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ABOUT THE COUPLING FACTOR OF THE GALLIUM ORTHOPHOSPHATE ($GAPO_4$) AND ITS INFLUENCE TO THE RESONANCE - FREQUENCY TEMPERATURE DEPENDENCE

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Abstract - **The quartz homeotype gallium orthophosphate ($GaPO_4$) is a representative of piezoelectric single crystals with large electromechanical coupling factor. It is known that its coupling factor k_{26} associated with the resonators vibrating in the thickness-shear mode is approximately two times greater than that of quartz. This property increases the spacing between the series and parallel resonance frequencies of resonators, and also the difference between the resonance frequency temperature dependencies of the fundamental and harmonic resonance frequencies of resonators vibrating in the thickness-shear mode. In this paper, the computed electromechanical coupling factors are compared with the measured ones, and the influences of the coupling coefficient to the resonance-frequency temperature dependencies of the fundamental and third harmonics of selected rotated Y-cut $GaPO_4$ resonators vibrating in the thickness-shear mode are presented. The precision of computation of the frequency-temperature dependencies of the fundamental and harmonic thickness-shear resonance is discussed. The purely elastic case for a laterally-unbounded plate, which corresponds closely to the limiting case of high harmonic resonance frequency-temperature behavior, was assumed for the calculations. The (YXl)0°, (YXl)-11°, and (YXl)-16.4° Y-cut orientations are used for the computations and measurements.**

Keywords – **GaPO4 single crystal, electromechanical coupling factor, temperature - frequency coefficients**

I. INTRODUCTION

The outstanding properties as remarkable temperature stability of the quartz homeotype with large electromechanical coupling factor - gallium orthophosphate ($GaPO_4$)- make possible to use it in some recent applications, as sensors at high temperatures in combustion machines, and VCXOs and SAW filters [1]. In the past, many authors give the attention to the basic properties [2], [3], and now to the nonlinear properties, namely to the methods for determination of some nonlinear constants of $GaPO_4$ [4]. The increased number of the papers indicates a significance of the $GaPO_4$ too. If the $GaPO_4$ single crystals are used in design of piezoelectric resonators, the knowledge of electromechanical coupling factor and resonance frequency temperature dependencies is very important. They are the reasons to develop the studies in our previously papers [4].

II. ROTATED Y-CUT $GAPO_4$ RESONATORS IN OUR STUDIES

In order to measure the important parameters of the $GaPO_4$ Y-cut resonators, sample plates of three different orientations were now obtained. The Y-cut = (YXl)0°, (YXl)-11°, and (YXl)-16.4° plates were prepared and electroded by AVL of Graz, Austria, and measured in our laboratory. The plates were 10 mm in diameter and 0.3 mm thick. The gold electrodes of 5 mm diameter were deposited on the major surfaces of the plates. The orientation of the plates was measured to ± 0.1°.

TABLE I
$GAPO_4$ RESONATOR PARAMETERS

Sample	Orientation Angle θ [°]	fs[Hz]	fp [Hz]
1-1	0.0	4 171 911	4 211 755
6	0.0	4 116 164	4 179 670
7	-11.0	4 092 603	4 115 280
2-1	-11.0	4 188 249	4 237 056
8	-16.4	4 058 879	4 092 180
3-1	-16.4	4 308 359	4 345 297

The reference temperature is 25°C, the fs is serial resonance frequency of fundamental harmonics (n = 1).

III. DETERMINATION OF THE ELECTROMECHANICAL COUPLING FACTOR

It is know, that the electromechanical coupling factor k_{26} can be determined from the measured resonance frequencies fs and fp (or from motional capacitance) - (A), from the measurements of the fundamental and overtone resonances of the thickness shear vibrations, using corrections for value of k_{26} and mass loading R - (B), and calculated from the relevant materials constants - (C). In this case the strain and electric field on piezoelectric body have a single non-zero component each, substitutions from the equations of state lead to the know form of the electromechanical coupling factor. In the equation for $GaPO_4$ ´s electromechanical factor k_{26}', the piezoelectric, dielectric and elastic constants must be transformed.

A) For thickness shear mode, there are three relevant materials constants: an elastic constant c^E_{66}, a piezoelectric constant e_{26}, and a dielectric constant ε^S_{22}.
The electromechanical coupling factor k_{26} is given in terms of these constants by equation

$$\frac{k_{26}^2}{1-k_{26}^2}=\frac{e_{26}^2}{\varepsilon_{22}^S\,c_{66}^E}\;,\qquad k_{26}^2=\frac{e_{26}^2}{\varepsilon_{22}^S\,c_{66}^D}\;,\tag{1}$$

$$c_{66}^E=\left(1-k_{26}^2\right)\rho\, f_p\, h^2\;,\tag{2}$$

where h is the plate thickness, and the electrical impedance is of the form

$$Z(\omega)=\frac{h}{j\omega\varepsilon^S A}\left[1-k^2\frac{\tan(\omega/4f_p)}{(\omega/4f_p)}\right],\tag{3}$$

where A is electrode area.

