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Surface Acoustic Wave Propagation in Relaxor-Based Ferroelectric Single Crystals $0.93Pb(Zn_{1/3}Nb_{2/3})O_3$-$0.07PbTiO_3$ Poled along $[011]_c$ *

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Surface acoustic wave (SAW) propagation in relaxor-based ferroelectric single crystals $0.93Pb(Zn_{1/3}Nb_{2/3})O_3$-$0.07PbTiO_3$ (PZN-7%PT) poled along $[011]_c$ has been analyzed theoretically. The results show that PZN-7%PT single crystals have excellent SAW properties, such as low phase velocities, very high electromechanical coupling coefficients and small power flow angles. It is also found that the SAW properties strongly depend on the propagation direction and the characteristic curves of SAW phase velocity, and the electromechanical coupling coefficients are symmetric with respect to $\theta = 90°$. Considering all related factors, the X-cut PZN-7%PT single crystal has the best performance. Based on our results, the X-cut PZN-7%PT single crystals poled along $[011]_c$ are an excellent candidate for ultra-wide bandwidth low-frequency SAW devices.

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In recent years, perovskite relaxorbased ferroelectric single crystal $(1-x)Pb(Zn_{1/3}Nb_{2/3})O_3-xPbTiO_3$ (PZN-xPT) has attracted a great deal of attention due to its excellent piezoelectric properties.[1−3] Near the morphotropic phase boundary (MPB, $x \approx 0.09$) composition, PZN-xPT single crystals possess superior dielectric and piezoelectric properties, and very high electromechanical coupling coefficients at room temperature.[4,5] It was reported that the $0.93Pb(Zn_{1/3}Nb_{2/3})O_3$-$0.07PbTiO_3$ (PZN-7%PT) single crystals, whose composition is slightly away from the MPB, have a higher rhombohedral-tetragonal phase transition temperature and more stable electromechanical properties.[6] Therefore, PZN-7%PT single crystals are more suitable for practical application. Experimental results also showed that a PZN-7%PT single crystal poled along $[011]_c$ can produce a super large transverse d_{32} (1460PC/N) piezoelectric coefficient and high electromechanical coupling coefficient k_{32} (0.86), which make it a promising multidomain piezoelectric material for electromechanical devices.[7]

Recently, various piezoelectric crystals such as $LiNbO_3$, $GdCa_4(BO_3)_3$ and $(1-x)Pb(Mg_{1/3}Nb_{2/3})O_3-xPbTiO_3$(PMN-$x$PT) have been investigated for surface acoustic wave (SAW) devices, such as filters, oscillators, resonator, etc.[8−10] In particular, relaxor-based ferroelectric single crystal PMN-33%PT has shown excellent SAW propagation properties, including low phase velocities, small power flow angles and very high electromechanical coupling coefficients.[10]

In this Letter, we report a theoretical study on the SAW propagation characteristics in PZN-7%PT crystals poled along $[011]_c$, which will facilitate the use of PZN-7%PT single crystal in future SAW devices.

At room temperature, the macroscopic symmetry of PZN-7%PT crystal changes from rhombohedral $3m$ to orthorhombic $mm2$ after being poled along $[011]_c$.[11−12] The coordinate system under investigation is illustrated in Fig. 1. The SAW propagation in a piezoelectric single crystal is governed by the Christoffel equation with semi-infinite boundary conditions.[13,14] Using the measured material parameters of $[011]_c$ polarized PZN-7%PT,[7] the SAW propagation characteristics in this single crystal can be calculated. When 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 power flow angle (PFA) ϕ for X-, Y- and Z-cut situations are shown in Figs. 2–4, respectively.

As shown in Fig. 2, the SAW phase velocities of PZN-7%PT single crystal are strongly dependent on the wave propagation direction. The maximum values of the SAW phase velocities for PZN-7%PT single crystal are 1679, 1542 and 1549 m/s, respectively, for the X-, Y- and Z-cut cases. The minimum values of

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the SAW phase velocities 980 and 733 m/s occur in the directions of 44° and 136° for the Y- and Z-cut situations, respectively. While for the X-cut crystals, the minimum SAW phase velocity 1038 m/s occurs at 90°. In comparison, the SAW phase velocity in the PZN-7%PT single crystal is much lower than those in traditional piezoelectric materials, such as quartz and $LiNbO_3$ crystals, which are around 3500 m/s and 3600 m/s, respectively.[15,16] This is similar to the situation of PMN-33%PT single crystal.[17,18] Therefore, this characteristic of PZN-7%PT single crystal poled along $[011]_c$ is suitable for true generation of miniaturized SAW devices.

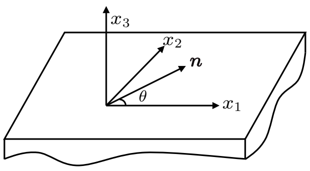

Fig. 1. Coordinate system used in this work.

