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Fundamental characteristics of thickness vibrations of langasite plates for baw resonators

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Abstract

Based on theoretical and experimental investigations further possibility of $\text{La}_3\text{Ga}_5\text{SiO}_{14}$ - langasite (LGS) application for BAW resonators is described. Anisotropy of frequency coefficients N_f , temperature-frequency coefficients (TCF), electromechanical coupling coefficients (k_g) for these modes of vibration of langasite has been investigated.

1. Introduction

For the first time langasite crystals have been grown up and investigated in Russia at the begin of eighties during the search of new promising crystals for lasers [1-5]. Later a high acoustic quality factor, a piezoelectric effect stronger than that of quartz and the orientation existence with zero temperature coefficient of frequency (TCF) for BAW have been discovered in this material. Resonators fabricated of these crystals had rather attractive parameters [6,7]. Moreover, langasite does not have phase transitions during heating from the room temperature up to the melting temperatures which gives the possibility to apply it in products operating under severe conditions. This has served as a basis for further investigation of langasite crystal properties and their application in piezoelectric engineering.

2. Main physical properties of crystals under investigation

Characteristics of thickness vibrations of single- and double-rotated cuts of langasite have been investigated (N_f , TCF, k_g) for the A, B, C -modes of vibration aimed at finding orientations with minimum temperature coefficient of frequency (TCF) and high electromechanical coupling factor.

Table 1
Elastic stiffnesses C_{ik}^E (10^{10} N/m²)

C_{11}	C_{12}	C_{13}	C_{14}	C_{33}	C_{44}	C_{66}	
19.09	10.63	10.42	1.52	26.19	5.24	4.32	[2]
19.02	10.63	9.19	1.47	26.21	5.382	4.20	[4]
18.89	10.46	9.68	1.43	26.22	5.39	4.22	[5]
19.01	10.30	9.83	1.57	26.83	5.331	4.35	[11]

Table 2
Elastic compliances S_{ik}^E (10^{-13} m²/N)

S_{11}	S_{12}	S_{13}	S_{14}	S_{33}	S_{44}	S_{66}	
87.64	-40.32	-18.51	-35.9	55.91	210	255.9	[2]
87.52	-40.21	-18.82	-37.9	53.15	219.86	255.4	[4]
87.7	-42.7	-16.6	-34.6	50.4	203	-	[5]

Table 3
Piezoelectric strain d_{ik} (10^{-12} C/N) and stress e_{ik} (C/m²) constants and electromechanical coupling factors k_s

d_{11}	d_{14}	e_{11}	e_{14}	k_{12}	k_{26}	k_t	
-6.16	5.36	-0.45	0.077	0.16	0.134	0.08	[2]

Table 4

Young's modulus E_{ii} (10^{10} N/m²), shear modulus G_{ii} (10^{10} N/m²) and Poisson's ratios σ_{ik}

G_{11}	G_{33}	E_{11}	E_{33}	σ_{12}	σ_{13}	σ_{31}	
4.21	4.45	11.13	18.81	0.459	0.35	0.215	[2]

Table 5

Dielectric permittivity constants $\epsilon_{ii}^T, \epsilon_{ii}^S$, specific resistance ρ_e (10^3 Ohm·cm) and dielectric losses $\text{tg}\delta$ (10^{-3}).

T ϵ_{11}	S ϵ_{11}	T ϵ_{33}	S ϵ_{33}	ρ_{11}	ρ_{33}	$\text{tg}\delta$	
18.99	18.87	49.32	49.32	1.5	0.8	-	[2]
18.86	-	49.10	-	-	-	0.11	[5]

Table 6

Density ρ (10^3 kg/m³) and linear expansion coefficients α_{ii} ($10^{-6}/^\circ\text{C}$)

ρ	α_{11}	α_{33}	
5.754	5.11	3.61	[2]
5.743	5.84	4.03	[5]

