Numerical investigation of surface and leaky acoustic wave properties in SrLaGa₃O₇ crystal

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Abstract. For surface acoustic wave (SAW) devices operating at elevated ambient temperatures, piezoelectric crystals that have stable material properties at high temperatures are desirable. The progress in the field of electronic technologies has increased the demand for high-temperature piezoelectric materials for the use in temperature and pressure sensors. Recently, SAW sensors have been operated at room temperature or 100°C-300°C at most. A new piezoelectric SrLaGa₃O₇ crystal belongs to tetragonal symmetry class, and has stability of its piezoelectric properties up to the melting temperature of 1650°C. Numerical simulation of the properties of surface and leaky acoustic waves in the SrLaGa₃O₇ single crystal is performed. The SAW has a maximum value of the electromechanical coupling coefficient (~0.25%) on Z+64°-cut and propagation direction along the X-axis. In the same propagation direction, the electromechanical coupling coefficient of the leaky wave is 3.5 times lower than that of SAW. The SAW has large electromechanical coupling coefficient value (~0.24%) on Z, X+45° -cut of the crystal. It is shown that these two cuts of the SrLaGa₃O₇ single crystal are promising for use in the SAW devices.

1. Introduction
New piezoelectric materials are grown and studied for various devices based on surface acoustic waves (SAWs) such as sensors and resonators with remote sensing at elevated temperatures and mechanical vibrations in machines [1-3]. Widely used piezoelectric materials, such as crystals of alpha-quartz (α-SiO₂) and lithium niobate (LiNbO₃), cannot be used at temperatures exceeding 600°C. The new piezoelectric crystal SrLaGa₃O₇ belongs to tetragonal crystal symmetry class (point group, 42m), and has stable piezoelectric properties up to its melting temperature ~1650°C [4]. This feature makes it as a suitable material for application in the SAW devices, operating in a high temperature range. Up-to-date, no detailed numerical modeling of SAW properties have been made in the SrLaGa₃O₇ single crystal.

2. Materials and Methods
The objective of the paper is numerically modeling the properties of surface and leaky acoustic waves in a new SrLaGa₃O₇ single crystal. For computation of surface and leaky acoustic wave properties, it is necessary to have full set material constants of SrLaGa₃O₇: 6 elastic constants, 2 piezoelectric constants and 2 dielectric constants [4]. The SAW and leaky wave properties (the phase velocity,
electromechanical coupling coefficient and power flow deflection angle) are calculated using our software [5].

The properties of surface and leaky acoustic waves are defined by solving the basic wave equations for displacements $u_i$ and electric potential $\varphi$ in an piezoelectric anisotropic medium [5,6]:

$$\rho \frac{\partial^2 u_i}{\partial t^2} - C_{ijkl} \frac{\partial^2 u_k}{\partial x_i \partial x_j} - e_{ikl} \frac{\partial^2 \varphi}{\partial x_i \partial x_j} = 0,$$

$$e_{ikl} \frac{\partial^2 u_k}{\partial x_i \partial x_j} - e_{ik} \frac{\partial^2 \varphi}{\partial x_i \partial x_j} = 0, \quad i, j, k, l = 1, 2, 3$$

with suitable boundary conditions on the free and metallized surfaces of the crystal. Here, $C_{ijkl}$, $e_{ikl}$ and $e_{ik}$ are the elastic, piezoelectric and dielectric constants; $\rho$ is the density of crystal. The electromechanical coupling coefficient for surface wave in the piezoelectric crystal is defined as:

$$K^2 / 2 = \Delta \frac{V_f - V_m}{V_f},$$

where $V_f$ and $V_m$ are the velocities for free and metallized surfaces of the crystal, respectively. The surface wave power flow deflection angle (or beam steering angle) $\phi$ is defined as:

$$\tan \phi = \frac{1}{V_f} \frac{\partial V_f}{\partial \theta}.$$

For SAW devices, it is important to search for piezoelectric substrate orientations with large electromechanical coupling coefficient and zero power flow angle of surface wave.

Numerical studies of the SAW properties were carried out on Z- and Y-cuts and on rotating Z-cut in the SrLaGa$_3$O$_7$ crystal. The three Euler angles ($\alpha$, $\mu$, $\theta$) are used for rotations of the system of coordinates. The first two Euler angles ($\alpha$, $\mu$) define the orientation of the crystal plane (the crystal cut). The third Euler angle $\theta$ defines the direction of SAW propagation on this crystal plane. Taking into account the SrLaGa$_3$O$_7$ tetragonal crystal symmetry (point group, $\bar{4}2m$), it is assumed that $\alpha = 0^\circ$, the angles $\theta$ and $\mu$ varies in the range from 0° to 90° with the discrete angular step of 2°.

![Figure 1](image_url)

**Figure 1.** Isolines of SAW a) phase velocity, b) electromechanical coupling coefficient (%), c) beam steering angle (degrees) in the SrLaGa$_3$O$_7$ crystal.

