# V(z) Evaluation of Crystallographic Orientations Effects on Elastic Properties of Sodium Cobalt Germanate Single Crystals

**Dr. Ibrahim Hamid Qassem AL-Suraihy**

Department of Physics, Faculty of Education, AL-Mahweet, Sana'a University, Al-Mahweet, Yemen.

**Abstract.** Herein we report on the effect of anisotropy on the elastic acoustic parameters (reflection coefficients R(θ), critical angles of wave excitation, acoustic signatures V(z), spatial periods, velocities) of sodium cobalt germanate $Na_2CoGeO_4$ single crystals with six crystallographic orientations [100], [001], [010], [110], [101], and [011]. Simulations were carried out in the case of a scanning acoustic microscope at an operating frequency of 142MHz, a half opening angle of 50° and water couplant. Interesting results were found. Shear modes were first excited at $\theta_S$ ~ 26.8° on [100] direction. However, at other propagation directions [001], [010], [110], [101], and [011] the shear mode appears at higher angles: $\theta_S$ ~27.1°, 31°, 33.9°, 40.5°, 43° respectively. Propagation of acoustic waves showed a decrease of longitudinal waves velocities from 5687 m/s for [101] direction to 4471 m/s for [011] direction. Similar behaviors were obtained with R(θ) and V(z) curves. These variations are due to either low or high atomic occupation of different orientations.

## 1. Introduction

Materials elastic properties are of great importance in industrial applications as well in basic research. In industry, elastic data are very much useful to determine the strength of the materials under various strained conditions while in basic research, the data are useful in obtaining an insight into the structure of the inter-atomic and inter-ionic forces in solids especially of the long-range type forces. These data can be obtained via static or dynamic methods; the latter case based on acoustic wave propagation is non destructive. However, elastic wave propagations strongly depend on the nature of propagating media, in particular in solids that could be homogeneous or inhomogeneous, isotropic or anisotropic [1-4].

Therefore, it is our aim to investigate anisotropy effects on several acoustic parameters: reflection coefficients R(θ), critical angles of wave excitation, acoustic signatures V(z), spatial periods Δz, velocities of propagating modes). This investigation is carried out, in the case of a scanning acoustic microscope, on sodium cobalt germanate $Na_2CoGeO_4$ single crystals that are playing very important roles in many modern applications.

## 2. Materials and computing procedure

### 2.1.Materials

Sodium-cobalt germanate single crystals, $Na_2CoGeO_4$, possess orthorhombic structure. These crystals are isomorphous to $Na_2ZnGe0_4$, whose monoclinic unit cell is strongly pseudo-orthorhombic; its lattice parameters are a = 7.175, b=5.605 and c =5.325 and the angles α, β and γ are equal to 90°. The characteristic equation of orthorhombic structure, as in case of sodium cobalt germanate $Na_2CoGeO_4$, is of the same form as for the hexagonal classes, but with more general stiffness coefficients [5, 6]. The idealized form [7] of sodium cobalt germanate $Na_2CoGeO_4$ single crystals and crystallographic orientations are schematically illustrated in Fig. 1. The single crystals considered in this work were prepared by direct synthesis of $Na_2CoGeO_4$ from the oxides as well as recrystallization of $Na_2CoGeO_4$ and seeded growth [8]. The spontaneous crystallization technique does not permit the stable production of large crystals with a high degree of perfection. It may be reasonable of seed growth or by the modified spontaneous crystallization method with the aim to suppress the nucleation and thus to produce somewhat larger single crystals. It was in these directions that work was carried out in search of the technique of growing single crystals [8].