Table 7
Thermal expansion coefficients $TC_{ik} (10^{-6}/^{\circ}C)$

TC_{11}	TC_{12}	TC_{13}	TC_{14}	TC_{33}	TC_{44}	TC_{66}	
-47	-100	-130	-370	-94	-30	+36	[4]
-58.7	-218	-101	-154	-135	-79.7	139	[5]
-52.7	-107.4	+0.7	-176	-105	-57.6	+12	[11]

Table 8
Thermal expansion coefficients $TS_{ik} (10^{-6}/^{\circ}C)$

TS_{11}	TS_{12}	TS_{13}	TS_{14}	TS_{33}	TS_{44}	TS_{66}	
-96.6	-337	165	-250	151	43.4	-	[5]

Table 9
Thermal expansion coefficients $Te_{ik} (10^{-6}/^{\circ}C)$,
 $Td_{ik} (10^{-6}/^{\circ}C)$, $se_{ik} (10^{-6}/^{\circ}C)$

Te_{11}	Te_{33}	Td_{11}	Td_{33}	se_{11}	se_{33}	
-2400	-5000	-2680	-3320	447	618	[5]
				153	-760	[4]

Table 10
Thermal expansion coefficients $T2C_{ik} (10^{-9}/^{\circ}C)$

$T2C_{11}$	$T2C_{12}$	$T2C_{13}$	$T2C_{14}$	$T2C_{33}$	$T2C_{44}$	$T2C_{66}$	
-113	+1085	-117	+452	+65	+102	-1564	[5]
-55.4	+48.1	+1294	-10.4	-62.8	-133	-178	[10]

Table 11

Phase velocity of elastic waves $v(10^3 \text{ m/c})$ and temperature dependence elastic waves $Tv(10^{-6}/^\circ\text{C})$, $T2v(10^{-9}/^\circ\text{C})$ of langasite crystals

Direction of propagation	Wave type	v			Tv	T2v
		[3]	[5]	[10]	[10]	[10]
X	XL	5.784	5.748	5.746	-24.9	-24.7
X	XFS	3.344	-	3.305	-53.2	-39.1
X	XS	2.344	2.380	2.394	+49.8	-42.0
Y	YQL	5.792	5.754	5.756	-31.0	-42.0
Y	YQS	2.971	3.015	3.003	-18.8	-57.5
Y	YS	2.767	2.745	2.750	+6.6	-89.0
Z	ZL	6.753	6.750	6.826	-50.0	-29.2
Z	ZS	3.021	3.061	3.043	-26.5	-64.9
[011]	+45YZQL	5.998	-	5.900	-40.1	-377.0
[011]	+45YZQS	3.141	-	3.281	-52.2	-87.0

Table 12

Acoustic characteristics: velocity $v_{lt}(10^3 \text{ m/s})$ and attenuation (dB/cm) of elastic waves in different crystals at the frequency of 830 MHz (20°C)

Crystal	Pure longitudinal		Pure transversal		
[3, 11]	along X-axis [1120]		along Y-axis [1010]		
	velocity	attenuation	velocity	attenuation	
SiO ₂	5.751	2.38	3.914	3.4	[3]
La ₃ Ga ₅ SiO ₁₄	5.784	0.45	2.767	1.6	[2]
Ca ₃ Ga ₅ Ge ₄ O ₁₄	5.85	0.6	2.757	3.9	[3]
Sr ₂ Ga ₂ Ge ₄ O ₁₄	5.576	0.8	2.791	2.8	[3]
Y ₃ Al ₅ O ₁₂	8.62	0.3	4.95	1.1	[3]

Table 13
Frequency constants of different crystals

Mode of vibration	SiO ₂	La ₃ Ga ₅ SiO ₁₄ [2]	Ca ₃ Ga ₂ Ge ₄ O ₁₄ [3]	Sr ₂ Ga ₂ Ge ₄ O ₁₄ [3]
Thickness-extensional mode				
X-cut plate	2715	2892	2964	2627
Thickness-shear mode	1660(AT) ⁽²³⁰⁰⁾			
Y-cut plate	2550(BT)	1382	1398	1364

