Surface acoustic wave propagation in Y- and Z-cut 0.67PbMgNbO₃–0.33PbTiO₃ single crystals

Xiuming Li,¹ Rui Zhang,^{2,a)} Naixing Huang,² Tianquan Lü,² and Wenwu Cao³

¹Department of Physics, Harbin Institute of Technology, Harbin, Heilongjiang 150080, China and

Department of Physics, Daqing Normal University, Daqing, Heilongjiang 163712, China

²Department of Physics, Harbin Institute of Technology, Harbin, Heilongjiang 150080, China

³Department of Physics, Harbin Institute of Technology, Harbin, Heilongjiang 150080, China and Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania 16802, USA

(Received 5 May 2009; accepted 29 July 2009; published online 11 September 2009)

Surface acoustic wave (SAW) propagation in Y-cut and Z-cut relaxor-based 0.67Pb(Mg_{1/3}Nb_{2/3})O₃–0.33PbTiO₃ (PMN-33%PT) ferroelectric single crystals poled along [001]_c cubic direction has been analyzed theoretically. Characteristic curves were obtained for the phase velocity, electromechanical coupling coefficient and PFA of SAW in Y-cut and Z-cut PMN-33%PT single crystals. It was found that the phase velocity is lower, while the electromechanical coupling coefficient is much higher, than that of traditional piezoelectric materials. The power flow angle (PFA) can be zero in certain directions, which makes this crystal system a promising material for future SAW devices with smaller size and enhanced performance. The directions near 45° and 135° of Y-cut PMN-33%PT crystals are found to be optimum directions for SAW device applications.

© 2009 American Institute of Physics. [doi:10.1063/1.3211922]

Surface acoustic wave (SAW) devices made of piezoelectric materials are widely used as radio-frequency filters, delay line oscillators, or resonators in communication systems, and there are many new applications in sensor area (gas or liquid pressure sensor, microfluidic systems, etc.).^{1–5} With fast developing technologies in information industry, there is always a need for better performance SAW devices. Therefore, the study of piezoelectric substrate for such SAW devices becomes one of the hot topics in recent years.

Generally speaking, lower phase velocity of surface waves in piezoelectric substrate can help reducing the size of SAW devices, while larger electromechanical coupling coefficient can reduce the insertion loss and increase the bandwidth.⁶ However, traditional piezoelectric materials used in current SAW devices all have some drawbacks. For example, quartz has low electromechanical energy conversion efficiency, LiNbO₃ has poor temperature stability, and severe diffraction has been observed in La₃Ga₅SiO₁₄ crystals.^{7,8}

In recent years, relaxor-based Pb(Mg_{1/3}Nb_{2/3})O₃–PbTiO₃ (PMN-PT) ferroelectric single crystals have become the center of attention due to their superior electromechanical properties.^{9,10} For example, when the crystal is poled along [001]_c its electromechanical coupling coefficient can reach more than 90% and its piezoelectric coefficient d_{33} is greater than 2500 pC/N.¹¹ These new crystals have been used in various electromechanical devices, such as medical ultrasonic transducers, large displacement actuators and ultrasonic motors, etc.^{12–14}

When being poled along the [001]_c direction, the relaxor-based PMN-33%PT single crystal has the best piezoelectric properties among all compositions of PMN-PT. Here

we try to investigate the possibility of using PMN-33%PT single crystals in high-performance SAW devices. SAW velocities of PMN-33%PT have been measured by Choi *et al.*¹⁵ However, there is no report on the literature on the detailed theoretical analysis of SAW propagation properties for PMN-33%PT single crystals. In this paper, we report a theoretical study on the SAW propagation characteristics in Y-cut and Z-cut PMN-33%PT crystals poled along [001]_c.