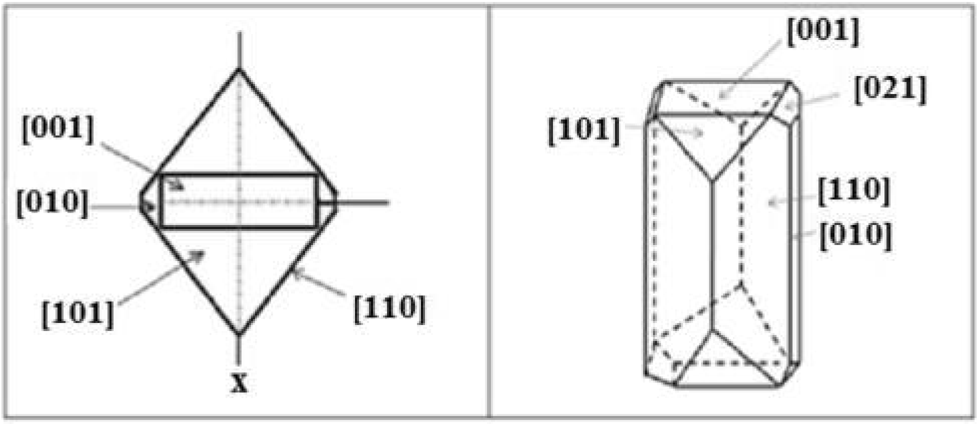


**Figure 1.** Schematic representation of crystallographic orientations of $Na_2CoGeO_4$ single crystals

By applying the pulse ultrasonic method in the frequency of 14 MHz and the synchronous ring method, it was reported [8, 9] that the velocities of longitudinal ($V_L$) and transverse ($V_S$) elastic waves can be experimentally measured (Table 1) along definite crystallographic directions: [100], [001], [010], [110], [101], and [011]. These published data are to be used in the present simulations to investigate all other acoustic parameters.

**Table 1.** Experimental data [8] of longitudinal and shear Velocities in sodium cobalt germanate $Na_2CoGeO_4$ directions.

| crystallographic orientations | $V_L$(m/s) | $V_S$(m/s) |
|---|---|---|
| **[100]** | 5540 | 3250 |
| **[001]** | 5260 | 3230 |
| **[010]** | 4480 | 2810 |
| **[110]** | 5790 | 2610 |
| **[101]** | 5430 | 2240 |
| **[011]** | 5690 | 2130 |

## 3. Calculating procedure

The calculation procedure, described in detail elsewhere [10-14], consists of several steps:

i. calculating the reflection coefficient, R(θ) from [14]:

$$R(\theta) = \frac{\left(Z_L \cos^2 2\vartheta_T + Z_T \sin^2 2\vartheta_T - \rho_{Liq} V_{Liq} / \cos\vartheta\right)}{\left(Z_L \cos^2 2\vartheta_T + Z_T \sin^2 2\vartheta_T + \rho_{Liq} V_{Liq} / \cos\vartheta\right)} \qquad (1)$$

where $Z_L$, $Z_S$, $\rho_{Liq}$ and $V_{Liq}$ are liquid impedance, solid impedance, coupling liquid density and the propagating wave velocity in the liquid, respectively.

ii. computing the V(z) curves of the whole specimen-lens system from the angular spectrum model [13] given by the expression:

$$V(z) = \int P^2\, R(\vartheta) e^{(2jk_\circ)} \sin\vartheta \cos\vartheta \, d\vartheta \qquad (2)$$

where $P^2(\theta)$ is the pupil function, θ is the half-opening angle of the lens, z is the defocusing distance and $k_0 = 2\pi/\lambda$ is the wave number in the coupling liquid, $j = \sqrt{-1}$.

iii. deducing V(z) of the sample by subtracting the response of the lens V1(z) from V(z),

iv. applying fast Fourier transform, FFT, a spectral technique to the obtained signal $V(z)-V_1(z)$, in order to determine spatial periods Δz,

v. deducing the phase velocity of the corresponding mode from the following relation [12]:

$$V_R = \frac{V_{Liq}}{\sqrt{\left[1 - \left(\frac{V_{Liq}}{2f\,\Delta z}\right)^2\right]}} \qquad (3)$$

where f is the operating frequency.