Table 14
Piezoelectric constants d_{ik} (10^{-12} C/N), e_{ik} (C/m²), k_s (%) of different crystals

Crystal[3,11]	d_{11}	d_{14}	e_{11}	e_{14}	k_{12}	k_t	k_{26}	e_{11}	e_{33}
SiO ₂	2.3	-0.68	-1.62	-0.41	10	9	14	4.52	4.64
La ₃ Ga ₅ SiO ₁₄	-6.16	5.36	-0.45	0.077	26	8	13.4	18.99	49.32
Ca ₃ Ga ₂ Ge ₄ O ₁₄	-5.38	2.58	-0.344	0.0014	14.5	10.2	12.5	15.5	24.22
Sr ₂ Ga ₂ Ge ₄ O ₁₄	-9.41	6.96	-0.567	0.055	26.64	13	26	13.8	18.21

The present paper utilizes the results of crystal properties measurement published in [1-5,10,11], several of them are represented in tables 1-14.

The analysis of main langasite crystal properties shows that in accordance with Mason's classification, this crystal belongs to piezoelectrics possessing a moderately strong piezoelectric effect. Piezoelectric moduli of langasite are 1.5 times greater than those of quartz, but considerably less than those of lithium tantalate.

A high acoustic quality factor is characteristic for langasite. In comparison with quartz langasite has higher acoustic quality factor. Hypersound attenuation of a shear wave in langasite at a frequency of 830 MHz along the Y-axis is 3 times less and that of longitudinal wave, is 5 times less than those of quartz and is comparable with the wave attenuation in YAG.

An important langasite property is the possibility of the substitution of the structure elements La, Ga, Si by other elements and in obtaining based thereon of new compositions and solid-state solutions with the calcium-gallium-germanate structure, for example:

Several physical characteristics of the above-mentioned langasite compositions in accordance with the data published in [1-3], are given in tables 12-14, from which it follows that the compositions of this type can possess a diverse physical characteristic spectrum, for example, to have κ_g near to that of LBO. Their application in piezoelectric engineering can enable development of resonators with necessary parameters based on the "basic" LGS-structure.

The analysis of acoustical and electromechanical of properties of langasite crystal shows, that langasite can be effectively used for resonators operating in longitudinal, flexural, face shear and thickness- shear modes.

3. Theoretical investigations of thickness - shear vibrations in langasite plates

Evaluation has been made by using a computer taking into account crystal properties measurement data obtained in [2,4].

Second -order temperature constants have not been used in this paper due to necessity of further investigations.

As the basis for the calculation method, one-dimensional model

of thickness vibrations of an infinite piezoelectric plate developed by Tiersten and Yamada [8,9] has been used.

The electrical impedance of a piezoelectric plate vibrating in thickness-shear mode can be written as:

$$Z = \frac{1}{jC_0\omega} \left[1 - \sum_{i=1}^3 k^{(i)2} \frac{\operatorname{tg}\theta^{(i)}}{\theta^{(i)}} \right] \quad (1)$$

where $\theta^{(i)} = \frac{\omega t}{2v^{(i)}} = \frac{\pi f t}{v^{(i)}}$, (2)

C_0 - is the static capacitance of the plate;

t - is the plate thickness;

$k^{(i)}$, $v^{(i)}$ - is the electromechanical coupling factor and the phase velocity of the i th mode of vibration;

ω, f - are angular and linear frequencies, respectively;

j - is an imaginary unit.

The expression for antiresonance frequencies is obtained from the condition $Z \rightarrow \infty$ ($\operatorname{tg}\theta^{(i)} \rightarrow \infty$).

$$f_a^{(i)} = \frac{n\theta^{(i)}}{2t}, \quad (3)$$

where n - is the overtone order ($n = 1, 3, 5, \dots$) and the condition $Z=0$ determines resonance frequencies $f_r^{(i)}$, which are the roots of the following equation:

$$1 - \sum_{i=1}^3 k^{(i)2} \frac{\operatorname{tg}\theta^{(i)}}{\theta^{(i)}} = 0 \quad (4)$$

Phase velocity and the electromechanical coupling coefficient of the i th mode are calculated as:

$$v^{(i)} = \sqrt{\frac{c^{(i)}}{\rho}}, \quad (5)$$

$$k^{(i)} = \frac{e^{(i)}}{e c^{(i)}}, \quad (6)$$

where ρ - is density.