From (3) one finds that the coupling factor can be determined from the frequencies *fs* and *fp*:

$$k_{26}^2=\frac{\pi}{2}\frac{f_s}{f_p}\tan\left(\frac{\pi}{2}\frac{\Delta f}{f_p}\right).\tag{4}$$

Due to the many spurious resonances from high overtone contour modes, it is not desirable to attempt a direct measurement of *fp*. It is preferable to determine *fp* from high overtone resonances.

An alternative procedure is to measure the frequencies of the fundamentals and first or higher overtone resonances and use the *ratio* to calculate the coupling factor. For materials with small coupling factors, however, Δf is small, and it may be more accurate to measure the motional capacitance.

$$\Gamma=\frac{8\varepsilon^S k^2}{\pi^2}\frac{(f_p/f_s)^2}{1-4k^2(1-k^2)(f_p/f_s)^2\frac{1}{\pi^2}}\tag{5}$$

When $k < 0.1$, $\Gamma=\frac{8\varepsilon^S k^2}{\pi^2}$, for $k > 0.1$ values of Γ/ε^2 versus k are given in the table in [5].

B) Analysis of free thickness-shear vibrations of the piezoelectric plates with the surfaces perpendicular to the thickness covered with short-circuited conducting electrodes indicate that the fundamental and overtone resonance frequencies are not related as a simple multiple and that this relation depends also on the piezoelectric properties of the plate. The relation for the resonance frequency of the n-th order thickness-shear mode of vibration in the x_1x_2 plane of crystal plate with hexagonal symmetry, class 32 derived Tiersten [6] in the form (6):

$$f_n=\frac{\eta_n\cdot n}{2\pi h}\cdot\sqrt{\frac{c_{66}^D}{\rho}}\;,\tag{6}$$

where n is the overtone order, h is the thickness of the plate, ρ is the density of the unstressed plate and the wave number η_n is given by the relation

$$\tan(\eta_n\cdot h)=\frac{\eta_n\cdot h}{k_{26}{}^2+R\cdot(\eta_n\cdot h)^2}\,.\tag{7}$$

In equations (6) and (7) c_{66}^D is the elastic stiffness by constant electric displacement, and k_{26} is electromechanical coupling coefficient

$$c_{66}^D=c_{66}^E+\frac{e_{26}{}^2}{\varepsilon_{22}^S}\,,\quad k_{26}{}^2=\frac{e_{26}{}^2}{c_{66}^D\varepsilon_{22}^S}\,.\tag{8}$$

In Eq. (7) R is the mass-loading of the plate caused by the deposited electrodes

$$R=\frac{2\rho' h'}{\rho h},\tag{9}$$

where ρ' is the density of electrodes and h' is the thickness of electrodes.

For a small electromechanical coupling factor k_{26} (for a quartz typically) the relations (6) and (7) can be replaced by one relation

$$f_n=\frac{n}{4h}\sqrt{\frac{c_{66}^D}{\rho}}\cdot\left(1-\frac{4k_{26}{}^2}{n^2\pi^2}-R\right),\tag{10}$$

(10)

from which for known resonance frequencies f_{n1} and f_{n3} and known R the electromechanical coupling coefficient k_{26} can be computed.

In the next part, the determination of the k_{26} of different levels will be presented.

a) The coefficient k_{26} is high ($k_{26} > 0.3$), and the influence of the mass loading R is neglected.

Using the Eq. (6) and (7) we get to expressions

$$\frac{f_n}{f_1}=\frac{\eta_n}{\eta_1}\;,\tag{11}$$

$$\frac{f_n}{f_1} tg(\eta_1 h) = tg\left(\frac{f_n}{f_1}\eta_1 h\right) \quad \text{and} \qquad (12)$$

$$F\, tg(\lambda) = tg(F\lambda) \qquad (13)$$

by substitutions $F = \frac{f_n}{f_1}$ and $\lambda = \eta_1 h$.

Finally, the $k_{26}^2 = \frac{\lambda}{tg\lambda}$. (14)

b) The coefficient k_{26} small (01< k_{26} < 0.3), and the influence of the mass loading R is not neglected.

Using Eq. (10), the rapport of frequencies F is given by

$$F = \frac{f_n}{f_1} = \frac{n\left(1 - \frac{4k_{26}^2}{n^2\pi^2} - R\right)}{\left(1 - \frac{4k_{26}^2}{\pi^2} - R\right)} \,, \qquad (15)$$

and the electromechanical coupling coefficient is expressed as

$$k_{26}^2 = \frac{(F-n)(1-R)}{\frac{4}{\pi^2}\left(F - \frac{1}{n}\right)} \,. \qquad (16)$$

For a fundamental and third overtone frequency

$$k_{26}^2 = \frac{F-3}{0.405F - 0.135} \,. \qquad (17)$$

c) The coefficient k_{26} is very small (k_{26} < 0.1) .

