Propagations of Rayleigh and Love waves in ZnO films/glass substrates analyzed by three-dimensional finite element method*

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Propagation characteristics of surface acoustic waves (SAWs) in ZnO films/glass substrates are theoretically investigated by the three-dimensional (3D) finite element method. At first, for $(11\bar{2}0)$ ZnO films/glass substrates, the simulation results confirm that the Rayleigh waves along the [0001] direction and Love waves along the $[1\bar{1}00]$ direction are successfully excited in the multilayered structures. Next, the crystal orientations of the ZnO films are rotated, and the influences of ZnO films with different crystal orientations on SAW characterizations, including the phase velocity, electromechanical coupling coefficient, and temperature coefficient of frequency, are investigated. The results show that at appropriate h/λ, Rayleigh wave has a maximum k^2 of 2.4% in (90°, 56.5°, 0°) ZnO film/glass substrate structure; Love wave has a maximum k^2 of 3.81% in (56°, 90°, 0°) ZnO film/glass substrate structure. Meantime, for Rayleigh wave and Love wave devices, zero temperature coefficient of frequency (TCF) can be achieved at appropriate ratio of film thickness to SAW wavelength. These results show that SAW devices with higher k^2 or lower TCF can be fabricated by flexibly selecting the crystal orientations of ZnO films on glass substrates.

Keywords: surface acoustic wave, ZnO films, electromechanical coupling coefficient, temperature coefficient of frequency, 3D finite element method

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1. Introduction

ZnO films have been widely applied to surface acoustic wave (SAW) and bulk acoustic wave (BAW) devices because of the superior piezoelectricity and higher electromechanical coupling coefficient. However, most of the acoustic devices were based on (0001) textured ZnO films, in which the *c* axis of the hexagonal crystal was perpendicular to the substrate plane, and the thickness vibration mode of BAW and Rayleigh mode of SAW were always used.[1–3] Recently, $(11\bar{2}0)$ ZnO films, with *c* axis parallel to the substrate plane, have attracted more attention, in which the shear horizontal (SH) mode waves can be excited.[4–6] The SAW devices based on $(11\bar{2}0)$ ZnO films have potential applications in liquid and biological sensors because of the disappearance of normal displacement and lack of coupling elastically with liquid medium to induce radiation loss.

The ZnO piezoelectric films can be deposited on various substrates to obtain different multi-layered structures for improving some of the characterizations of SAW devices. Matsuo *et al.*,[7] Krishnaswany *et al.*[8] and Wang and Lakin[9] have deposited ZnO films with *c* axis tilted by different angles with respect to the normal of fused quartz, glass, and Si substrates, respectively. However, both longitudinal and shear bulk waves were generated in these films, which resulted in poor quality factor (Q) and sensing resolution in sensor applications. In addition, it was reported that the pure shear mode of SAW has been excited when the *c* axis of ZnO films lied in the substrate plane.[10,11] Furthermore, Wang *et al.* have investigated experimentally characterizations of Love waves excited in $(11\bar{2}0)$ ZnO films/R-sapphire substrates and the Love wave humidity sensors.[12,13] On the other hand, Yanagitani *et al.* have successfully deposited $(11\bar{2}0)$ ZnO films on SiO_2 substrates and pure shear horizontal waves in the VHF-UHF range have been excited in the films.[14]

A few theoretical researches have been reported on the propagations of SAWs in ZnO films with different textures.[15–17] However, it is necessary to carry out the theoretical investigations on acoustic characterizations, such as the phase velocity v_p, electromechanical coupling coefficient k^2, and temperature coefficient of frequency (TCF) for designing and optimizing the properties of acoustic devices.

In this work, a three-dimensional (3D) FEM model based on COMSOL 4.3b is employed to study the propagation characterizations of SAWs in ZnO film/glass substrate structures. The dependence of v_p, k^2, and TCF on the thicknesses of ZnO films is studied in detail, especially, the influences of ZnO films with different crystal orientations on SAW properties are

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calculated numerically.