ϵ , $e^{(i)}$, $c^{(i)}$, are effective values of dielectric permeability, piezoelectric constant and stiffness modulus for BAW, propagating in the direction $\vec{n} = (n_1, n_2, n_3)$ with polarization vector $\vec{p} = (p_1, p_2, p_3)$.

The values of $c^{(i)}$ and ρ are eigenvalues and eigenvectors respectively of Green-Kristoffel G_{ik} , the components of which are determined for the piezoelectric medium as:

$$G_{ik} = C_{ijkl}n_jn_l + \frac{\gamma_i\gamma_k}{\epsilon} \quad (7)$$

$$\text{where } \gamma_i = e_{kij}n_jn_k, \quad (8)$$

$$\epsilon = \epsilon_{jk}^s n_jn_k, \quad i, j, k, l = 1, 2, 3, \quad (9)$$

and C_{ijkl}^E , e_{kij} , ϵ_{jk}^s are the components of stiffness tensors, piezoelectric constants and dielectric permeability, respectively.

In such a way the roots of eq. (4) are resonance frequency of A, B- and C-modes, corresponding to longitudinal, quick shear and slow shear BAW, propagating in the direction of the normal n to the plate. For calculation of the 1st- and the 2nd-order temperature coefficients of resonance frequency, temperature constants of crystal have been used and the roots of eq. (4) have been found at several different temperatures. Temperature coefficients of frequency of the k th order ($k=1, 2$) have been calculated as the 2nd order polynomial coefficients $f = f(T)$.

Calculations have been made by using a computer. The crystal properties measured data are published in [2, 4].

BAW propagation direction was specified by means of two angles γ and β (figure 1) for the plate of $xyb1/\gamma/\beta$ -cut.

Figure 1. BAW propagation direction for the plate of $xyb1/\gamma/\beta$ -cut.

Mode A

Mode B

Mode C

$\gamma=60^\circ(1), \gamma=70^\circ(2), \gamma=80^\circ(3), \gamma=90^\circ(4)$

Figure 4. Electromechanical coupling coefficients (k_g) of A, B and C-modes of langasite crystal, xy1/ γ / β -cuts.

Figure 3. Electromechanical coupling coefficients (k_g) of A, B and C-modes of langasite crystal, xy1/ β -cuts.

Mode A

Mode B

Mode C

 $\gamma=60^\circ(1), \gamma=70^\circ(2), \gamma=80^\circ(3), \gamma=90^\circ(4)$

Figure 6. Frequency coefficient of A, B and C-mode of langasite crystal, $xy1/\gamma/\beta$ -cuts.

Figure 7. Frequency coefficient of A, B and C-mode of langasite crystal, $yx1/\beta$ -cuts.

Based on the calculation results, it was found that the A-mode of thickness vibrations of langasite plates, analogous to quartz and berlinite, does not have temperature compensated cuts and its temperature coefficient of frequency (TCF) varies from $-40 \cdot 10^{-6}$ to $-10 \cdot 10^{-6}/^{\circ}\text{C}$ (figure 2,3).

The electromechanical coupling coefficient for the A-mode is not over 8% and it takes the highest value in the direction of the second order axis. Over the angle range β from 50° to 90° (cone around the Z-axis) the electromechanical coupling coefficient is less than 1% (figure 4,5).

The frequency coefficient decreases nearly monotonously from 3380 to 2800 kHz mm in the direction from the Z-axis towards the XY-plane (figure 6,7).

Therefore the A-mode can find a limited application in langasite resonators because the orientation with zero TCF is absent for it.

