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Enlarged phase velocities of ultra-wideband surface acoustic wave devices with relaxor based ferroelectric single crystal/diamond layered structure

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ABSTRACT

The surface acoustic wave (SAW) characteristics of Y-cut X propagating $Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (YX-PIMNT) single crystals on a diamond substrate have been theoretically calculated. The simulated results show that the phase velocity of the shear horizontal (SH) SAW may be greatly enhanced from the 1350 m/s to 3350 m/s by reducing the thickness of the PIMNT from 0.5λ to 0.05λ, with a corresponding decrease in the electromechanical coupling factor (K^2) from 73.6% to 19.6%. The dispersion curves of phase velocity and K^2 as a function of PIMNT thickness are given for the proposed layered structure. Besides the SH SAW, there are also higher order modes that would cause unwanted responses in the pass-band of wideband SAW filters. These were suppressed by properly controlling structural parameters including top electrode thickness, thickness and Euler angle (θ) of PIMNT substrate. The calculated results demonstrate the effectiveness of this approach to enlarge the phase velocity of the SH SAW without dramatically sacrificing its K^2, which makes relaxor based ferroelectric single crystals promising for realizing ultra-wideband SAW devices working in ~GHz range.

1. Introduction

Relaxor based ferroelectric single crystals, such as $Pb(Mg_{1/3}Nb_{2/3})O_3$-$xPbTiO_3$ (PMNT or PMN-xPT) and $Pb(Zn_{1/3}Nb_{2/3})O_3$-$xPbTiO_3$(PZNT or PZN-xPT) have triggered revolutionary changes in piezoelectric devices over the past few decades. This is because of their ultrahigh electromechanical coupling factor k_{33} (>94%) and piezoelectric constant d_{33} (>2500pC/N) near the morphotropic phase boundary (MPB) at room temperature [1–5].

One of the drawbacks of PMNT single crystals is their relatively low Curie temperature ($T_c \approx 130$ °C) and phase transition temperature ($T_{rT} \approx 85$ °C) from the rhombohedral to tetragonal phase, which limits their high temperature applications. Recently, a ternary compound $Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PIMNT or PIN-PMN-xPT) has attracted great attention because it exhibits a higher T_c ($\approx$200 °C) and T_{rT} ($\approx$110 °C) with comparable piezoelectric performance to that of PMNT single crystals [6–7].

The authors have previously achieved a large K^2 ($\approx$60%) by fabricating a SAW resonator on YX-PIMNT substrate [8–9]. However, the barrier to its application in radio frequency (RF) SAW filters is its low phase velocity ($\approx$1350 m/s) that results in low resonance frequency f_r ($\approx$355 MHz) at a wavelength $\lambda \approx 4$ μm. The direct approach to achieve higher frequency operation is to reduce the width of the electrodes, but this has a limit imposed by the resolution of lithography. Another effective approach is to use a substrate with higher acoustic wave propagating velocity as a bottom substrate, such as SiC or diamond. F. Bénédic et al. reported that the SAW phase velocity can be increased from 5700 m/s to 11,000 m/s by using a layered structure of AlN/diamond substrate [10].

In this paper, we propose a similar layered structure of YX-PIMNT/diamond substrate to increase propagating SAW velocity. Numerical analysis of SAW propagation on the layered structure was performed using the finite element method (FEM) with the commercial software package Multiphysics COMSOL. The structure admittance response was calculated, and dispersion curves of phase velocity and K^2 for the SAW modes were estimated from the admittance. The structural parameters, among which top electrode thickness, and thickness and Euler angle (θ) of the PIMNT crystals were optimized to achieve large phase velocity without dramatically sacrificing K^2.

2. Modeling and simulation

Fig. 1(a) shows the modeled structure of an electrode layer/YX-PIMNT/diamond substrate configuration. The thickness of each layer is respectively denoted as h_e, h_{PIMNT}, and h_D. Fig. 1(b) shows a schematic diagram of a wave propagating along a rotated Euler angle θ on the YX-PIMNT crystals.