2. Modeling and simulation

A 3D FEM model of delay lines used to simulate the characteristics of SAWs is shown in Fig. 1(a). The material constants of ZnO films are generally given in the crystal coordinate system, which corresponds to the global coordinate system (x, y, z) in COMSOL. In order to obtain the parameters of ZnO films with different crystalline orientations, the rotated local coordinate system must be defined, which then corresponds to the orientations of the crystal axes within the model. The local system is often defined by the rotated system. As illustrated in Fig. 1(b), starting from the Global axis (x, y, z), this local system (X, Y, Z) can be set by a set of Euler angles (α, β, γ), in which the intersection line of xy-plane and XY-plane is denoted with N. After the coordinate rotation, the c axis of ZnO is aligned with the Z axis as illustrated in Fig. 1(a).

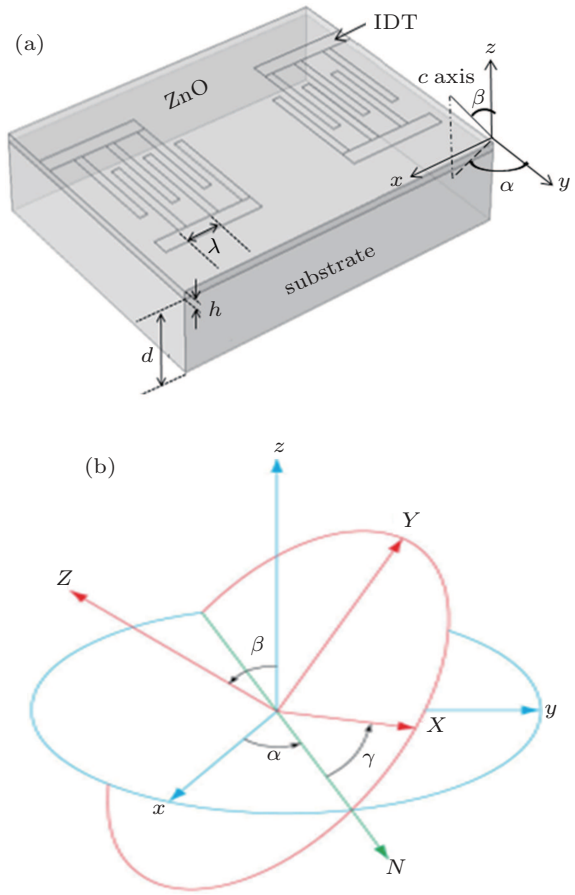


Fig. 1. (color online) Schematic diagram of ZnO film/glass substrate structure and coordinate system used in calculations.

In the numerical analysis, the model of the SAW devices shown in Fig. 1(a) is meshed with triangular elements. The mesh density of the device is kept at 16 nodes per wavelength (i.e., 1 node for 1 μm).

The boundary conditions of the devices are chosen as follows: the top surface is free of mechanical boundary, the bottom surface is fixed boundary, and the other 4 side faces are periodic boundaries, and none of the boundaries has charge, which is used for electrical boundary condition. Besides, all of the interfaces are under the condition of continuous mechanical boundary.

The phase velocity of SAWs can be calculated from the following relation:[12]

$$v_{\mathrm{p}} = \lambda \times f_0, \tag{1}$$

where λ is the wavelength and f_0 is the resonance frequency of delay lines.

The electromechanical coupling coefficient k^2 can be calculated from[5]

$$k^2 = 2\frac{v_{\mathrm{f}} - v_{\mathrm{m}}}{v_{\mathrm{f}}}, \tag{2}$$

where v_{f} and v_{m} are the velocities of SAWs corresponding to electrically free surface and electrically metallized surface, respectively.

The TCF is an important factor to characterize the temperature stabilization of SAW device, which can be calculated from the following equation:[18]

$$\mathrm{TCF} = \frac{1}{T - T_0} \cdot \frac{\Delta f}{f_{T_0}}, \tag{3}$$

where T_0 is the reference temperature, which is set to be 20 °C for the simulations, f_{T_0} is the resonance frequency at 20 °C, and Δf is the frequency shift caused by the variation of temperature. The important material constants and temperature coefficients used in the calculations are listed in Table 1.

