Numerical analysis of SAW propagation characteristics in Ca$_2$Al$_2$SiO$_7$ crystal

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Abstract. The importance of surface acoustic wave (SAW) technology is to integrate signal processing with sensor functions. Recently, SAW sensors can operate at room temperature or around 100°C-200°C. The task associated with materials becomes relevant if it is necessary to increase the operating temperature of the device to 1000°C. A new piezoelectric calcium aluminate silicate (Ca$_2$Al$_2$SiO$_7$) crystal of the tetragonal symmetry has stable piezoelectric properties up to the melting point temperature of 1500°C. The properties of surface acoustic waves a new Ca$_2$Al$_2$SiO$_7$ single crystal are numerically modeled in the paper. The SAW velocity, the electromechanical coupling coefficient, and the power flow angle are modeled for various cuts of the Ca$_2$Al$_2$SiO$_7$ crystal. The SAW has the maximal electromechanical coupling coefficient value (~0.1%) on Z.X+45° -cut of the crystal. In the Z+63°, X-cut, the SAW electromechanical coupling coefficient is equal to 0.08%. Both of these crystal cuts show the absence of bulk acoustic wave generation by an interdigital transducer, and the Ca$_2$Al$_2$SiO$_7$ crystal is a promising piezoelectric material for use in the SAW device applications.

1. Introduction
For sensors operating in an environment with elevated temperature, piezoelectric crystals are required that have stable material properties at high temperatures. Advances in electronic technology have increased the demand for high-temperature piezoelectric materials for use in temperature and pressure sensors. Recently, the following widely-used piezoelectric crystals were used as sensor materials: GaPO$_4$, La$_3$Ga$_5$SiO$_14$ (langasite, LGS) and rare-earth calcium oxoborate ReCa$_4$O(BO$_3$)$_3$ (RCOB) (Re- rare-earth elements) [1-7].

The new piezoelectric Ca$_2$Al$_2$SiO$_7$ crystal belongs to tetragonal symmetry (point group $42m$) crystal class and has stable its piezoelectric properties up to the melting point temperature of 1500°C [8]. The high-temperature piezoelectric stability makes the Ca$_2$Al$_2$SiO$_7$ crystal as a good candidate for use in the SAW sensors operating in a wide temperature range. The full set of material constants of this crystal is represented by 10 material coefficients: 6 elastic constants, 2 piezoelectric and 2 dielectric constants [9]. To date, no extensive numerical calculations of SAW properties have been made in this crystal.

2. Materials and Methods
The aim of the paper is a numerical investigation of the SAW properties in new Ca$_2$Al$_2$SiO$_7$ single crystal. In our numerical modeling, the full set of Ca$_2$Al$_2$SiO$_7$ elastic, piezoelectric and dielectric
constants were used [9]. Our software were used for numerical modeling of the SAW phase velocity, the electromechanical coupling factor and power flow deflection angle [10].

The propagation properties of a surface acoustic wave in an anisotropic piezoelectric crystal are determined by the following system of wave equations [10, 11]:

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial T_{ij}}{\partial x_j}, \quad i, j = 1, 2, 3;$$

and constitutive material relations:

$$T_{ij} = C_{ijkl} \frac{\partial u_k}{\partial x_l} + e_{klj} \frac{\partial \varphi}{\partial x_k};$$

$$D_i = e_{ijkl} \frac{\partial u_k}{\partial x_l} - e_{ik} \frac{\partial \varphi}{\partial x_k};$$

with taking into account the appropriate boundary conditions on the free or metallized surfaces of crystal. Here, $C_{ijkl}, e_{klj}$ and $e_{ik}$ are the elastic, piezoelectric and dielectric material constants; $D_i$ and $u_i$ are the electric and mechanical displacements; $\varphi$ and $T_{ij}$ are the electric potential and mechanical stress tensor; $\rho$ is the crystal density.

The value $(V_f - V_m)/V_f$ (or $\Delta V/V$) is a very important parameter, which is well known as the SAW electromechanical coupling coefficient (or factor) in piezoelectric crystals, where $V_f$ and $V_m$ are the phase velocities on the free and electrically shorted (metallized) crystal surfaces by thin metal film. It defines the value of surface acoustic wave energy generation by interdigital transducers. Another important SAW parameter is the power flow deflection angle or beam steering angle. The power flow deflection angle (or beam steering angle) is the angle between the power flow vector and the direction of wave vector. It is determined by the formula [11]:

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

here, $\phi$ is the power flow deflection angle, $\theta$ is the SAW propagation direction on the free crystal surface. To design the surface acoustic wave devices, it is desirable to find the crystal orientations (the cut and the wave propagation direction) with large SAW electromechanical coupling coefficient and zero power flow deflection angle. In our numerical modeling, the orientation of the crystal plane (crystal cut) is determined by two Euler angles ($\alpha$, $\mu$), and the third angle $\theta$ is the wave propagation direction on this crystal plane. For the given crystal symmetry ($\bar{4}2m$), it is assumed that $\alpha = 0^\circ$, but the angles $\mu$ and $\theta$ vary from $0^\circ$ to $90^\circ$ with a discrete step of $2^\circ$.