The SAW propagation in a piezoelectric single crystal is governed by the Christoffel equation with semi-infinite boundary conditions. The coordinate system under investigation is illustrated in Fig. 1. Due to piezoelectric coupling, the equations of motion for elastic and electromagnetic fields must be solved simultaneously for piezoelectric media. The coupled-wave equations are

$$\left. \begin{aligned} \rho \frac{\partial^2 u_i}{\partial t^2} - c_{ijkl}^E \frac{\partial^2 u_k}{\partial x_l \partial x_j} - e_{kil} \frac{\partial^2 \Phi}{\partial x_k \partial x_j} &= 0 \\ e_{jkl} \frac{\partial^2 u_k}{\partial x_i \partial x_j} - \epsilon_{ijk} \frac{\partial^2 \Phi}{\partial x_k \partial x_j} &= 0 \end{aligned} \right\} \quad (i, j, k, l = 1, 2, 3), \quad (1)$$

where u_i is the vibration displacement, Φ is the electrical

FIG. 1. Coordinate system used in this work. θ is the angle between propagation direction $\vec{n}$ and x_1 axis.

^{a)}Electronic mail: ruizhang_ccmst@hit.edu.cn.

FIG. 2. The SAW phase velocity of PMN-33%PT at the Y-cut.

potential, c_{ijkl} is the elastic stiffness tensor measured under constant electric field, e_{kil} is the piezoelectric strain tensor, ε_{jk} is the dielectric tensor measured under constant strain, and ρ is the density of the medium.

Using linear combinations of partial waves, the displacements and the electric potential can be written as:

$$\begin{aligned} u_i &= \alpha_i \exp\{j\beta[(l_1x_1 + l_2x_2 + l_3x_3) - vt]\} \\ \Phi &= \alpha_4 \exp\{j\beta[(l_1x_1 + l_2x_2 + l_3x_3) - vt]\} \end{aligned} \quad (i = 1, 2, 3), \quad (2)$$

where v is the phase velocity of acoustic wave, β is the scalar wave vector, l_i is the direction cosine for wave propagation, and α_i and α_4 are the amplitudes.

Using Eqs. (1) and (2), we can get the following Christoffel equation:

$$\begin{bmatrix} \Gamma_{11} - \rho v^2 & \Gamma_{12} & \Gamma_{13} & \Gamma_{14} \\ \Gamma_{21} & \Gamma_{22} - \rho v^2 & \Gamma_{23} & \Gamma_{24} \\ \Gamma_{31} & \Gamma_{32} & \Gamma_{33} - \rho v^2 & \Gamma_{34} \\ \Gamma_{41} & \Gamma_{42} & \Gamma_{43} & \Gamma_{44} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} = 0, \quad (3)$$

where $\Gamma_{ik} = c_{ijkl}l_jl_k$, $\Gamma_{i4} = e_{kij}l_kl_j$, and $\Gamma_{44} = -\varepsilon_{ik}l_i l_k$ ($i, k, j, l = 1, 2, 3$).

SAW velocities under free boundaries and with metal surface coatings are defined as v_s and v_m , respectively, which can be obtained by solving Eq. (3) for a semi-infinite crystal. For piezoelectric materials, the strength of piezoelectric effect is determined by the electromechanical coupling coefficient k , which can be quantified by the formula

$$k^2 = 2(v_s - v_m)/v_s. \quad (4)$$

The power flow angle (PFA) φ is defined as the separation angle between power flow and phase propagation wave vector, it reflects the diffracted intensity of sound wave. The PFA φ is given by the following equation:

$$\tan \varphi = \frac{1}{v} \frac{dv}{d\theta}. \quad (5)$$

Using the Eq. (3) and the PMN-33%PT material parameters,¹² the SAW propagation characteristics in PMN-33%PT single crystals were calculated at room temperature for a crystal being poled along $[001]_c$ cubic direction. When

FIG. 3. The SAW phase velocity of PMN-33%PT at the Z-cut.

the propagation angle θ changes in the range of 0° – 180° , the corresponding values of the phase velocity v in free surface, the electromechanical coupling coefficient k , and PFA φ for Y-cut and Z-cut situations are shown in Figs. 2–4, respectively. Characteristic curves of quartz, $\text{La}_3\text{Ga}_{5.5}\text{Ta}_{0.5}\text{O}_{14}$ (LGT) and LiNbO_3 crystals are also cited for comparison.^{16,17}

