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Theoretical calculation of the surface acoustic wave characteristics of GdCOB single crystals

Takashi Nishida *, Hiroyuki Shimizu, Tadashi Shiosaki

Graduate School of Materials Science, Nara Institute of Science and Technology, 8916-5 Takayama-cho, Ikoma, Nara 630-0101, Japan

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Abstract

Fabrication and crystalline characteristics for various piezoelectic materials have been studied. In particular, quartz, $LiNbO_3$, $LiTaO_3$ and LiB_4O_7 crystals have been investigated, and their piezoelectric properties for applications such as surface acoustic wave (SAW) devices have been evaluated in detail; however, there has been interest in new materials with improved properties. Recently, new rare earth crystalline materials, such as $ReCa_4O(BO_3)_3$ (Re: Y, Gd, La and others) have been grown, and excellent nonlinear optical properties have been reported. It is expected that these materials may also have good piezoelectric properties; however, few studies of the piezoelectricity of these materials have been performed. Of particular interest is that a large electric-mechanical coupling coefficient may be obtained in $GdCa_4(BO_3)_3$ (GdCOB).

In this study, a theoretical analysis of the SAW characteristics, and investigation of the piezoelectric properties is reported in detail. The analysis was performed using material constants obtained from resonance–anti-resonance method by Wang et al. [J. Wang, X. Hu, X. Yin, R. Song, J. Wei, Z. Shao, Y. Liu, M. Jiang, J. Mater. Res. 16 (2001) 790–796]; SAW velocities and coupling constants were calculated at several crystalline cuts and propagation directions. In particular, the result calculated at the *Z*-cut of GdCOB was substantially in accordance with the measured results. Two SAW propagation modes (lower and higher) existed on the cut. From comparison between measured and calculated results, the lower and higher modes were identified as the Rayleigh mode and the leaky mode, respectively. From the theoretical analysis of Rayleigh SAW for all crystalline cuts and propagation directions, the maximum velocity and coupling coefficients were obtained for GdCOB *Y*-cuts, revealing that the *Y*-cut will be suitable for SAW device applications.

Keywords: GdCOB; ReCOB; YCOB; SAW; Piezoelectric

1. Introduction

Various piezoelectric crystals such as $LiNbO_3$, $LiTaO_3$ and LiB_4O_7 have been grown and their piezoelectric properties investigated, because of the interest in the SAW application for filter and resonator devices.

In recent years, new rare earth materials $RCa_4O(BO_3)_3$ (R = La, Nd, Sm, Gd, Er and Y) have been studied, and the crystal growth conditions have been investigated [1–7]. There is interest in using these materials for nonlinear optical devices, because the crystals exhibit not only excellent nonlinear properties but also non-hygroscopic and chemically stable with good mechanical properties. In particular, $GdCa_4O(BO_3)_3$ (GdCOB) exhibits excellent optical second harmonic generation (SHG) characteristics, and single crystals can be grown with the Czochralski (CZ) technique at a low cost.

However, few studies on the piezoelectricity and SAW properties of these materials have been reported. Therefore, in this study, inter-digital transducers are fabricated on *X*, *Y* and *Z* cuts of GdCOB crystals, and SAW characteristics such as velocity, coupling constants and temperature coefficients are evaluated. It is expected that SAW properties comparable to those of $LiTaO_3$ can be obtained with GdCOB [8].

In this paper, the simulations are performed with various crystalline cuts and propagation directions, and the optimum

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* Corresponding author.
E-mail address: tnishida@ms.aist-nara.ac.jp (T. Nishida).

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Table 1
The material constant used for SAW simulation [9]

Elastic constants s (10^{-12} m^2/N)

s_{11}	s_{12}	s_{13}	s_{15}	s_{22}	s_{23}	s_{25}	s_{33}	s_{35}	s_{44}	s_{46}	s_{55}	s_{66}
7.7	0.44	0.13	0.04	7.3	−1.9	1.6	8.9	−1.1	13.6	10	18.1	15

Piezoelectric constants d (10^{-12} C/N)

d_{11}	d_{12}	d_{13}	d_{15}	d_{24}	d_{26}	d_{31}	d_{32}	d_{33}	d_{35}
−2.4	−3.8	4.3	2.4	2.9	3.5	−2.6	−4.5	2.6	5.7