The TCF of B-mode varies from $-45 \cdot 10^{-6}/^{\circ}\text{C}$ to $15 \cdot 10^{-6}/^{\circ}\text{C}$. Over the angle range γ from 15° to 45° and β from 0° to $+35^{\circ}$ TCF of B-mode is positive and at the boundary of this region it is equal to zero (figure 2,3).

For these cuts with zero TCF the coupling coefficient varies from 0% ($\gamma = 30^{\circ}$) to 7% ($\beta = 15^{\circ}$, $\gamma = 45^{\circ}$).

The electromechanical coupling coefficient of B-mode has minima over the angle range β from 0° to 30° (γ from 60° to 120°) and away from these angles it takes higher value (figure 4,5).

The frequency coefficient of B-mode increases from 1500 kHz mm to 1700 kHz mm (figure 6,7). The greatest value the frequency constant N_f takes over the angle range β from 20° to 40° ($\gamma = 90^{\circ}$) and β from 40° to 70° ($\gamma = 30^{\circ}$).

Thus, the B-mode in langasite has piezoelectrically active zones with TCF equal to zero (with $k_g > 0$) and can be perspective for resonator application.

The TCF of the C-mode (figure 2,3) varies from $-40 \cdot 10^{-6}/^{\circ}\text{C}$ to $100 \cdot 10^{-6}/^{\circ}\text{C}$. This mode is the most interesting one from the point of view of completeness of temperature - and piezoelectric properties. At the graph of lines of the TCF level there are two regions where it becomes equal to zero. The electromechanical coupling coefficient of TCF with zero cuts, lying in the region $\beta \sim 80^{\circ}$ to 90° does not exceed 1%.

The region located over the angle range $\beta \sim 5^{\circ}$ to 50° and $\gamma \sim 65^{\circ}$ to 90°

is of greater interest for resonator applications. At the boundary of this angle range the zero TCF is "supplemented" by the electromechanical coupling coefficient which is relatively large for this material. For such cuts with the direction of normal near to that of the Y_c -axis, the electromechanical coupling coefficient ranges from 12% to 15% (figure 4,5).

The frequency coefficient for the C-mode varies from 1200 to 1600 kHz·mm for the above-mentioned directions (figure 6,7). Figure 8 represents more detailed dependencies of N_f , k_g and TCF for a single-rotated Y-cut of langasite, because just the cuts of $yx1/\beta$ type of this crystal have been used for designing first samples of temperature compensated resonators, operating in thickness shear mode. Analogous dependencies for quartz and berlinite are given. The designed TCF curve of langasite (figure 8,9) passes through zero at $\beta \approx 5^\circ$. Certain difference in designed and experimental values of temperature compensated cuts can be explained by the difference in properties of crystals from which resonators have been fabricated and of those crystals which have been used for acoustoelectrical characteristics measurement.

In such a way the condition of minimum TCF and maximum k_g satisfy single-rotated $yx1/\beta$ -cuts, where β takes the value of the angle range from 0° - 5° . The frequency coefficient N_f for these cuts is equal to 1360-1400 kHz·mm.

TCF and k_g analysis of langasite for A, B, and C-modes has shown the existence of large areas with zero 1st-order TCF and high k_g , therefore further investigations of langasite as a promising material for BAW resonators are of great interest.

4. Experimental

4.1. Theoretical estimation checking

Experimental checking of theoretical TCF, N_f and k_g estimation have been made by using resonators of $yx1/\beta$ -cut for different β -angles. The measurement data are shown in figure 9 and coincide satisfactorily with the theoretical results.

4.2. Experimental langasite resonators operating in thickness - shear mode C.

For resonators with crystal elements of $yx1/0^\circ$ - cut the temperature of FTC inflection point corresponds to $30-35^\circ$, and the

Figure 8. Dependencies of frequency coefficient (a), of electromechanical coupling factor (b) and temperature coefficient of frequency (c) on the rotation angle of Y-cut for: — langasite, - - quartz, - · - berlinite.