3. Numerical results and discussion

Figure 1 shows the contour maps of SAW properties in the SrLaGa$_3$O$_7$ crystal, defined by the Euler’s angles $\mu = 0^\circ \div 90^\circ$, $\theta = 0^\circ \div 90^\circ$. As can be seen in Figure 1 the SAW has the following extreme values: the velocity is in the range of 2600 m/s to 2950 m/s, the electromechanical coupling coefficient varies is in the range of 0% to 0.25%, the power flow angle is in the range from $-14^\circ$ to $14^\circ$. In Figure 1c, blue lines show beam steering angle isolines with zero value.
Figure 2 shows the SAW characteristics as a function of the wave propagation direction $\theta$ on Y-cut of SrLaGa$_3$O$_7$ crystal. It is seen that surface acoustic wave has the maximum value of the electromechanical coupling coefficient ($\sim 0.28\%$) for the wave propagation direction along the X$+50^\circ$ axis (see Figure 2b). Unfortunately, SAW beam steering angle is large ($\sim 14^\circ$) for this wave propagation direction (see Figure 2b), and for this reason this orientation is not suitable for SAW device applications. For the Z-cut of the SrLaGa$_3$O$_7$ crystal, the SAW has a small beam steering angle ($\sim 3^\circ$) in all directions of wave propagation (see Figure 3b). Figure 3b shows that the SAW has the maximum value of the electromechanical coupling coefficient ($\sim 0.24\%$) for the wave propagation direction along the X$+45^\circ$ axis in the SrLaGa$_3$O$_7$ crystal. For this wave propagation direction, the SAW beam steering angle is equal to zero (see Figure 3b) which is preferable for SAW device applications.

![Figure 2](image1.png) ![Figure 3](image2.png)

**Figure 2.** a) SAW phase velocity, b) SAW electromechanical coupling coefficient and beam steering angle (degrees) as a function of wave propagation direction $\theta$ on the Y-cut of the SrLaGa$_3$O$_7$ crystal.

**Figure 3.** a) SAW phase velocity, b) SAW electromechanical coupling coefficient and beam steering angle (degrees) as a function of wave propagation direction $\theta$ on the Z-cut of the SrLaGa$_3$O$_7$ crystal.
Figure 4. a) SAW phase velocity and b) SAW electromechanical coupling coefficient as a function of cut angle $\mu$ on rotated Z-cut of the SrLaGa$_3$O$_7$ crystal.

Figure 5. Leaky acoustic wave a) phase velocity, b) electromechanical coupling coefficient and attenuation (dB/wavelength) as a function of the cut angle $\mu$ and wave propagation direction along the X-axis in the SrLaGa$_3$O$_7$ crystal.

Figure 6. IDT conductance as a function of frequency for a) the Z-cut and wave propagation direction along the X+45° axis and b) for the Z+64°-cut and wave propagation direction along the X-axis in the single SrLaGa$_3$O$_7$ crystal.
Figures 4 and 5 show the SAW and leaky wave characteristics on the rotated Z-cut and the wave propagation direction along the X-axis of crystal. Figure 4b shows that the SAW electromechanical coupling coefficient reaches the maximum value (~0.25%) at cut angle μ=64° (Z+64°- cut), which is comparable to that for well-known langasite crystal [3]. Leaky wave has small electromechanical coupling coefficient (~0.08%), which is much lower than that for SAW (see Figure 5b).

The interdigital transducer (IDT) conductances are shown in Figure 6 for two above discussed cuts of SrLaGa₃O₇ crystal. Interdigital transducers have 100 electrodes with the wavelength period of 20 microns, the transducer aperture is equal to 1600 microns. The thickness of the aluminum transducer electrodes is equal to 0.4 microns. For the Z-cut and wave propagation direction along the X+45°-axis, there are no leaky and bulk acoustic wave excitation responses from transducer (see Figure 6a). It should be noted that the SAW mechanical reflections between electrodes in the transducer are very small for this crystal cut. That allows one to minimize the influence of wave reflections on the SAW filter characteristics. For the Z+64°-cut and wave propagation direction along X-axis, there is a weak response due to radiation of the leaky wave from the transducer (see Figure 6b). There are no bulk acoustic wave generation by the transducer in the both crystal cuts, and therefore these crystal cuts are more suitable for use in the SAW devices.

4. Conclusion

In summary, the results of numerical simulation of the surface and leaky wave characteristics in the SrLaGa₃O₇ crystal have been presented in the paper. It was shown that the maximum value of SAW electromechanical coupling factor (~0.25%) was on the Z+64°-cut and wave propagation direction along the X-axis. In the same propagation direction, the leaky acoustic wave had 3.5 times lower electromechanical coupling coefficient than that for SAW. For the Z-cut, the SAW electromechanical coupling coefficient reached the maximum value of ~0.24% along X+45°-axis wave propagation direction. It was shown that bulk acoustic waves were not generated by the transducer in the both cuts of the SrLaGa₃O₇ single crystal. Thus, these two cuts of the SrLaGa₃O₇ crystal could be useful in the SAW device applications.

References

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