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A Numerical Investigation of HVPSAW in $LiTaO_3$ with Uniform Gold Film and Periodic Gold Grating

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Abstract The paper reports on the results of numerical investigation of high-velocity pseudo-surface waves (HVPSAW) in θ-rotated Y-cuts of lithium tantalate (LT), 90°-propagation. Attenuation coefficients of HVPSAW are compared for LT with Au uniform film and with Au periodic grating. The results are presented as contour plots of attenuation versus film or electrode thickness and rotation angle. HVPSAW degenerates into a pure HVSAW when θ=29° and 127°, with Au film thickness h/λ=4.8% and 5.0%, respectively. These optimal orientations move to θ=39° and θ=118°, in a substrate with Au grating, with optimal electrode thickness reduced to h/λ=2.55%. In both orientations low-attenuated HVPSAWs exhibit fairly high piezoelectric coupling (2-6%). Analysis of strip admittance confirmed that HVPSAW resonator with high quality factor can be built on the found orientations. Velocity dispersion curve was calculated for the optimal cut with the grating of optimized thickness.

I. Introduction

High propagation velocity of a surface acoustic wave (SAW) is an important requirement to piezoelectric substrates of SAW devices used in communication systems. This requirement is caused by continuously increasing operating frequencies in such systems. Utilization of high-velocity pseudo-surface (leaky) waves (HVPSAW) provides the highest velocities, compared to common SAW or low-velocity PSAW. Though such waves exist in any crystal, in general they are strongly attenuated due to the leakage of acoustic energy into the bulk of crystal and therefore they are not suitable for low-loss SAW devices.

The attenuation coefficient of a pseudo-surface wave tends to zero if it degenerates into a pure bulk wave, called in this case “exceptional”, or into a true SAW, due to vanishing contributions of either inhomogeneous or homogeneous (bulk) partial waves, respectively. True SAW solutions can occur on a low-velocity PSAW branch but they are not allowed to exist on a high-velocity (HVPSAW) branch [1]. On the other side, HVPSAW can degenerate into a pure bulk wave only in crystals with sufficiently strong anisotropy. A simple criterion, which determines the relation between the elastic stiffness constants of a crystal, necessary for the existence of non-attenuated HVPSAW, was derived in [2], $c_{44}/c_{13}>>1$. This criterion is satisfied, for example, in quartz and $Li_2B_4O_7$ and it is not satisfied in $LiNbO_3$ and $LiTaO_3$, though these crystals are more attractive for low-loss SAW devices, due to high piezoelectric coupling. As a result, in $LiNbO_3$ and $LiTaO_3$ attenuation of HVPSAW is usually higher than 0.5 dB/wavelength.

Recently, it was found that deposition of a thin film on the substrate surface could result in propagation of non-attenuated high velocity surface acoustic wave (HVSAW) [3-5]. The energy of such a wave is localized near the surface and it behaves like a true SAW. Some numerical examples of the HVSAW were reported. One can assume that HVPSAW with negligible attenuation can also exist if a periodic metal grating is deposited on a substrate, instead of uniform metal film. This assumption agrees with recently reported numerical results [6,7]. It was found that in some orientations of $LiNbO_3$ and $LiTaO_3$ with periodic Al grating of sufficiently high thickness, the propagation loss of HVPSAW becomes fairly low, and SAW resonators with high Q-factors can be built.

The present paper reports the results of numerical investigation of HVPSAWs propagating in $LiTaO_3$ with Au grating. Orientations, in which low-attenuated HVPSAW can exist, were predicted based on analysis of exceptional wave criterion. Then attenuation coefficients of HVPSAWs were calculated for two cases, with uniform gold layer, and with periodic gold grating, and compared. In both cases, attenuation tends to zero at certain film (or electrode) thickness and certain orientation. These optimal orientation and thickness are different for uniform film and grating. Analysis of contributions of the bulk partial waves into HVPSAW solution, in the case of uniform Au film, confirmed that HVPSAW degenerates into the pure surface wave at the optimal point. Other important characteristics of the found low-attenuated HVPSAWs were calculated: velocities, electromechanical coupling coefficients, Q-factors of SAW resonators. Harmonic (strip) admittance and velocity dispersion curve are presented for one of the optimal cuts with the grating of optimized thickness.