Dielectric constants ε				Density ρ (g/cm^3)
ε_{11}	ε_{13}	ε_{22}	ε_{33}	
11.1	0.97	1.5	12.1	3.74

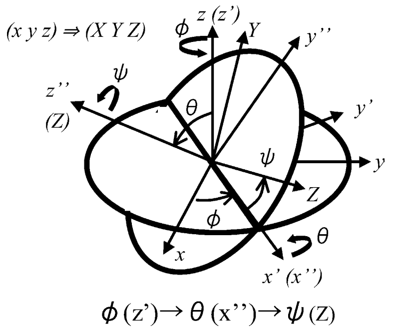
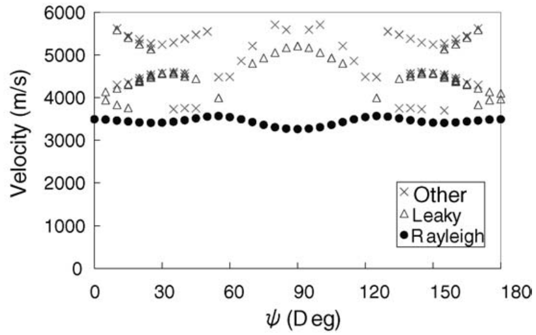
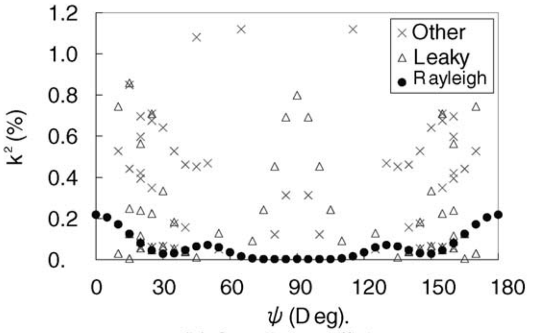


Fig. 1. Euler angle (right hand system) used for simulation.

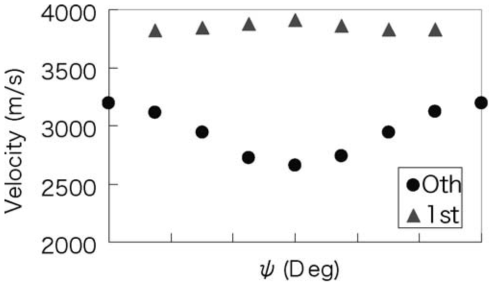


(a) Velocity

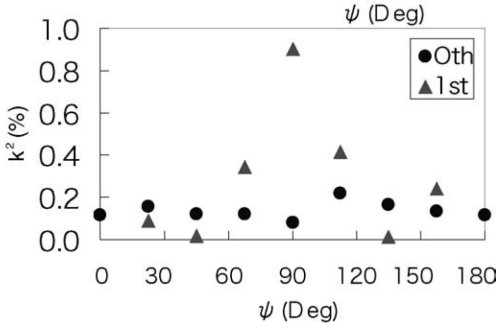


(b) Coupling coefficient

Fig. 2. The relationships SAW properties calculated on GdCOB *Z* cut and propagation direction (ψ). (a) Velocity and (b) coupling coefficient.



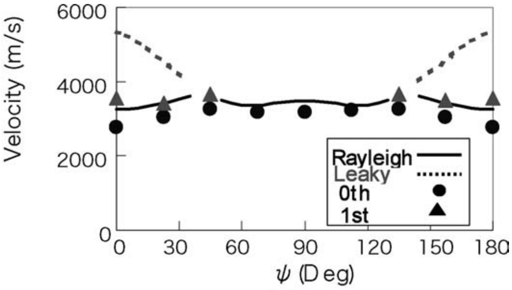
(a) Velocity



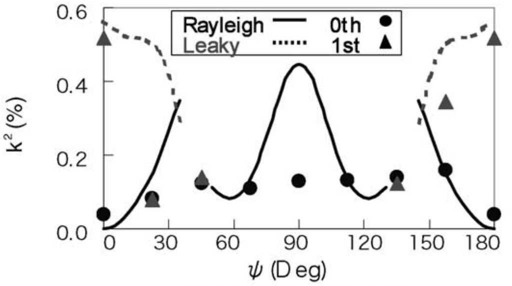
(b) Coupling coefficient

Fig. 3. The relationships SAW properties measured on GdCOB *Z* cut and propagation direction (ψ) [7], (a) Velocity and (b) coupling coefficient.

cut for GdCOB is revealed. The calculated results are compared with measured values [8], and the SAW propagation properties of the GdCOB crystal are discussed in detail.