Now, under approximation

$$\sqrt{c_{66}^D} = \sqrt{\frac{c_{66}^E}{1-k_{26}^2}} = \sqrt{c_{66}^E}\left(1 + \frac{1}{2}k_{26}^2\right) \qquad (18)$$

the Eq. (10) get to expression

$$f_n = \frac{1}{4h}\sqrt{\frac{c_{66}^E}{\rho}}\left(1 + k_{26}^2\left(\frac{1}{2} - \frac{4}{n^2\pi^2}\right) - R\right). \qquad (19)$$

We use the difference $f_n - nf_1$ for determination k_{26} :

$$f_n - nf_1 = k_{26}^2\left(\frac{4}{\pi^2} - \frac{4}{n^2\pi^2}\right)\frac{n}{4h}\sqrt{\frac{c_{66}^E}{\rho}} \qquad (20)$$

$$k_{26}^2 = \frac{f_n - nf_1}{\frac{4}{\pi^2}\left(1 - \frac{1}{n^2}\right)}\frac{4h}{n}\sqrt{\frac{\rho}{c_{66}^E}} \qquad (21)$$

For a fundamental and third overtone frequency

$$k_{26}^2 = \frac{f_3 - 3f_1}{1.08}\frac{4h}{n}\sqrt{\frac{\rho}{c_{66}^E}} \,. \qquad (22)$$

C) To calculate k_{26} for different rotation angles of rotated Y-cut $GaPO_4$ resonators, the material constants given in [1] and now also in Table 4 in [4] are used. We express the piezoelectric constants e_{11} and e_{14} as

$$e_{11} = d_{11}\left(c_{11}^E - c_{12}^E\right) + d_{14}c_{14}^E = 0.209 \;\; C/m^2 \quad \text{and}$$
$$e_{14} = d_{14}c_{14}^E = 0.072 \;\; C/m^2 \,. \qquad (23)$$

In the Eq. (23) the values of $d_{11} = 4.5 \times 10^{-12}$ m/V, $d_{12} = -d_{11}$, $d_{14} = 1.9 \times 10^{-12}$ m/V, $d_{24} = -d_{14}$, and $c_{11} = 66.58 \times 10^9$ N/m^2, $c_{12} = 21.81 \times 10^9$ N/m^2, $c_{14} = 3.91 \times 10^9$ N/m^2, $c_{44} = 37.66 \times 10^9$ N/m^2, and $c_{24} = -c_{14}$ were used.

For different rotation angles θ, the material constants of $GaPO_4$ were transformed by the equations given in [4] and designed as symbols with prime.

We read the electromechanical coupling factor k_{26}' as

$$(k_{26})' = \sqrt{\frac{(e_{26})'^2}{(c_{66}^D)'(\varepsilon_{22}^S)'}} \,. \qquad (24)$$

The transformed material constants including k_{26}' computed by Eq. (24) are given in Table 2.

TABLE II
TRANSFORMED MATERIAL CONSTANTS CALCULATED FOR DIFFERENT ORIENTATION ANGLES θ FOR ROTATED Y-CUTS OF $GaPO_4$.

θ [°]	$(c_{66}^E)'$ [GPa]	$(c_{66}^D)'$ [GPa]	$(\varepsilon_{22}^S)'$	$(e_{26})'$ [C/m^2]	$(k_{26})'$
0.0	22.38	23.28	5.8	-0.209	0.192
-11.0	21.47	22.16	5.83	-0.188	0.176
-16.4	21.48	22.06	5.86	-0.173	0.162

The values are calculated for room temperature 25 ºC.

for the $Tf^{(n)}$ is 25ºC.

IV. INFLUENCE OF THE ELECTROMECHANICAL COUPLING COEFFICIENT TO THE RESONANCE-FREQUENCY TEMPERATURE DEPENDENCIES

TABLE III

TEMPERATURE-FREQUENCY COEFFICIENTS AND TURNOVER POINT TEMPERATURES CALCULATED FOR DIFFERENT ORIENTATION ANGLES θ FOR ROTATED Y-CUTS OF $GaPO_4$.