II. Numerical Results and Discussion

In quartz and LBO the branches of low-attenuated HVPSAWs exist in the vicinity of orientations, in which a quasi-longitudinal bulk wave becomes exceptional. A numerical technique of search for exceptional waves (EW) was described in [2]. An existence criterion of EW derived in [8],

$$D=Det(c_{ijkl}\, n_k\, u_l)=0, \qquad (1)$$

was analytically investigated for trigonal crystals. In equation (1), c_{ijkl} is the elasic stiffness tensor, $\boldsymbol{u}$ is the mechanical polarization vector of a bulk wave propagating in direction defined by unit wave vector $\boldsymbol{n}$. By way of example, all symmetric EW orientations were determined in quartz. In particular, it was found that in orientations, defined by the Euler angles (0°,θ, 90°), there can exist an even number of quasi-longitudinal EW orientations, which give rise to the branches of low-attenuated HVPSAW.

Fig. 1 shows the determinant D calculated for quasi-longitudinal bulk mode, as a function of the Euler angle θ. In quartz, D crosses zero value few

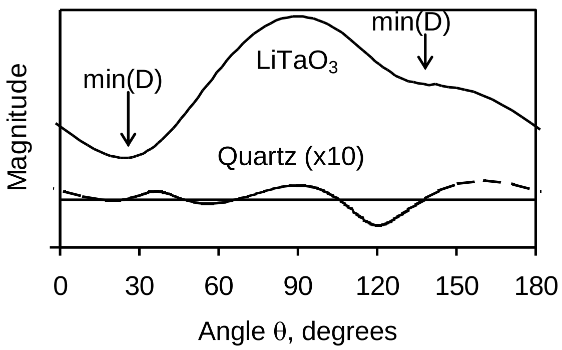

Fig.1.Determinant of mechanical boundary conditions D calculated for the quasi-longitudinal SSBW propagating in orientations of $LiTaO_3$ and quartz with Euler angles (0°,θ, 90°).

times, indicating EW orientations. As a result, even slight perturbation of the boundary conditions (e.g. mass loading produced by uniform film or grating) results in propagation of low-attenuated HVPSAWs.

In $LiTaO_3$, the determinant D is always positive and its absolute value is much larger than in quartz. Therefore, HVPSAWs are strongly attenuated in any orientation. However, D exhibits two local minimums, when θ is about 30° and 130°. These minimums can give rise to low-attenuated HVPSAW branches, provided that the boundary condition is considerably perturbed. Such perturbation can occur, for example, due to heavy or sufficiently thick film.

To verify this assumption, HVPSAWs were investigated in LT orientations with Euler angles (0°,θ, 90°), and uniform Au film. The results of calculations are shown in Fig.2 as contour plots of HVPSAW attenuation (in dB/λ), versus angle θ and normalized Au film thickness h/λ. Attenuation tends to zero when θ=29° and θ=127°, with Au thickness h/λ=4.8% and h/λ=5.0%, respectively.

The same orientations were investigated with short-circuited periodic grating of Au electrodes built on LT substrates. A numerical technique based on matrix formalism [9] was utilized to find Green functions in a piezoelectric substrate, combined with FEM analysis of electrode region [10], to obtain harmonic admittance of infinite periodic grating. Attenuation coefficients were then extracted from the real part of harmonic admittance at resonance