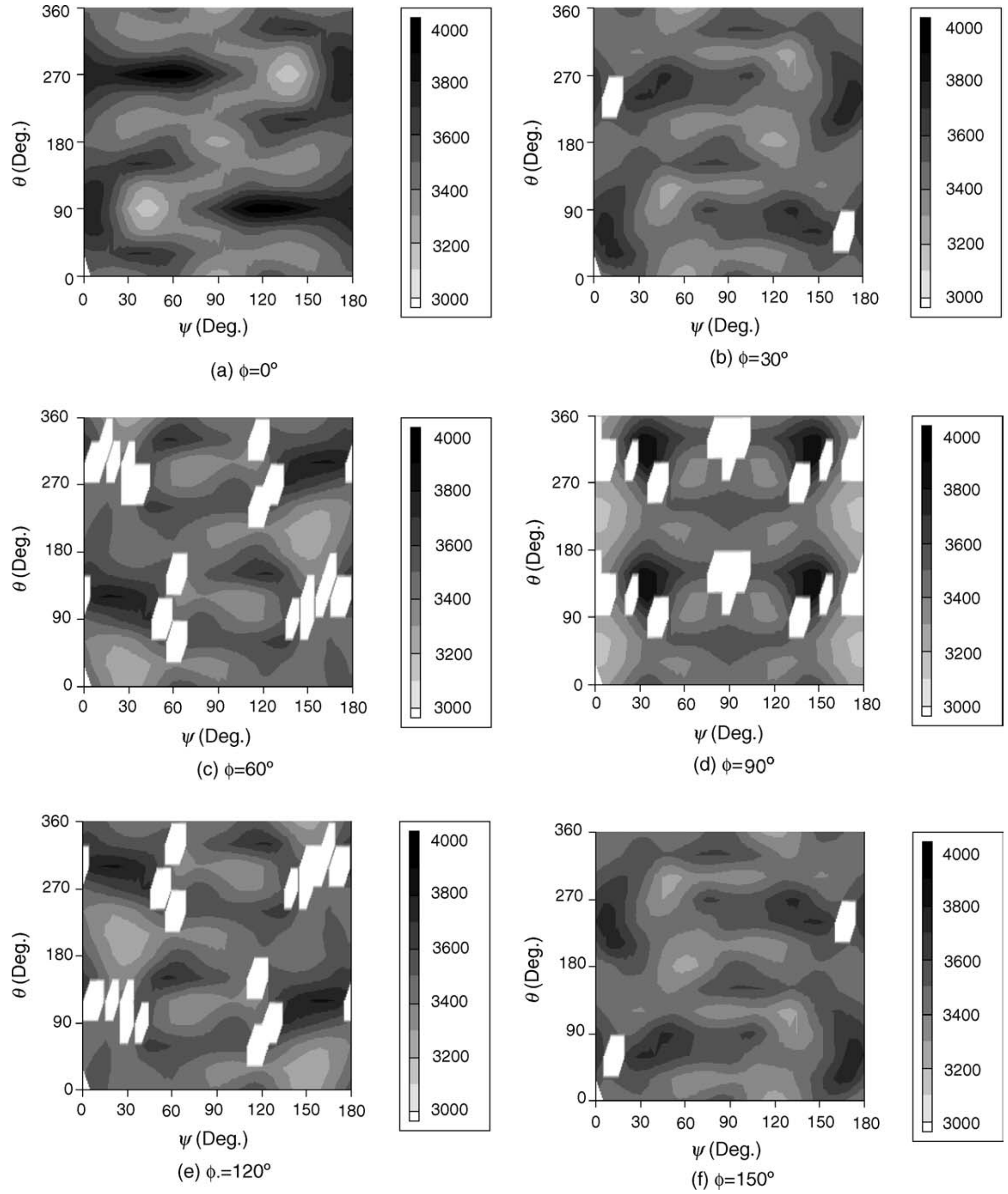


(a) Velocity



(b) Coupling coefficient

Fig. 4. The relationships SAW properties of GdCOB *X* cut and propagation direction (ψ). (a) Velocity and (b) coupling coefficient.