# 4. Simulation conditions

Theoretical simulations were carried out in the case of a scanning acoustic microscope in the reflection mode under normal operating conditions: an operating frequency of 142 MHz, a half opening angle of 50° and water as the coupling liquid whose density, $\rho = 1000$ kg/m$^3$ and longitudinal velocity $V_L$ = 1500 m/s.

# 5. Results and discussions

## 5.1. crystallographic orientations effects on R(θ)

Reflection coefficients of sodium germanate $Na_2CoGeO_4$ along definite crystallographic directions: [100], [001], [010], [110], [101], and [011] were calculated. Figure 2 illustrates typical results of the amplitude (Fig. 2a) and the phase (Fig. 2b) as a function of incidence angle. It is clear that, as the angle of incidence increases we notice important changes in both amplitude and phase.

In amplitude, the change occurs at the critical angle, $\theta_S$, at which the shear mode is excited for every crystallographic direction. Beyond these critical angles all the energy is reflected. The modulus of R(θ) becomes equal to unity as a result of total reflection and a null transmission. It can readily be deduced that shear modes are excited at $\theta_S \sim 26.8°$, 27.1°, 31°, 33.9°, 40.5° and 43° for [100], [001], [010], [110], [101], and [011], respectively.

In phase, the most important fluctuation, with $\Delta\varphi = 2\pi$, occurs at the critical angle, $\theta_R$, at which Rayleigh modes are excited. Thus, one can easily determine that $\theta_R \sim 30.5°$, 31°, 36.2°, 38.2°, 45.4° and 48.2° for wave propagation in the directions [100], [001], [010], [110], [101], and [011], respectively. It should be noted that the onset of the 2 phase change corresponds to the shear critical angle $\theta_S$, (as indicated by the arrow in Fig. 2b). The slight shift between $\theta_S$ and $\theta_R$ is due to the fact that the Rayleigh velocity varies slightly from 87 to 95 per cent of the shear velocity [14]. The degree of fluctuations in phase and amplitude in R(θ) in the different crystallographic directions of each critical angle are indicative of the generation efficiency of different modes.

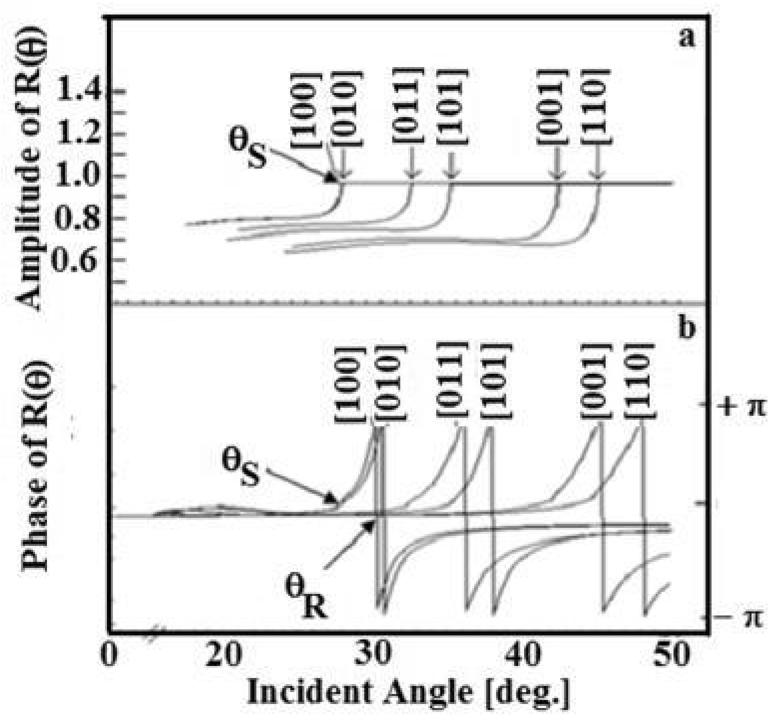


**Figure 2.** Amplitude (a) and phase (b) of refection coefficient of $Na_2CoGeO_4$ at different crystallographic directions.