Two dimensional models are insufficient in analyzing SH SAW component, thus a three dimensional periodical model of the layered

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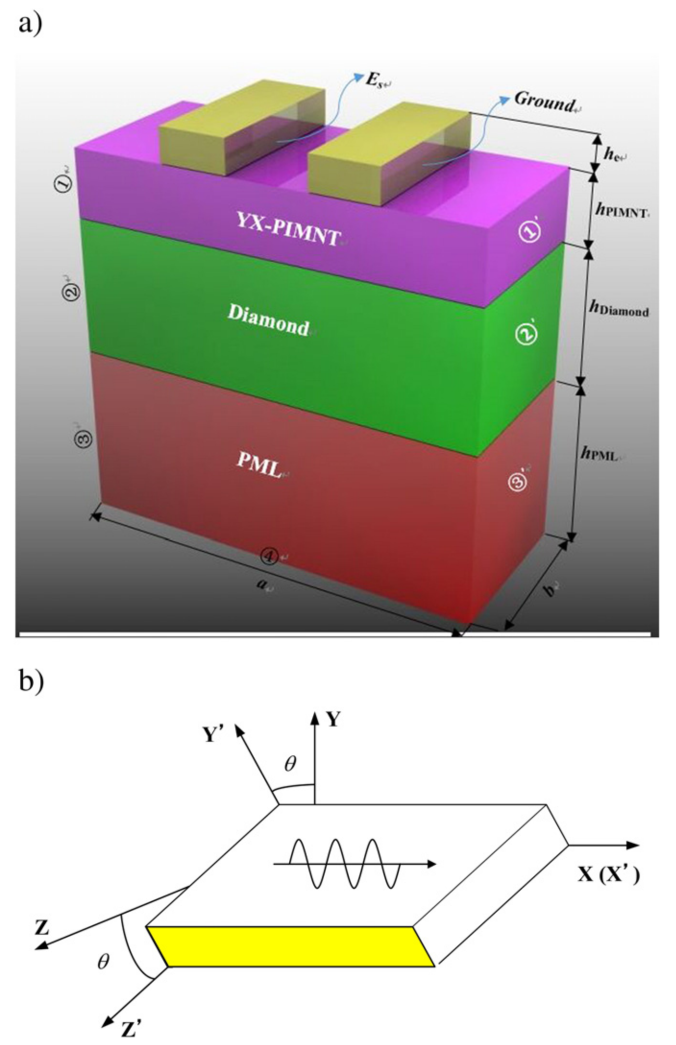

Fig. 1. Schematic diagrams of (*a*) electrode/PIMNT/diamond substrate layered structure, ①①’,②②’,③③’ are with periodic boundary conditions for displacements and electric potential, ④ is with free constrain, E_s is excited source of sinusoidal signal; (b) wave propagating at rotated angle θ on YX PIMNT substrate, displacement components of L (u_x), SH (u_y) and SV (u_z), φ is the potental.

structure was established in COMSOL using the FEM [11]. The material constants of PIMNT crystal and diamond are taken from Refs. [12,13]. Gold was set as the top electrode material.

The resonator was characterized by harmonic analysis under the condition of application of a sinusoidal signal with voltage $E_s/2$ to the electrode. The harmonic admittance Y per iDT period is then given by $Y = j2\pi fQ/E_s$, where f is the driving frequency and Q is the total charge induced on the electrode.

3. Results and discussion

Fig. 2 shows the calculated relative admittance in decibels, namely, $20\log_{10}|Y(f)/\omega C_0|$ per period of infinitely long Interdigital transducers (IDTs) on the layered structure of YX-PIMNT/diamond substrate as a function of frequency, where ω is the main angular resonance frequency, and C_0 (=0.02 pF) is the static capacitance of the IDT per periodic length λ (=4 μm). In the calculation, $h_e = 1.5\%\lambda$, h_{PIMNT} of 0.15λ and 0.225λ were used for comparison, $h_D = 35\lambda$ and the layer was set to be semi-infinite. The frequencies of f_r and f_a for each eigenmode were obtained for $Y(f)^{-1} = 0$ and $Y(f) = 0$, respectively. K^2 is a measure of the electro-acoustic energy conversion efficiency of a resonator, and