(a) ϕ=0°

(b) ϕ=30°

(c) ϕ=60°

(d) ϕ=90°

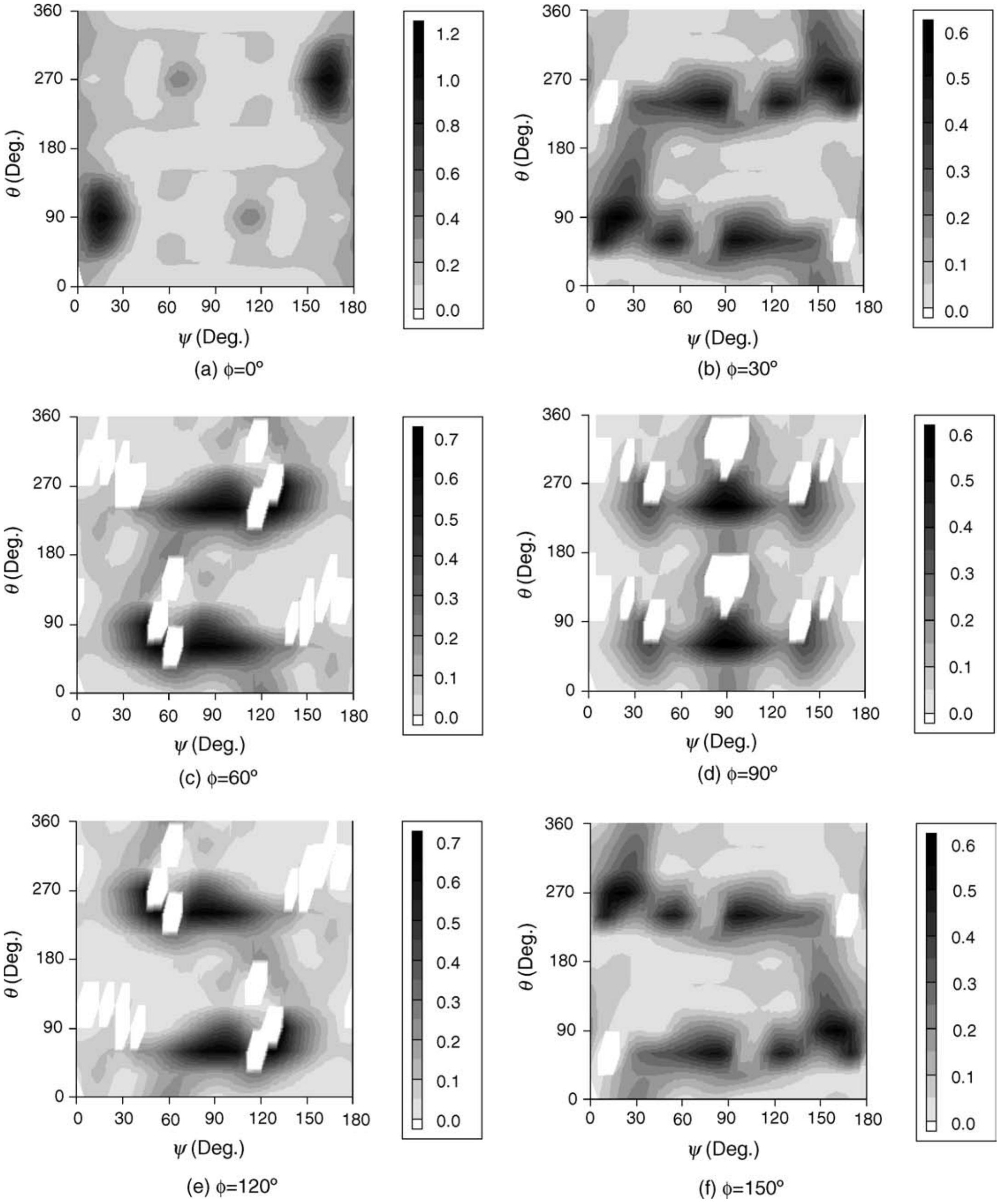
(e) ϕ.=120°

(f) ϕ=150°

Fig. 5. The SAW velocity calculated on all crystalline cuts. (a) $\phi = 0^\circ$, (b) $\phi = 30^\circ$, (c) $\phi = 60^\circ$, (d) $\phi = 90^\circ$, (e) $\phi = 120^\circ$ and (f) $\phi = 150^\circ$.