Figure 1. Contour maps of surface wave properties as a function of two Euler angles $\mu$ and $\theta$: a) phase velocity (m/s), b) electromechanical coupling coefficient (%) and c) beam steering angle (degrees) in the Ca$_2$Al$_2$SiO$_7$ crystal, respectively.
3. Numerical results and discussion

Figure 1 shows the contour maps of the SAW properties for different Ca\textsubscript{2}Al\textsubscript{2}SiO\textsubscript{7} crystal cuts defined by two Euler angles: \( \mu = 0^\circ \div 90^\circ \) and \( \theta = 0^\circ \div 90^\circ \). It can be seen that the SAW parameters are in the following ranges:

1. The phase velocity is in the range from 3450 m/s to 4150 m/s.
2. The electromechanical coupling factor is in the range from 0 to 0.14%.
3. The beam steering angle ranges from -28\(^\circ\) to 28\(^\circ\).

The blue isolines indicate the beam steering angle lines with zero value. Unfortunately, they are in the region defined by two Euler angles \( \mu \) and \( \theta \), where the value of the SAW electromechanical coupling coefficient is small (<0.1%). This can be seen by comparing the contour maps in Fig. 1b, c.

The SAW properties as a function of wave propagation direction \( \theta \) in the Y-cut of the Ca\textsubscript{2}Al\textsubscript{2}SiO\textsubscript{7} crystal are shown in Figure 2. The SAW has the maximum value of electromechanical coupling coefficient (~0.14%) for the wave propagation direction along the X+51\(^\circ\)-axis (see Figure 2b). For this orientation, the SAW beam steering angle is large (~13\(^\circ\)) (see Figure 2b). Therefore, this crystal cut is not suitable for the SAW device applications. Fortunately, the SAW has zero power flow deflection angle in Z-cut of the crystal (see Figure 3). The second advantage of this cut is a large SAW electromechanical coupling coefficient (~0.1%) for the wave propagation direction along the X+45\(^\circ\)-axis in the Ca\textsubscript{2}Al\textsubscript{2}SiO\textsubscript{7} crystal. All of these features make this crystal cut suitable for SAW device applications.

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 Ca\textsubscript{2}Al\textsubscript{2}SiO\textsubscript{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 Ca$_2$Al$_2$SiO$_7$ crystal.

Figure 4. a) SAW phase velocity and b) SAW electromechanical coupling coefficient as a function of cut angle $\mu$ on rotated Z-cut in the Ca$_2$Al$_2$SiO$_7$ crystal.

Figure 5. Effective permittivity on a) Z, X+45°-cut and b) Z+63°, X-cut as a function of slowness in the Ca$_2$Al$_2$SiO$_7$ crystal.
Figure 6. Transducer conductance as a function of frequency for a) Z, X+45°-cut and b) Z+63°, X-cut in the Ca$_2$Al$_2$SiO$_7$ crystal.

Figure 4 shows the SAW properties on the rotated Z-cut and wave propagation direction along the X-axis of the crystal. It should be noted that SAW beam steering angle is zero for wave propagation direction along the X-axis for rotated Z-cut of the crystal. One can see that the Z+63°-cut of the crystal (α=0°, μ = 63°, θ=0°) is potential interest for SAW device applications. In this crystal orientation, the SAW has the maximum value of electromechanical coupling coefficient (0.08%) which is close to that for a well-known langasite crystal [1].

Figure 5 shows the effective permittivities for Z, X+45°-cut and Z+63°, X-cut in Ca$_2$Al$_2$SiO$_7$ crystal. There are no bulk acoustic wave excitations in the both crystal cuts. The interdigital transducer (IDT) conductances as a function of frequency on both Ca$_2$Al$_2$SiO$_7$ crystal cuts are shown in Figure 6. The transducer has a periodic grating with a number of electrodes of 100 and a wavelength of 20 microns. The aperture of the transducer is 1600 microns, and the thickness of the aluminum electrode is 0.4 microns. The simulations of transducer conductances as a function of frequency show that there are no bulk acoustic wave responses generated by the IDT on the both crystal cuts. Finally, the numerical simulation of the SAW properties in the Ca$_2$Al$_2$SiO$_7$ crystal shows that only two Ca$_2$Al$_2$SiO$_7$ crystal cuts are more suitable for SAW device applications.

4. Conclusion
The properties of surface acoustic waves have been numerically simulated in a new piezoelectric Ca$_2$Al$_2$SiO$_7$ crystal. The SAW phase velocity, electromechanical coupling coefficient and beam steering angle have been calculated for various Ca$_2$Al$_2$SiO$_7$ crystal cuts. It was shown that the SAW has the maximum value of electromechanical coupling coefficient value (~0.1%) in the Z, X+45°-cut of crystal. For the Z+63°, X-cut of the crystal, the SAW electromechanical coupling coefficient was equal to 0.08%. It was shown that these both crystal cuts could be useful for SAW device applications.

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