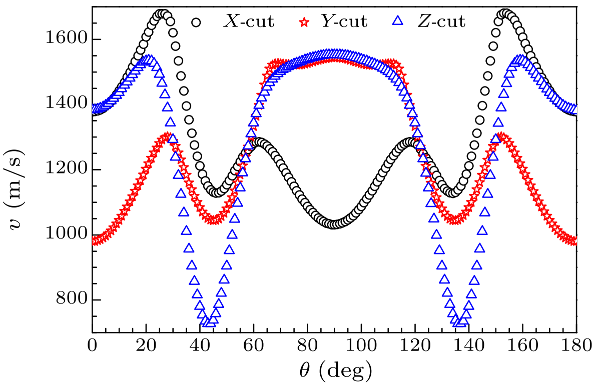

Fig. 2. The SAW phase velocity of PZN-7%PT single crystals poled along $[011]_c$.

For low-frequency and wide band applications, piezoelectric materials with lower phase velocity and higher electromechanical coupling coefficient are required. The characteristics of the SAW electromechanical coupling coefficients k in the PZN-7%PT single crystal poled along $[011]_c$ for the X-, Y- and Z-cut situations are given in Fig. 3. It can be noticed from Fig. 3 that the k^2 value of PZN-7%PT single crystal poled along $[011]_c$ for the X-cut is as high as 25.16% in the directions of 30° and 150° canted from $[011]_c$. Moreover, the range of high k^2 values is very wide. This SAW parameter is very attractive compared to the conventional materials in terms of high electromechanical coupling coefficient.[15,16] However, for the Z-cut and Y-cut cases, the k^2 values are below 6.64% and 1.91%, respectively. Therefore, the X-cut PZN-7%PT single crystal poled along $[011]_c$ is more suitable for ultra-wide bandwidth applications in low-frequency SAW devices. In addition, the macroscopic symmetry of the PZN-7%PT single crystal poled along $[011]_c$ is orthorhombic $mm2$, so that a pattern of symmetry appears on the maps, and a bilateral symmetry is obtained centered at $\theta = 90°$.[12]

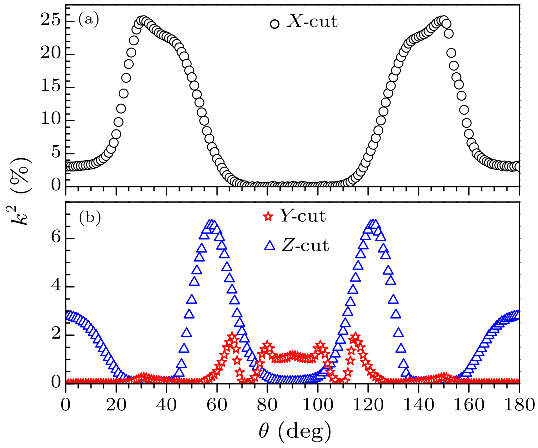

Fig. 3. Electromechanical coupling coefficient of PZN-7%PT single crystals poled along $[011]_c$.

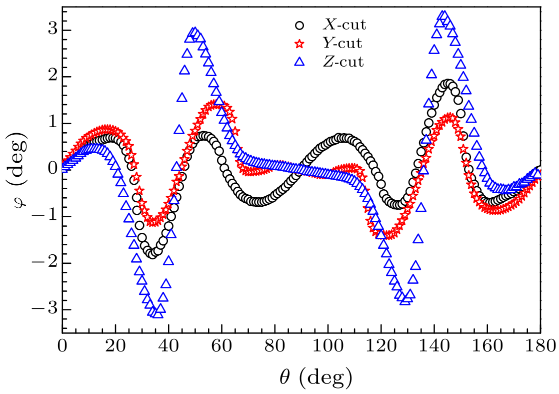

Fig. 4. Power flow angle of PZN-7%PT single crystals poled along $[011]_c$.

Figure 4 shows the characteristics of the SAW power flow angle (PFA) φ for the PZN-7%PT single crystal poled along $[011]_c$. One can see that the PFA values are less than 1.92°, 1.45° and 3.37° for the X-, Y- and Z-cut situations, respectively. Moreover, the PFA values become zero in certain directions for the three cases. Such small PFA values can significantly reduce the acoustic attenuation and improve the electromechanical performance of SAW devices. In addition, it can be noticed from Fig. 4 that the PFA values for the PZN-7%PT single crystal poled along $[011]_c$ are also strongly dependent on the propagation direction.

In summary, the SAW properties of the PZN-7%PT single crystals poled along $[011]_c$ have been evaluated theoretically. In order to determine the optimum crystalline cuts, the calculation is performed on three cut directions. The maximum k^2 value (25.16%) has been obtained on the X-cut crystal. In addition, the X-cut PZN-7%PT single crystal has very small PFA and low phase velocities. These SAW parameters are very attractive compared to the conventional piezoelectric materials, making the $[011]_c$ poled X-cut PZN-7%PT single crystal an excellent candidate for use in wide band low frequency SAW devices.

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