Table 1. Material constants and temperature coefficients used in simulations.[19,20]

Parameter	Symbol	ZnO	Glass
Elastic constant/(10^9 N/m^2)	C_{11}	209.7	78.5
	C_{12}	121.1	16.1
	C_{13}	105.3	16.1
	C_{33}	211.2	78.5
	C_{44}	423.7	31.2
Temperature coefficients/(10^4/°C)	TC(C_{11})	−1.12	2.39
	TC(C_{13})	−1.61	5.84
	TC(C_{33})	−1.23	2.39
	TC(C_{44})	−0.70	1.51
Piezoelectric constants/(c/m^2)	e_{24}	−0.48	–
	e_{31}	−0.57	–
	e_{33}	1.32	–
Relative dielectric constants	$\varepsilon_{11}/\varepsilon_0$	7.57	3.32
	$\varepsilon_{11}/\varepsilon_0$	10.2	3.32
Density/(kg/m^3)	ρ	5670	2200

3. Results and discussion

3.1. Characteristics of v_{p} and k^2 in ZnO film/glass substrate structures

The fundamental and higher order modes of Rayleigh and Love waves in the ZnO film/glass structures are calculated by

3D FEM. The propagation characterizations of SAW, including v_p, k^2, and TCF, are analyzed theoretically and plotted each as a function of the film thickness-to-wavelength ratio (h/λ).

(i) At first, the characteristics of fundamental (mode 0) and first order (mode 1) Rayleigh waves propagating along the [0001] direction in the structure of $(11\bar{2}0)$ ZnO film/glass substrate are simulated. As shown in Fig. 2, the phase velocity of each mode decreases rapidly with increasing h/λ. For mode 0, the phase velocity equals the SAW velocity of glass (3379 m/s)[20] at $h/\lambda = 0$, and the phase velocity is 2700 m/s at $h/\lambda = 0.5$, which is close to the SAW velocity of the ZnO film, i.e., Rayleigh wave almost propagates in the film. The mode 1 shows cutoff at a critical point of $h/\lambda = 0.7$, where the phase velocity corresponds to acoustic radiation in the glass (3783 m/s).[15,20] On the other hand, for k^2 of mode 0, there is a small peak corresponding to a relative maximum k^2 of 1.19% at $h/\lambda = 0.11$, and then k^2 increases with the further increase of h/λ and the maximum k^2 of 1.81% is obtained at $h/\lambda = 0.51$. Meanwhile, the k^2 values of mode 1 are all less than 0.1%, which is much smaller than those of mode 0.

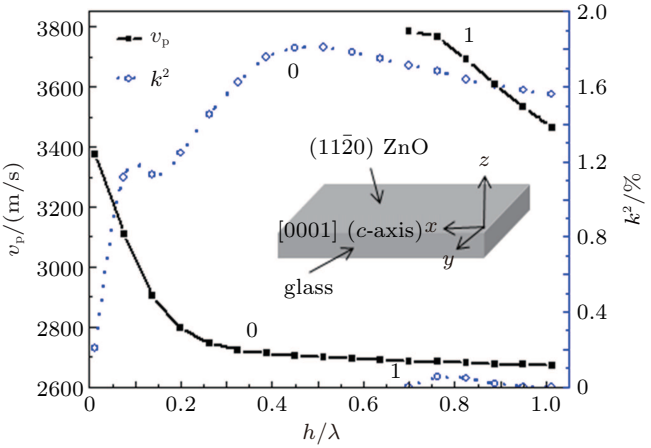


Fig. 2. (color online) Variations of v_p and k^2 with h/λ for Rayleigh waves in $(11\bar{2}0)$ ZnO films/glass substrates.

(ii) For comparison, Rayleigh waves in (0002) ZnO film/glass substrate structures are also investigated, and the characteristics of mode 0 and mode 1 are shown in Fig. 3. For mode 0 of Rayleigh wave, the phase velocity equals the SAW velocity of glass (3379 m/s) at $h/\lambda = 0$, and decreases rapidly with the increase of h/λ. Mode 1 appears at a critical cutoff point of $h/\lambda = 0.58$, where the phase velocity corresponds to acoustic radiation in the glass (3783 m/s). The k^2 values of mode 0 are larger than those of mode 1, and the maximum k^2 is 1.33% when the thickness of ZnO film is 0.39λ. Comparing Fig. 2 with Fig. 3, it is found that the fundamental Rayleigh waves in $(11\bar{2}0)$ ZnO films have higher phase velocities and larger k^2 than in (0002) ZnO films with the same values of ratio h/λ.