Figures 2 and 3 demonstrate the characteristics of SAW phase velocity in the PMN-33%PT single crystal for Y-cut and Z-cut situations. The maximum values of the SAW phase velocities for PMN-33%PT single crystal are 1741 and 1644 m/s, respectively, for the two cases. The minimum values of the SAW phase velocities 1156.6 and 868 m/s occur in the directions of 45° and 135° for the Y-cut and Z-cut situations, respectively, the theoretical results agree well with the measured results of Choi *et al.*¹⁵ In comparison, the SAW phase velocity in PMN-33%PT single crystal is dramatically lower than those of traditional piezoelectric materials. For example, the SAW phase velocities of quartz and LGT crystals are about 3300–4000 m/s and 2224–2697 m/s, respectively,¹⁶ and the SAW phase velocities of LiNbO_3 crystals are about 3300–3900 m/s.¹⁷ Therefore, the low SAW phase velocity of PMN-33%PT single crystal make it a very favorable candidate for further miniaturized SAW devices.

FIG. 4. Electromechanical coupling coefficient of PMN-33%PT at the Y-cut.

FIG. 5. Electromechanical coupling coefficient of PMN-33%PT at the Z-cut.

The electromechanical coupling coefficients of PMN-33%PT single crystal for the *Y*-cut and *Z*-cut situations are strongly dependent on wave propagation directions, as shown in Figs. 4 and 5, which implies that the electromechanical coupling coefficients strongly depend on the propagation direction. In comparison, the electromechanical coupling coefficients of PMN-33%PT single crystal are much higher than that of the traditional piezoelectric materials in most propagation directions. The maximum values of k^2 of PMN-33%PT single crystal are 12% and 9%, respectively, for the *Y*-cut and *Z*-cut situations, while the k^2 values of quartz, LGT and LiNbO₃ crystals are less than 0.1%, 0.45% and 6%, respectively.^{16,17}

Similar to electromechanical coupling coefficients, the PFA value φ is also strongly dependent on the propagation direction, Figs. 6 and 7 shows the calculate φ values for the *Y*- and *Z*-cut cases. Since the PFA reflects diffracted intensity of the SAW power, reducing the PFA can reduce acoustic attenuation and meliorate electromechanical performance of SAW devices. Traditional piezoelectric materials usually have large PFA, for example, the maximum values of PFA of quartz and LGT are close to 20°, and that of LiNbO₃ crystals are around 7°. On the other hand, the PFA values of PMN-33%PT single crystal at *Y*-cut and *Z*-cut are less than 1.5°, as shown in Fig. 4. We also found that the PFA values become zero in the directions of 16.35°, 46°, 63.88°, 90°, 115°, 133.3°, and 162° for the *Y*-cut case, and in the directions of 0°, 19.3°, 44.78°, 69°, 89.6°, 110.1°, 135.2°, 159°, and 180° for the *Z*-cut case. These findings will help SAW device designers to make better use of these PMN-PT single crystals.

FIG. 6. PFA of PMN-33%PT at the *Y*-cut.

FIG. 7. PFA of PMN-33%PT at the *Z*-cut.

115°, 133.3°, and 162° for the *Y*-cut case, and in the directions of 0°, 19.3°, 44.78°, 69°, 89.6°, 110.1°, 135.2°, 159°, and 180° for the *Z*-cut case. These findings will help SAW device designers to make better use of these PMN-PT single crystals.