## 5.2.crystallographic orientations effects on V(z) curves

Acoustic materials signatures, V(z), are the most important parameter that can be experimentally measured by a scanning acoustic microscope. These signatures represent the output signal, V, as a function of the defocusing distance, z, when the sample is moved vertically in the z axis towards the acoustic lens. The V(z) curves can also be calculated from equation 2 and previously determined reflection coefficients (Fig. 2). Typical obtained curves are illustrated in Fig. 3a for $Na_2CoGeO_4$ at six crystallographic directions [110], [001], [101], [011], [010] and [100].

It can clearly be seen that all the curves show oscillatory behavior due to constructive and destructive interference between different propagating modes in different direction. The difference between two successive minima (or maxima) is known as the spatial period, Δz, related to the velocity the of propagating mode by equation 3. Thus, it is obvious (Fig. 3a) that the spatial period Δz decreases gradually from direction [100] to [110]. The deduced values are assembled in Table 2.

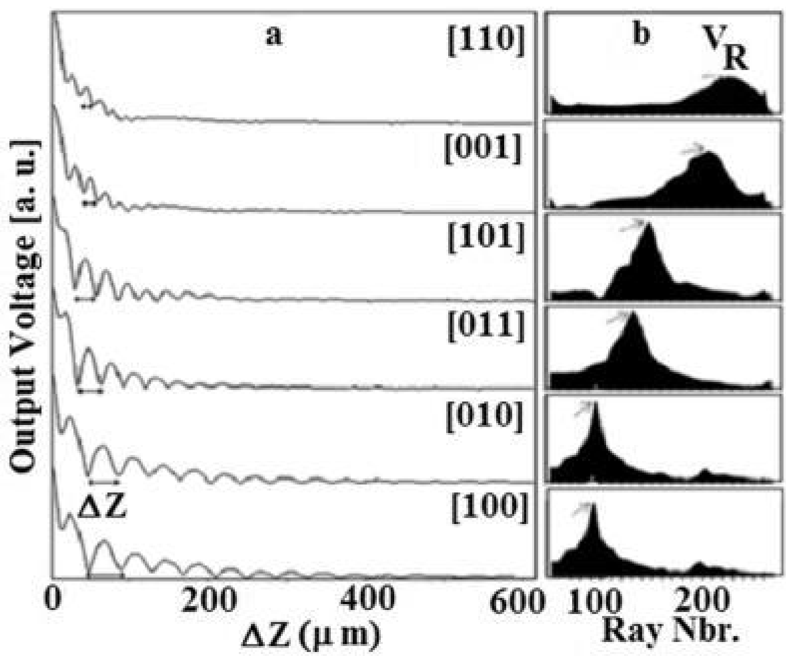


**Figure 3.** Acoustic materials signatures (a) and their FFT spectra (b) at different crystallographic directions on $Na_2CoGeO_4$ .

## 5.3.crystallographic orientations effects on wave velocities

The variations in Δz is better put into evidence by the spectral treatment of V(z) periodic signals (Fig. 3a) via fast Fourier transform analysis. Figure 3b illustrates FFT spectra of the corresponding V(z) curves of sodium germanate $Na_2CoGeO_4$ at different orientations. The principal peak corresponds to the most dominant propagating mode. It is well established that under the simulating conditions the propagating mode corresponds to that of leaky Rayleigh waves. It can be noticed that the height as well as the position of the peak change with crystallographic orientations. The height indicates that generation efficiency of the mode; whereas, the position corresponds to the value of Rayleigh wave velocity, $V_R$. The determined values (Eq. 3), regrouped in Table 2, put clearly into evidence the anisotropy effects on such acoustic parameters.