(iii) The properties of Love waves in $(11\bar{2}0)$ ZnO film/glass substrate structures are theoretically investigated and the results are shown in Fig. 4. For mode 0, the phase velocity equals the shear bulk wave velocity of glass (3766 m/s)[20] at $h/\lambda = 0$. The phase velocity decreases rapidly and tends gradually to be stable with increasing h/λ. The mode 1 shows a cutoff at a point of $h/\lambda = 0.58$ with a phase velocity of 3781 m/s. The k^2 of mode 0 shows a relative maximum value of 3.0% at $h/\lambda = 0.25$, where the phase velocity is 3075 m/s. Furthermore, the k^2 values are larger than 1% in a wide range of $h/\lambda > 0.06$, which is considered to be high enough for the applications of SAW devices from a viewpoint of practical application. Mode 1 has a maximum k^2 of 1.48% at $h/\lambda = 0.7$ with a velocity of 3574 m/s, and the k^2 values are smaller than those of mode 0.

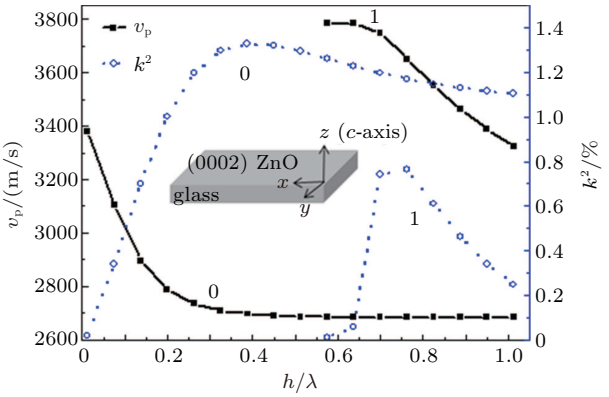


Fig. 3. (color online) Variations of v_p and k^2 with h/λ for Rayleigh waves in (0002) ZnO films/glass substrates.

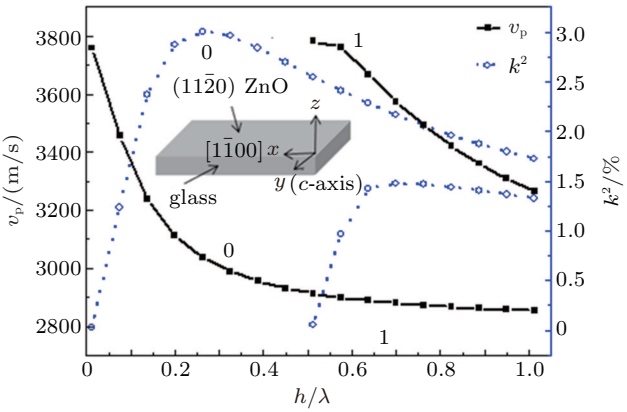


Fig. 4. (color online) Variations of v_p and k^2 with h/λ for Love waves in $(11\bar{2}0)$ ZnO films/glass substrates.

From the descriptions above, the k^2 values of mode 0 are larger than those of mode 1 for both Rayleigh waves and Love waves, thus the following discussion focuses on 0th modes of Rayleigh wave and Love wave.

3.2. Influences of crystal orientations of ZnO films on SAW properties

i) The textures with different crystal orientations of ZnO films strongly influence SAW properties in the layered struc-

tures. In the first case, the properties of SAWs in the structures of (α, 90°, 0°) (11$\bar{2}$0) ZnO films/glass substrates are investigated, in which c axis of ZnO film is parallel to the substrate plane. And α is the angle between N and x direction (Fig. 1(b)), which equals the angle between the projection of c axis of ZnO film in the xy-plane and the y direction as shown in Fig. 1(a). It can be indicated that for each α value, there is a maximum $k^2_{\max}$ as h is changed. The maximal values of $k^2_{\max}$ of SAWs propagating in ZnO films/glass substrates each as a function of angle α are calculated and the results are shown in Fig. 5.