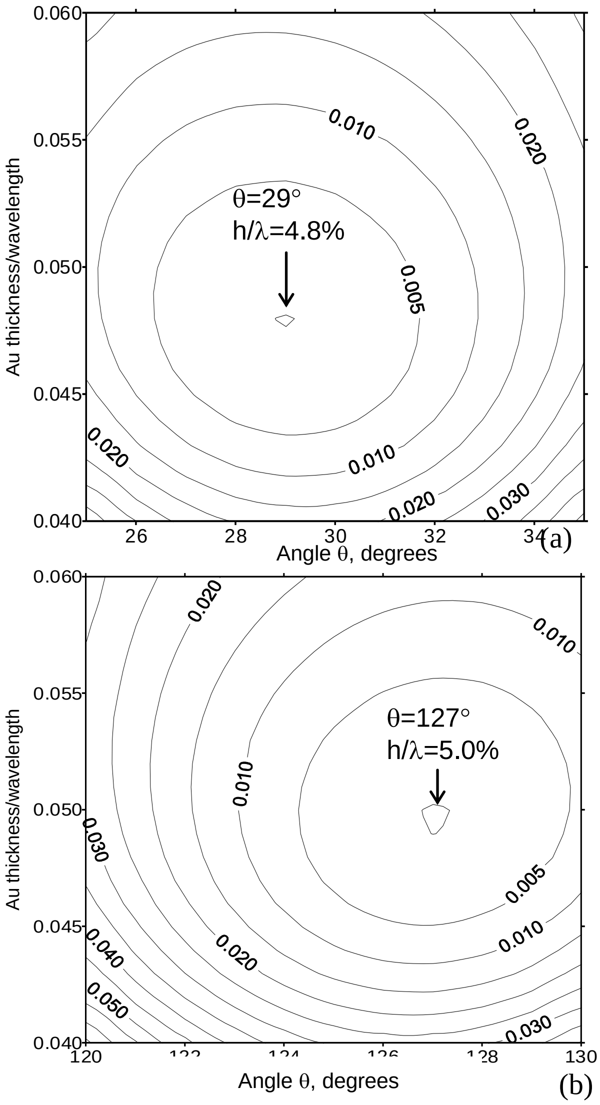

Fig.2. Contour plots of attenuation coefficients (dB/λ) of HVPSAW propagating in $LiTaO_3$, Euler angles (0°,θ, 90°), with ***uniform gold film****, versus Euler angle θ and normalized film thickness: a) θ=25-35°, b) θ=120-130°.*

