from Fig. 3 that the k^2 of PMN-33%PT single crystal poled along $[111]_c$ for the Z-cut is less than 1.4%, however, the k^2 value for the X-cut crystals is as high as 34.98% in the direction 5° canted from $[111]_c$. The theoretical results of SAW are in good agreement with the measured results of bulk waves.[10] This k^2 value is much higher than that of the traditional piezoelectric materials, such as quartz (0.14%) and $LiNbO_3$ (5%) crystals.[12,13] In addition, the maximum k^2 value of PMN-33%PT single crystal poled along $[111]_c$ is higher than that of the same crystal poled along $[001]_c$.[6] Therefore, X-cut PMN-33%PT crystals poled along $[111]_c$ have a good potential for making high efficiency SAW devices with much broader bandwidth than traditional SAW devices.

The PFA φ values for the X-cut and Z-cut cases are also found to be strongly dependent on the propagation direction, as shown in Fig. 4. The PFA values are less than 0.075°, which is only about 0.4% and 7.5% of that of conventional piezoelectric materials and PMN-33%PT single crystal poled along $[001]_c$, respectively.[6,12,14] For example, the maximum PFA values of quartz and $La_3Ga_{5.5}Ta_{0.5}O_{14}$ are about 20°,[12] and $LiNbO_3$ crystals around 7°.[13] Moreover, it was found that the PFA values become zero in the directions of 5.7°, 33.6°, 56.6°, 83.7°, 107.9°, and 141.6° for the X-cut case and in the directions of 18.8°, 28.7°, 38.5°, 59°, 77.9°, 88.6°, 99.7°, 118.6°, 138.3°, 148.5°, 159°, and 179° for the Z-cut case. Since PFA reflects the diffracted intensity of the SAW power, zero PFA are necessary for designing SAW devices with superior performance. This crystal gives us a lot of flexibility in SAW device designs.

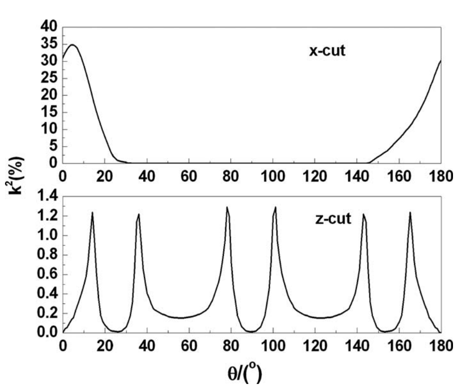

FIG. 3. Electromechanical coupling coefficients of PMN-33%PT single crystals poled along $[111]_c$.

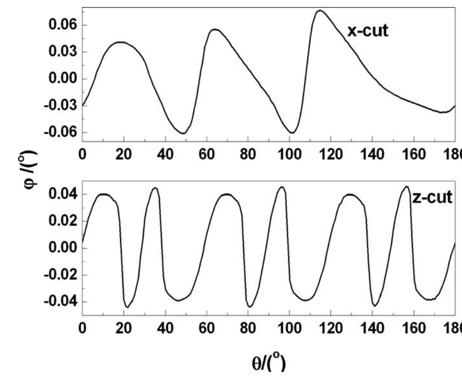

FIG. 4. PFA of PMN-33%PT single crystals poled along $[111]_c$.

One drawback of PMN-PT crystals is their limited temperature range because the rhombohedral to tetragonal phase transition temperature for the PMN-33%PT is about 70 °C.[15] Recent studies have demonstrated that the rhombohedral to tetragonal transition temperature could be increased to more than 100 °C by the heavy doping of indium, which can greatly improve the temperature stability.[16]

In summary, the properties of SAWs propagating in X-cut and Z-cut single domain PMN-33%PT single crystals poled along $[111]_c$ were theoretically investigated based on the experimentally measured material properties. The results showed that SAW propagating in Z-cut and X-cut PMN-33%PT single domain single crystals poled aong $[111]_c$ can have very low phase velocities, and the electromechanical coupling coefficients are much higher than that of the traditional piezoelectric materials in most propagation directions. The maximum k^2 value for the X-cut PMN-33%PT single domain single crystal could reach as high as 34.98% in the direction 5° canted from $[111]_c$. In addition, the X-cut single crystal has very small PFAs. In comparison, SAW propagation properties of PMN-33%PT single domain single crystals poled along $[111]_c$ are even better than that of the same crystals poled along $[001]_c$ for the X-cut. These superior properties make the X-cut $[111]_c$ poled PMN-33%PT single crystals excellent candidates for making next generation SAW devices.

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