Figure 9. Theoretical and experimental curves TCF, N_f and k_s of langasite crystal: □ - theoretical data, · - experimental data.

frequency coefficient is equal to 1380 kHz·mm. With enlarging angle of cut the inflection point of FTC shifts towards negative temperatures and the frequency coefficient becomes greater, the resonance spacing becomes narrower. The main resonator characteristics are shown in table 15.

Table 15

Parameters of langasite resonators operating in thickness-shear mode

Frequency MHz	Q	R_1 Ohm	L_1 H	C_1 pF	C_0 pF	Resonance spacing value, %	Maximum relative frequency deviation, 10^{-6} (-60÷85°C)
10.7	15000	6	0.0052	0.038	3.19	0.7	-(300-400)
21.4	12000	30	0.0045	0.012	1.31	0.6	-(300-400)

Langasite resonators operating at 8-10 MHz have been also manufactured for VCXO application.

It is expected that in the oscillator circuit the pulling range and the pulling sensitivity characteristics can be improved by 2-3 times.

4.3. Langasite resonators operating in longitudinal mode.

Resonators 350 kHz of yxs/α -cut, where α° varies from 0° to -4° , in metal enclosure $V=1.5 \text{ cm}^3$ ($C_0 \sim 0.3 \text{ pF}$) and resonators at 128 kHz in glass enclosure $V=1.5 \text{ cm}^3$ ($C_0 \sim 1.7 \text{ pF}$), for $w/l \leq 0.17$ and $t=0.45 \text{ mm}$ thickness (1) and $t=0.65 \text{ mm}$ (2) have the parameters presented in table 16.

Table 16

Parameters of langasite resonators operating in longitudinal mode

Frequency kHz	Q	R_1 Ohm	L_1 H	C_1 pF	C_0 pF	Resonance spacing %	N_f kHz·mm	Maximum relative frequency deviation, 10^{-6} (-60÷85°C)
128(1)	50000	100	5.9	0.27	17.1	0.8	2300	-450
128(2)	50000	70	3.7	0.41	26.2	0.8	~2300	-350
350(1)	25000	400	6.1	0.07	3.9	0.8	~2300	-400

Langasite resonator dependence on piezoelectric element design is analogous to that of quartz resonators. The steepness coefficient of

frequency-temperature characteristic for the left branch is equal to $-5 \cdot 10^{-8}/^{\circ}\text{C}^2$ and for the right branch it is equal to $-7 \cdot 10^{-8}/^{\circ}\text{C}^2$ (3.5 and $4.5 \cdot 10^{-8}/^{\circ}\text{C}^2$ for quartz resonators, respectively).

The extremum point of frequency - temperature characteristic (FTC) shifts towards positive temperatures with the increase of width (w) to length (l) ratio, thickness (t) and rotation angle α of elements. The frequency coefficient of resonators $N_f \approx 2300 \text{ kHz} \cdot \text{mm}$ decreases slowly with the w/l and α^0 increase. Resonator inductance decreases with w/l and increase, with the quality factor and resonance spacing values increase being increased to 0.8-1 %. The main difference of these resonators from the quartz crystal ones is in their lower by approximately 1.5 times and by twice lower inductance and resistance, 4-5 times greater resonance spacing.

The steepness of resonator frequency - temperature characteristic curve decreases with the increase of piezoelectric element thickness. FTC extremum shifts towards positive temperatures with the increase of w/l , S and α^0 . Resonator frequency coefficient $N_f \approx 2300 \text{ kHz} \cdot \text{mm}$ slowly increases with w/l and α^0 decrease.

The TCF and k_g analysis of langasite for A, B, and C -modes has shown the existence of large areas with zero 1st-order TCF and high k_g , therefore further investigations of langasite as a promising material for BAW resonators are of great interest.

For more exact LGS-resonator perspectivity evaluation for application in piezoelectronic engineering application further experimental and theoretical investigations are necessary aimed at obtaining higher frequency stability, higher Q and improvement of electrical characteristics of the resonators.

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