2. Calculation

A simulation of the propagation of a surface acoustic wave (SAW) was performed using the methods of Campbell [9]. The propagation velocity (v) and coupling coefficient (k^2) of the SAW can be obtained by simulation. In order to perform the calculation, material constants such as elastic and piezoelectric constants are required. The constants measured by Wang et al. [1] were used for the present simulation, and are given in Table 1. The material constants are comprised of 13 elastic constants, 10 piezoelectric constants and four dielectric constants, as the crystalline symmetry of the ReCOB crystal is monoclinic (m). The simulation methods are improved, because of the availability of various propagation modes, such as the Rayleigh mode, leaky mode and others [10]. The simulation was performed for various crystalline cuts. The cuts and propagation directions are indicated by the Euler angles (ϕ, θ, ψ), as shown in Fig. 1.



(a) ϕ=0°

(b) ϕ=30°

(c) ϕ=60°

(d) ϕ=90°

(e) ϕ=120°

(f) ϕ=150°

Fig. 6. The coupling coefficients (k^2) calculated on all crystalline cuts. (a) $\phi = 0°$, (b) $\phi = 30°$, (c) $\phi = 60°$, (d) $\phi = 90°$, (e) $\phi = 120°$ and (f) $\phi = 150°$.

3. Results and discussion

At first, the SAW velocity and coupling coefficient (k^2) of the GdCOB *Z* cut were calculated, and many propagation modes could be obtained. The bulk mode and the low coupling mode ($k^2 \sim 0$) were removed from the calculated results, and a valid mode was obtainable. The dependence of the obtained SAW properties (v, k^2) on the propagation direction (ψ) is shown in Fig. 2. The results were compared with the measured value of the *X* and *Z* cuts given in our previous report [8]. The measured SAW properties of the *Z* cut are shown in Fig. 3. The two propagation modes, lower mode (0th) and higher mode (1st), were evident. In the case of the lower mode, the highest velocities of 3200 and 3488 m/s were obtained at $\psi = 0°$ (*X*-axis propagation) from the measured and theoretical results, respectively, as shown in Figs. 2(a) and 3(a). Both results also revealed that the higher mode could not propagate in this direction. In the case of the higher mode, the highest velocities and coupling (measured: 0.9%, calculated: 0.8%) were obtained at the *Y*-axis ($\psi = 90°$). From comparison between Figs. 2 and 3, it is revealed that the 0th mode is a Rayleigh mode, and the 1st mode is a leaky mode. The SAW properties of the GdCOB *X* cut are also shown in Fig. 4. The angular dependence of the calculated results also agreed with that of the measured results. However, the calculated velocities were higher than the measured values, and this could be the case because the material constants used may contain errors. Therefore, precise measurement of the material constants is a future subject for investigation due to the SAW device application of the GdCOB material.

In order to evaluate all cut and propagation directions, the calculations were also performed at a ϕ range between 0 and 180°, and at a θ range between 0 and 360°, and at ψ ranging between 0 and 180°. The velocities and coupling coefficients obtained are summarized with contour maps shown in Figs. 5 and 6, respectively. The white areas in the contour maps indicate that a solution is not converged in the simulation due to the overlap of several solutions. The plane of symmetry is the *Y*-plane in the monoclinic *m* crystal symmetry, so that a pattern of symmetry appeared on the maps, and a bilateral symmetry is obtained at $\phi = 90°$ as shown in Fig. 5(d). The crystalline cuts that obtained optimum properties can also be found from the contour maps. From these results, it was found that the maximum velocity ∼4000 m/s, and coupling ∼1.1% may be obtained on the *Y* cut ($\phi = 0°$, $\theta = 90°$), revealing that the *Y* cut will be suitable for SAW devices using the Rayleigh mode.

4. Conclusion

In this study, the piezoelectric SAW properties of GdCOB were evaluated using a simulation method. The propagation angular dependences of the simulated results were in agreement with the measured results. Two propagation modes existed on GdCOB crystalline cuts, and are identified as Rayleigh wave and leaky wave modes. In order to determine the optimum crystalline cuts, the calculation was performed on all cut directions, revealing that the maximum velocity ∼4000 m/s and coupling ∼1.1% will be obtained on the *Y* cut.

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