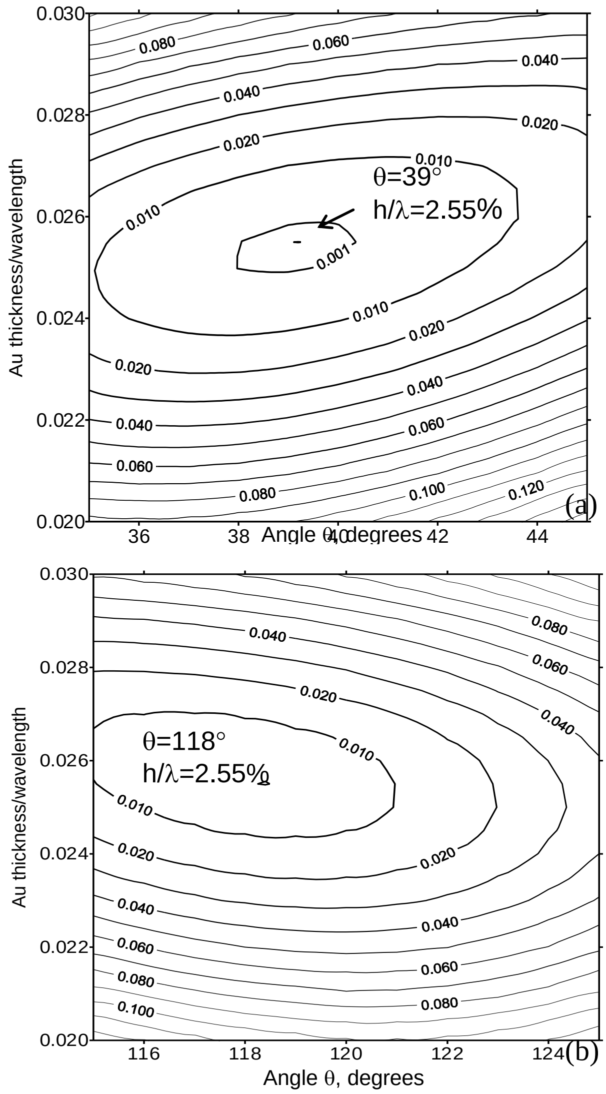

Fig.3. Contour plots of attenuation coefficients (dB/λ) of HVPSAW propagating in $LiTaO_3$, Euler angles (0°,θ, 90°), with ***periodic gold grating****, versus Euler angle θ and normalized film thickness: a) θ=25-35°, b) θ=115-125°.*

frequency. Metallization ratio μ=0.5 was used.

The results are shown in Fig.3, as contour plots of HVPSAW attenuation versus normalized electrode thickness h/λ and the Euler angle θ. The behavior of HVPSAW looks similar with the uniform film and with the grating, but orientations and thicknesses providing minimum HVPSAW attenuation are different. In the grating, the optimal thickness decreases twice and the optimal angle θ shifts approximately by 10°, compared to the uniform film.

It should be mentioned that the typical behavior of HVPSAW attenuation in the two-dimensional space (θ, h/λ) is different from that of low-velocity PSAW. The latter always exhibits the optimal line $\theta(h/\lambda)$, the example of which was previously reported for rotated YX-cuts of LT [11]. It can be explained by stricter requirement of vanishing attenuation in the case of

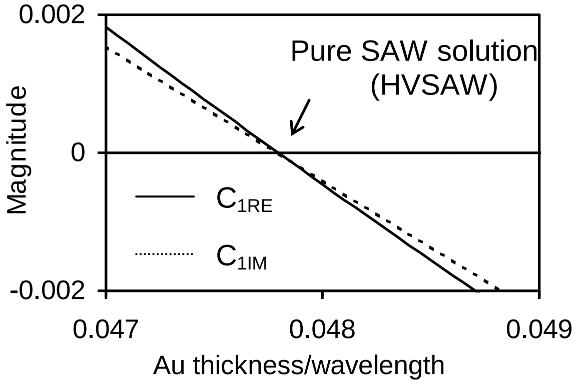

Fig.4. Real and imaginary parts of coefficient C_1 illustrating contribution of quasi-shear bulk partial wave into HVPSAW solution in LT cut (0°,29°,90°) with uniform Au film, versus film thickness.

HVPSAW, compared to that of PSAW. The number of partial bulk waves involved in PSAW solution increases from one to two. Therefore, two complex coefficients must vanish simultaneously, instead of one.

Moreover, pure HVSAW can exist in layered structures when orientations of a substrate and a layer have certain symmetry [5]. For example, in rotated Y-cuts of LT, 90°-propagation, analyzed in the present paper, the sagittal plane is parallel to the plane of crystal symmetry. Therefore, the shear bulk wave polarized normally to this plane is uncoupled. As a result, the HVPSAW includes only one partial bulk wave, which is responsible for HVPSAW attenuation. Fig.4 shows the complex contribution coefficient associated with this wave, in LT cut (0°, 29°, 90°), with uniform Au film, as a function of film thickness. The contribution of a bulk wave vanishes when $h/\lambda \approx 4.78\%$. It means that the pure surface wave occurs on the HVPSAW branch. This wave has a specific structure of a one-partial mode perturbed by piezoelectric effect [3-4].

The electromechanical coupling coefficient k^2 was extracted from harmonic admittance of LT cuts with Au grating. Fig.5 shows this characteristic as contour plots versus angle θ and electrode thickness, in the vicinity of two orientations providing minimum HVPSAW attenuation. The following values have