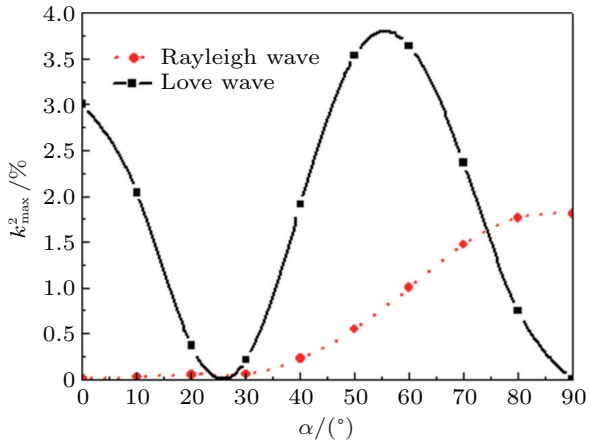


Fig. 5. (color online) Variations of maximum $k^2_{\max}$ with α for SAWs in (α, 90°, 0°) (11$\bar{2}$0) ZnO films/glass substrates.

For Rayleigh waves, the $k^2_{\max}$ monotonically increases with increasing α. The largest $k^2_{\max}$ of 1.81% is obtained when $\alpha = 90°$. It means that Rayleigh wave propagating along the [0001] direction of (11$\bar{2}$0) ZnO film/glass substrate has a maximum $k^2_{\max}$. But k^2 equals zero when $\alpha = 0°$, i.e., Rayleigh wave cannot be excited in the [1$\bar{1}$00] direction.

The results of Love waves show that the largest $k^2_{\max}$ is 3.81% when $\alpha = 56°$, which means that Love wave has a maximum $k^2_{\max}$ in (56°, 90°, 0°) (11$\bar{2}$0) ZnO film/glass substrate. However, k^2 equals zero when $\alpha = 26°$ and $\alpha = 90°$, i.e., no Love waves propagate in (11$\bar{2}$0) ZnO films on glass substrates with (26°, 90°, 0°) texture and (90°, 90°, 0°) texture.

ii) Then, theoretical investigations on SAWs in ZnO films with tilted c axis are also carried out. Figure 6 shows the characterizations of SAWs in (α, β, 0°) ZnO film/glass substrate structures, in which β is the angle between c axis of ZnO film and the z direction (normal of substrates) as shown in Fig. 1(a). In the following calculations, the values of α are set to be 90° and 56° for Rayleigh waves and Love waves, respectively, where the maximal values of $k^2_{\max}$ can be obtained for both waves according to the results shown in Fig. 5.

The calculated results demonstrate that Rayleigh waves can be excited in ZnO films with the tilted c axis and for each β value, there is also a maximum $k^2_{\max}$ as h is changed. Meanwhile, with β increasing from 0° to 90°, the values of maximum $k^2_{\max}$ first increase and then decrease. The largest $k^2_{\max}$ of 2.4% is achieved when $\beta = 56.5°$ and $h/\lambda = 0.39$.

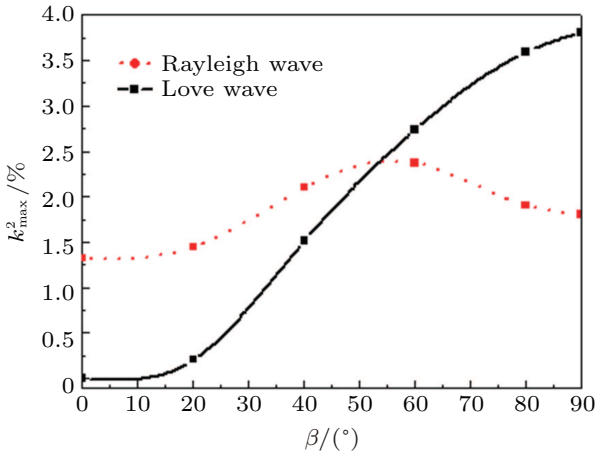


Fig. 6. (color online) Variations of maximum $k^2_{\max}$ with β for SAWs in (α, β, 0°) ZnO films/glass substrates.