**Table 2:** Calculated elastic parameters of Na2CoGeO4 in different crystallographic directions

| | Longitudinal | | | Rayleigh | | |
|---|---|---|---|---|---|---|
| **Crystallographic directions** | **$\theta_R$(deg.)** | **Δz (µm)** | **$V_R$(m/s)** | **$\theta_L$(deg.)** | **Δz (µm)** | **$V_L$(m/s)** |
| **[100]** | 30.2 | 39.7 | 2993 | 15.6 | 141.3 | 5501 |
| **[001]** | 30.7 | 38.9 | 2965 | 16.7 | 128.5 | 5253 |
| **[010]** | 36.1 | 28.7 | 2583 | 19.6 | 92.4 | 4472 |
| **[110]** | 37.8 | 25.1 | 2464 | 15.1 | 151.3 | 5686 |
| **[101]** | 45.3 | 18.9 | 2157 | 16.1 | 133.3 | 5353 |
| **[011]** | 48.2 | 17.3 | 2075 | 15.3 | 147.5 | 5616 |

To enrich this investigation, we considered longitudinal acoustic waves which are a type of acoustic modes that can propagate in materials faster than shear and Rayleigh modes. To put into evidence anisotropy effects on such mode, we first calculated R(θ) in the vicinity of longitudinal critical angles, then the corresponding V(z) curves and finally their FFT spectra. Typical obtained results are displayed in Fig. 4. Similar behaviors were obtained as those of Rayleigh modes for different crystallographic orientations:

a) variations in longitudinal critical angles, changes of spatial periods,
b) changes in positions of FFT principal rays,
c) variations in peak heights
d) variations in the values of longitudinal velocities.

All these observations are regrouped in Table 2. This behavior could be explained by the atomic occupation of different planes. For denser directions the velocity is higher.

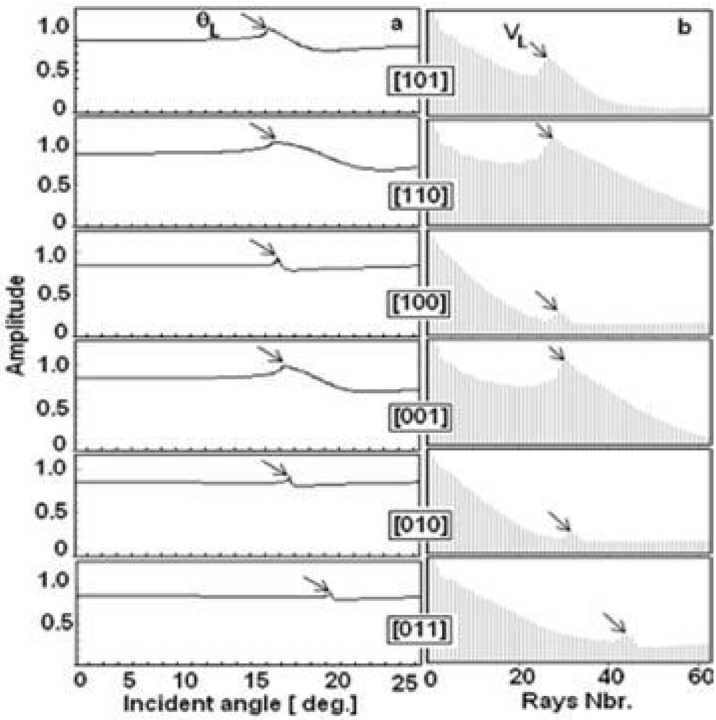


**Figure 4.** Effects of crystallographic orientations on (a) amplitude of reflection function in the vicinity of the longitudinal mode and (b) FFT spectra extracted from the corresponding V(z) curves.

## 6. Conclusions

The crystallographic direction effects in $Na_2CoGeO_4$ crystals are put into evidence for reflections coefficients, acoustic signatures, critical angles of mode excitation, spatial periods as well as velocities of different modes. For example, the propagation of acoustic waves in six crystallographic directions [101], [110], [100], [001], [010] and [011] of $Na_2CoGeO_4$ shows a decrease of the velocity of longitudinal waves from 5687 m/s to 4471 m/s due to the decreasing the atomic occupations of these planes.

# 7. References

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