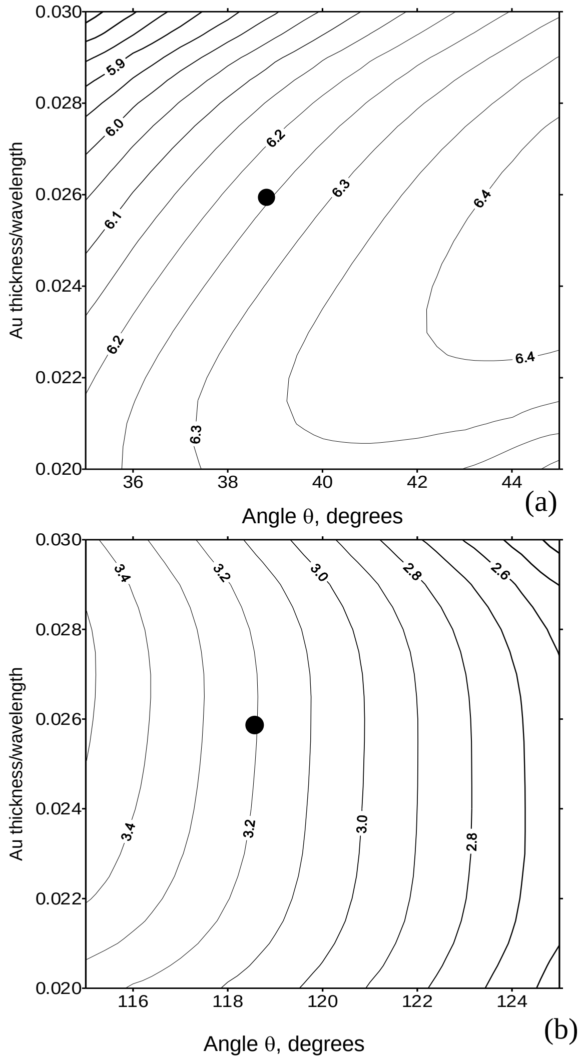

Fig.5. Contour plots of electromechanical coupling coefficient k^2 (%) of HVPSAW propagating in $LiTaO_3$, Euler angles (0°,θ, 90°), with ***periodic gold grating****, versus Euler angle θ and normalized film thickness: a) θ=35-45°, b) θ=115-125°. The sign "•" marks the optimal angle θ and thickness, providing minimum propagation loss,* according to Fig.4.

been obtained for the optimal points indicated on the plots: k^2 =6.27% for θ=39° (Fig.5a) and k^2 =3.21% for θ=118° (Fig.5b), with the optimal electrode thickness $h/\lambda \approx 2.55\%$ in both cases.

Fig. 6 shows variation of HVPSAW velocity and attenuation coefficient, estimated at resonance

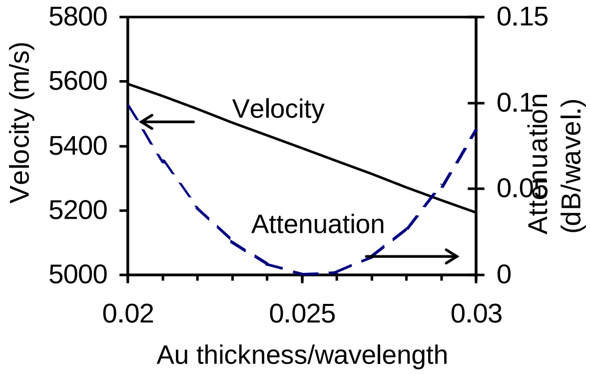

Fig.6. Propagation velocity and attenuation at resonance frequency in LT orientation with Euler angles (0°,39°, 90°), versus normalized thickness of Au grating.

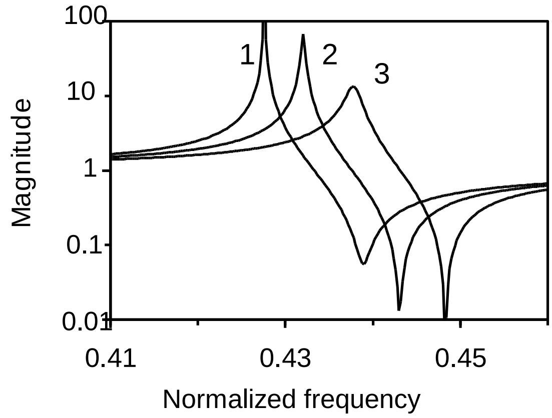

Fig.7. Amplitude of strip admittance Y versus normalized frequency $f'=fp/v_{BAW}$, in three LT orientations (0°, θ, 90°) with optimized thickness of Au grating: 1 - θ=39°, h/λ=2.55%, 2 - *θ=34°, h/λ=2.4%,*
3 - θ=28.5°, h/λ=2.25%,