Meanwhile, the $k^2_{\max}$ values of Love waves monotonically increase from 0% to 3.81% with angle β increasing from 0° to 90°. The results indicate that there is no Love wave in (0002) ZnO film with the c axis perpendicular to the substrate plane ($\beta = 0°$), and Love wave has the maximum $k^2_{\max}$ in (11$\bar{2}$0) ZnO film with the c axis parallel to the substrate plane ($\beta = 90°$). Therefore, ZnO films with (90°, 56.5°, 0°) texture and (56°, 90°, 0°) texture are optimal for exciting Rayleigh wave and Love wave, respectively.

3.3. TCF characterizations in ZnO film/glass substrate structures

TCF curves for 0th modes of Rayleigh wave and Love wave in ZnO film/glass substrate structures are calculated each as a function of h/λ. As shown in Fig. 7(a), all of the TCF values change from positive values to negative values with the thickness of ZnO film increasing because glass substrate with a positive TCF is compensated by ZnO films with a negative TCF. For Rayleigh waves, zero TCF can be achieved when $h/\lambda = 0.41$ and $h/\lambda = 0.43$ in (11$\bar{2}$0) ZnO films and (0002) ZnO films on glass substrates, respectively. The TCF of Love waves in (11$\bar{2}$0) ZnO films/glass substrates decreases to zero at $h/\lambda = 0.2$, where a relative high k^2 of 2.87% is obtained. Figure 7(b) shows the frequency shifts versus operating temperature for Rayleigh waves and Love waves as h is selected at zero TCF. From the results mentioned above, it can be concluded that the temperature compensation can be realized by the structure of ZnO films/glass substrates, and the temperature compensation effect of (11$\bar{2}$0) ZnO films for Rayleigh wave is better than that of (0002) ZnO films.

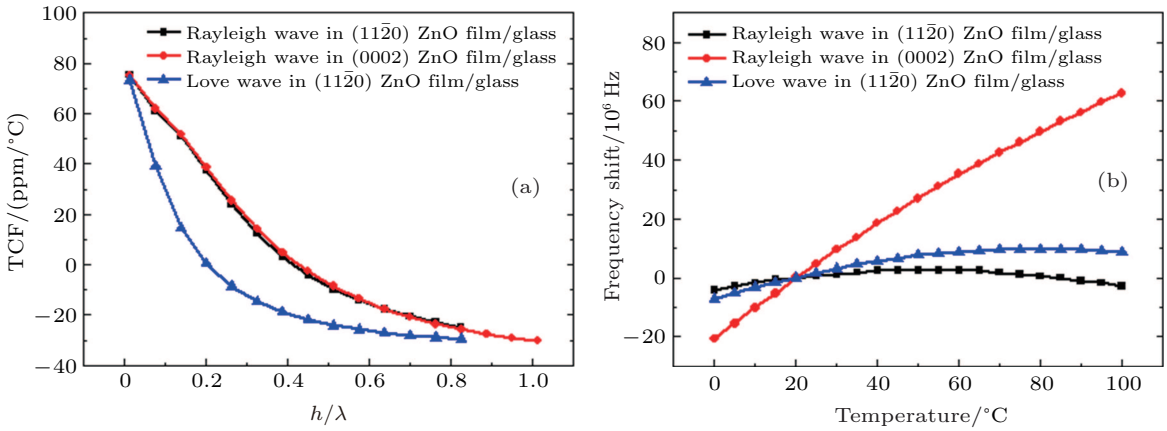


Fig. 7. (color online) Plots of (a) calculated TCF versus h/λ and (b) frequency shift versus temperature for SAWs in ZnO films/glass substrates.

The influences of ZnO films with different crystal orientations (various angles of α and β) on the TCF characteristics of Rayleigh waves and Love waves can be obtained by the similar calculations as described in the above sections, such as the variations of TCF as functions of h/λ, and zero TCF can be obtained at suitable h/λ. So, with the consideration of the influence of temperature, the SAW devices with optimized TCF can also be fabricated by selecting the textures of ZnO films.