In summary, the properties of SAWs propagating in *Y*-cut and *Z*-cut PMN-33%PT single crystals poled along [001]_c were theoretically investigated based on the experimentally measured material properties. The results showed that *Y*-cut and *Z*-cut PMN-33%PT single crystals have excellent properties, such as low phase velocities, small power flow angles and very high electromechanical coupling coefficients, which are crucial factors for making better SAW devices with broader bandwidth, lower insertion loss and lower acoustic attenuation. It was found that the characteristic curves of SAW in *Y*-cut and *Z*-cut PMN-33%PT single crystals are symmetric with respect to $\theta=90^\circ$, reflecting the symmetric nature of the PMN-33%PT crystals. The angular dependence of SAW propagation has been calculated and the theoretical results are in good agreement with measured results. Considering all related factors, it was concluded that the *Y*-cut PMN-33%PT single crystals possess superior performance in the directions of 45° and 135°. In other words, 45° and 135° of *Y*-cut PMN-33%PT are excellent piezoelectric materials for making miniaturized SAW devices.

This research was supported in part by the NSFC under Grant No. 50602009, Program of the Ministry of Education of China for New Century Excellent Talents in University under Grant No. NCET-06-0345, Postdoctoral Science Research Developmental Foundation of Heilongjiang Province under Grant No. LBH-Q06068, and NIH Grant No. P41-EB21820.

¹J. R. Gell, M. B. Ward, R. J. Young, R. M. Stevenson, P. Atkinson, D. Anderson, G. A. C. Jones, D. A. Ritchie, and A. J. Shields, *Appl. Phys. Lett.* **93**, 081115 (2008).

²H. Takeda, H. Sako, H. Shimizu, K. Kodama, M. Nishida, H. Nakao, T. Nishida, S. Okamura, T. Shikida, and T. Shiosaki, *J. Appl. Phys.* **42**, 6081 (2003).

³K. Sriharan, C. J. Strobl, M. F. Schneider, A. Wixforth, and Z. Guttenberg, *Appl. Phys. Lett.* **88**, 054102 (2006).

- ⁴R. Shilton, M. K. Tan, L. y. Yeo, and J. R. Friend, *J. Appl. Phys.* **104**, 014910 (2008).
- ⁵X. Y. Du, Y. Q. Fu, S. C. Tan, J. K. Luo, A. J. Flewitt, W. I. Milne, D. S. Lee, N. M. Park, J. Park, Y. J. Choi, S. H. Kim, and S. Maeng, *Appl. Phys. Lett.* **93**, 094105 (2008).
- ⁶N. Naumenko and L. Solie, *IEEE Trans. Ultrason. Ferroelectr. Freq. Control* **48**, 530 (2001).
- ⁷G. Zhang, T. Han, X. Ji, and W. Shi, *J. Shanghai Jiaotong Univ.* **38**, 116 (2004).
- ⁸J. Bohm, E. Chilla, C. Flannery, H.-J. Fröhlich, T. Hauke, R. B. Heimann, M. Hengst, and U. Straube, *J. Cryst. Growth* **216**, 293 (2000).
- ⁹R. E. Service, *Science* **275**, 1878 (1997).
- ¹⁰Y. Jia, S. W. Or, H. L. W. Chan, X. Zhao, and H. Luo, *Appl. Phys. Lett.* **88**, 242902 (2006).
- ¹¹H. Fu and R. E. Cohen, *Nature (London)* **403**, 281 (2000).
- ¹²R. Zhang, B. Jiang, and W. Cao, *J. Appl. Phys.* **90**, 3471 (2001).
- ¹³K. C. Cheng, H. L. W. Chan, C. L. Choy, Q. Yin, H. Luo, and Z. Yin, *IEEE Trans. Ultrason. Ferroelectr. Freq. Control* **50**, 1177 (2003).
- ¹⁴S. T. Lau, K. H. Lam, H. L. W. Chan, C. L. Choy, H. S. Luo, Q. R. Yin, and Z. W. Yin, *Mater. Sci. Eng., B* **111**, 25 (2004).
- ¹⁵K. H. Choi, J. H. Oh, H. J. Kim, J. Y. Kim, S. G. Lee, and S. M. Rhim, *Proc.-IEEE Ultrason. Symp.* **1**, 161 (2001).
- ¹⁶G. Zhang, T. Han, X. Ji, and W. Shi, *Acta Acust.* **29**, 12 (2004).
- ¹⁷C. Wen, M.S. thesis, Tianjin University, 2006.