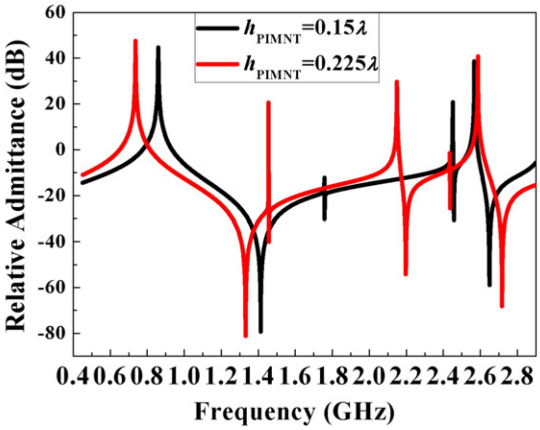

Fig. 2. Calculated relative admittance $Y(f)$ per period of infinitely long IDTs on layered structure as a function working frequency for $h_{PIMNT} = 0.15\lambda$ and 0.225λ.

can be estimated using the following formula derived from equivalent circuit analysis [14]:

$$K^2 = (\pi f_r/2f_a)/\tan(\pi f_r/2f_a).$$

Large K^2 indicates a large difference between f_r and f_a, which is of great importance for achieving wideband SAW filters [15].

It is clear that several eigenmodes exist in the layered structure. The first eigenmode with $f_r \approx 700$ MHz is the main mode corresponding to SH SAW [8], whose displacement component u_y couples with potential φ, as depicted in Fig. 1(b). The K^2 of SH SAW is as large as 73.6% and phase velocity of 1590 m/s are obtained when $h_{PIMNT} = 0.225\lambda$. These values are almost the same as those achieved for SAW resonators on bulk YX-PIMNT substrate. Interestingly, the phase velocity can be doubled simply by thinning the YX-PIMNT crystal to 0.15λ, while the K^2 drops to 66.8%. Such large K^2 with enhanced phase velocity is of great merit for achieving ultra-wideband SAW devices that operate in the GHz range [16–17]. The second eigenmode can be associated with traditional Rayleigh SAW, whose displacement components u_x and u_z compled each other. The $f_r \approx 1.33$ GHz when $h_{PIMNT} = 0.225\lambda$ and increases to 1.55 GHz at a smaller h_{PIMNT} of 0.15λ. The f_r of the Rayleigh SAW is very close to that of the SH SAW, which would produce unwanted responses in the pass-band of such a ultra-wideband SAW filter. Fortunately, it could be suppressed by properly selecting the thickness of the YX-PIMNT substrate, such as the K^2 of the Rayleigh SAW is almost zero when $h_{PIMNT} = 0.15\lambda$.

There are also higher order eigenmodes, and the dispersion curves of phase velocity and K^2 as a function of PIMNT thickness estimated by the calculated admittance are given in Fig. 3(a) and (b), respectively. The phase velocity of SH SAW can reach a value of 3325 m/s when $h_{PIMNT} = 0.05\lambda$, while its K^2 drops to 19.6%, indicating limited applicability for wideband SAW devices. Although higher modes travel a larger phase velocities, their maximum K^2 is <7%, as shown in the inset of Fig. 3(b).

It should be noted that effects of mass loading by the electrode layer could not be neglected, because the thickness of the electrode layer was comparable to that of the thinned YX-PIMNT substrate. Therefore, the dependence of the K^2 of the SH and Rayleigh SAWs on the Au electrode thickness was investigated, as shown in Fig. 4. The maximum K^2 of the SH SAW is about 68.7% when $h_e = 2.25\%\lambda$, at which the value of the Raleigh SAW's K^2 is almost zero. As the electrode thickness is increased, the value of K^2 for the SH SAW decreases and that of the Rayleigh SAW increases.

Fig. 5(a) and (b) shows the variation in the calculated effective velocities and K^2 of the SH and Rayleigh SAW with Euler angle θ from 0° to 180°. In this case, $h_{PIMNT} = 0.15\lambda$ and $h_e = 2.25\%\lambda$. The effective velocities are defined by $V_r = f_r\lambda$ and $V_a = f_a\lambda$ at the resonance and antiresonance frequencies, respectively. The V_r of the SH SAW gradually