frequency, versus electrode thickness, in LT orientation (0°,39°,90°). At the point $h/\lambda \approx 2.55\%$, attenuation is less than 0.0001 dB/λ and v=5373 m/s.

The amplitude of strip admittance Y(f) is shown in Fig.7 for this and two additional orientations with optimized Au thickness. For the curve 1, the Q-factor is maximum at resonance ($Q_R \approx 3\cdot10^5$, $Q_A \approx 195$). For the curve 3, there is an opposite relation between Q_R and Q_A .The curve 2 corresponds to orientation and thickness which provide approximately equal Q-factors at resonance and at anti-resonance, $Q_R \approx Q_A \approx 900$.

Fig.8 shows the velocity dispersion curve for HVPSAW in LT orientation (0°, 39°,90°) with h/λ=2.55%. The real and imaginary parts of velocity are shown as functions of normalized frequency $f'=fp/v_{BAW}$, where v_{BAW}=6283 m/s is the velocity of the quasi-longitudinal surface-skimming bulk wave, and p is the period of the grating. The lower edge of the Bragg stopband occurs at f'=0.428. The imaginary part of velocity is nonzero for the analyzed frequencies, thus indicating propagation loss. However, it reaches minimum value at the resonance frequency f_R, which coincides with the lower edge of the Bragg stopband. With further increasing frequency, in the stopband, the propagation loss caused by leaky wave nature increases, which results in strongly asymmetric Im(v). The cut-off frequency of bulk wave radiation

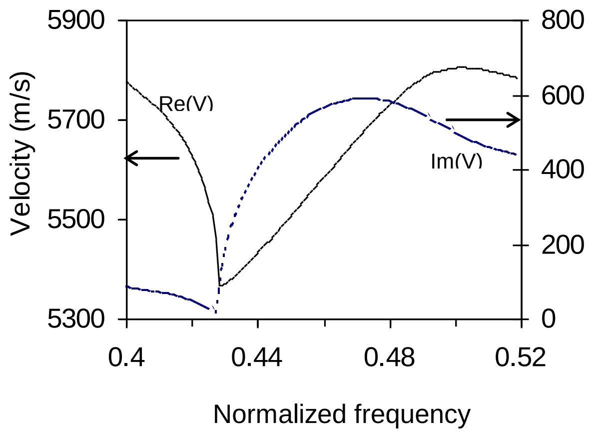

Fig.8. Velocity dispersion of HVPSAW propagating in $LiTaO_3$,, Euler angles (0°,39°,90°), with Au grating h/λ=2.55%, versus normalized frequency.

f'=0.5 occurs within the stopband and makes the upper edge of the stopband uncertain.

The typical features of the behavior of velocity, attenuation, harmonic admittance and velocity dispersion in the grating, shown in Fig.6-8, were also observed for another orientation which supports propagation of low-attenuated HVPSAW, with the Euler angles (0°, 118°, 90°).

III. Conclusions

The numerical investigation of HVPSAWs, which propagate in rotated Y-cuts of LT, 90°-propagation, has shown that, when uniform Au film or periodic grating of Au electrodes is deposited on the surface, attenuation of the wave tends to zero at certain rotation angle and certain film or electrode thickness. These optimal values are different for uniform metal film and infinite periodic grating. Two cuts providing negligible attenuation have been found. In these cuts, the HVPSAW exhibits high propagation velocity and strong piezoelectric coupling. Analysis of harmonic admittance and velocity dispersion of HVPSAW in the grating confirmed that the found orientations could be used in resonator structures, with expected high values of Q-factor.

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