3.4. Love wave displacement in (11$\bar{2}$0) ZnO film/glass substrate structures

Figure 8 shows the normalized displacement (u) field distributions for Love waves as a function of normalized depth z/λ, which propagates in (0°, 90°, 0°) (11$\bar{2}$0) ZnO film/glass substrate structure with $h/\lambda = 0.25$ and (56°, 90°, 0°) (11$\bar{2}$0) ZnO film/glass substrate structure with k^2 of 3.81% at $h/\lambda = 0.26$, respectively. The u_z components equal zero for both Love waves in (0°, 90°, 0°) and (56°, 90°, 0°) (11$\bar{2}$0) ZnO films. It means that Love wave device consisting of (α, 90°, 0°) (11$\bar{2}$0) ZnO films/glass substrate structures is a promising candidate for sensors operated in liquid circumstance, due to the disappearance of normal displacement and lack of coupling elastically with liquid medium to induce radiation loss.

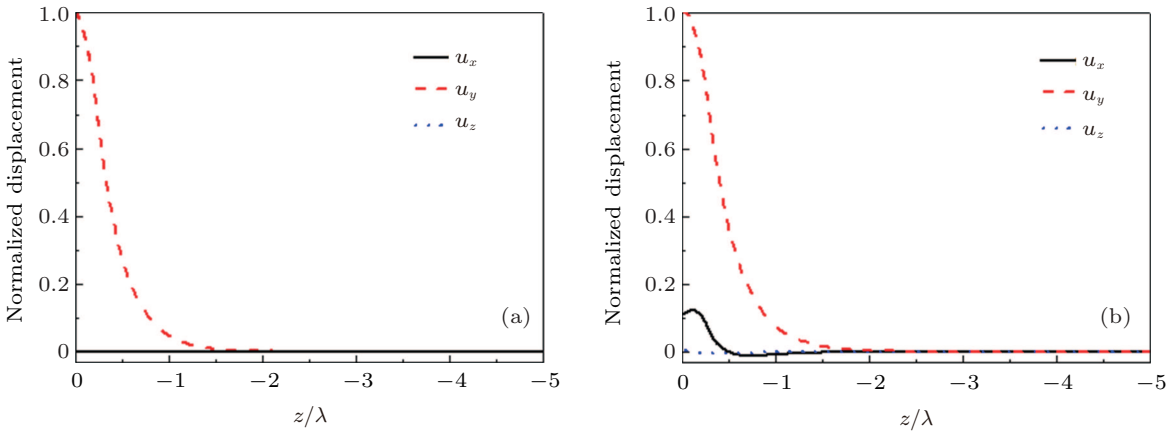


Fig. 8. (color online) Normalized displacements of Love waves each as a function of normalized depth z/λ in (11$\bar{2}$0) ZnO films with (a) (0°, 90°, 0°) texture at $h/\lambda = 0.25$ and (b) (56°, 90°, 0°) texture at $h/\lambda = 0.26$.

4. Conclusions

The propagation characteristics of SAWs (Rayleigh waves and Love waves), including the phase velocity, electromechanical coupling coefficient and TCF, in ZnO film/glass substrate structures are calculated by 3D finite element method. At first, Rayleigh waves and Love waves are theoretically studied in (11$\bar{2}$0) ZnO films on glass substrates along the [0001] and [1$\bar{1}$00] directions, respectively. Especially, the influences of ZnO textures (various α and β) on properties of SAWs are analyzed. It is found that the maximum k^2 of 2.4% can be achieved for Rayleigh wave in (90°, 56.5°, 0°) ZnO film when $h/\lambda = 0.39$, and the maximum k^2 of 3.81% can be achieved for Love wave in (56°, 90°, 0°) (11$\bar{2}$0) ZnO film as $h/\lambda = 0.26$. Furthermore, TCFs of the SAW devices composed of ZnO film/glass substrate structures with different ZnO film textures (i.e., different ZnO crystal orientations) are also calculated similarly. The results show that the performances of SAW devices, such as higher k^2 and lower TCF, can

be optimized by suitably selecting crystal orientations of ZnO films on glass substrates, which provides important theoretical bases for extending application scope of SAW devices.

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