θ [°]	$Tf^{(1)}$ [10^{-6} K^{-1}]	$Tf^{(2)}$ [10^{-9} K^{-2}]	$Tf^{(3)}$ [10^{-12} K^{-3}]	T_{TP} [°C]
-20.00	-6.078	-20.767	3.693	-121.34
-19.00	-4.699	-19.791	4.066	-93.71
-18.00	-3.280	-18.799	4.402	-62.24
-17.00	-1.827	-17.795	4.703	-26.32
-16.40	-0.939	-17.187	4.865	-2.32
-16.00	-0.342	-16.781	4.966	14.82
-15.00	1.171	-15.761	5.190	62.15
-14.00	2.707	-14.738	5.376	116.83
-13.00	4.262	-13.714	5.522	180.37
-12.00	5.831	-12.693	5.629	254.71
-11.00	7.411	-11.677	5.695	342.35
-10.00	8.998	-10.670	5.722	446.64
-9.00	10.586	-9.674	5.709	572.15
-8.00	12.172	-8.691	5.657	725.24
-7.00	13.751	-7.724	5.566	915.10
-6.00	15.320	-6.776	5.438	
-5.00	16.873	-5.848	5.272	
-4.00	18.409	-4.942	5.069	
-3.00	19.922	-4.060	4.832	
-2.00	21.410	-3.203	4.561	
-1.00	22.868	-2.374	4.257	
0.00	24.295	-1.572	3.922	
1.00	25.687	-0.799	3.557	
2.00	27.041	-0.056	3.163	
3.00	28.356	0.656	2.743	
4.00	29.628	1.337	2.299	
5.00	30.857	1.987	1.830	

T_{TP} denotes the turnover point temperature. The reference temperature

To study of the influence of electromechanical coupling coefficient to the resonance frequency temperature dependencies the results of our previously work [4] are used. The computed temperature coefficients for the Y-cut orientation, and calculated turnover point temperatures T_{TP} for the (YXl) orientation are summarized in Table 3.

The purely elastic case for a laterally-unbounded plate, which corresponds closely to the limiting case of high harmonic resonance frequency-temperature behavior, was assumed for the calculations since the only available temperature coefficients were those of the elastic stiffnesses (see Table 4 in [4]). For the calculations of the $T_{TP,}$ the values of the $Tf_1^{(1)}$, $Tf_1^{(2)}$, and $Tf_1^{(3)}$, and T_0 =25°C were used. The difference between the first order resonance frequency temperature coefficients of the fundamental ($Tf_1^{(1)}$) and third harmonic ($Tf_3^{(1)}$) is caused by the temperature coefficient of the electromechanical coupling factor k_{26}. From the measured data we observe that the difference between $Tf_1^{(1)}$ and $Tf_3^{(1)}$ is smaller for these $GaPO_4$ orientations than for AT-cut quartz, which implies that the temperature coefficient $Tk_{26}^{(1)}$ is also relatively small.

Similarly to the method using Eqs. (6)-(10) the temperature coefficient of the electromechanical coupling factor $Tk_{26}{}^{(i)}$ can be also computed from the resonance frequency temperature coefficients $T_{fn}{}^{(1)}$ and $T_{fn}{}^{(3)}$.
The average value of the computed first order temperature coefficient of the electromechanical coupling coefficient $Tk_{26}{}^{(1)}$ is

$$Tk_{26}{}^{(1)} = +4.52 \times 10^{-4} \ K^{-1}$$

Using the method described under A) and Eq.(4), the following results are obtained for different orientation angles θ of rotated $GaPO_4$ Y-cuts. The resonance frequencies for Y-cut orientations angles (YXl)-13.03°(*) , (YXl) 0° (*), and (YXl)+14.15°(*) presented here in Table 4 were published in [3]. The Y-cut orientations angles (YXl)-16.4°, (YXl)-11.0°, and (YXl) 0° are valid for samples No. 8, 7 and 6 respectively, which are measured in our laboratory.

TABLE IV

ELECTROMECHANICAL COUPLING FACTOR DETERMINED FROM THE MEASURED FREQUENCIES FS AND FP FOR DIFFERENT ORIENTATION ANGLES θ OF THE ROTATED Y-CUTS OF $GaPO_4$.

θ[°]	fs [Hz]	fp[Hz]	$(k_{26})'$ meas.fs,fp	/comp. by (24)
-16.4 (S8)	4058879	4092180	0.141	0.162
-11.0 (S7)	4092603	4115280	0.116	0.176
-13.03 (*)	7894200	7971620	0.154	
0 (*)	8751762	8874059	0.183	
0 (S6)	4116164	4179670	0.191	0.192
+14.15 (*)	9485855	9594238	0.166	
+15 (*)	9169240	9273918	0.166	
+21 (*)	5039750	5094200	0.162	

The reference temperature is 25 ºC.

V. Discussion

Generally it is possible to compute the shear piezoelectric coupling factor k_{26} of $GaPO_4$ from the measured resonance frequencies of the arbitrary two harmonics of the thickness-shear vibrations. But from the point of the accuracy of the computation, it is suitable to measure the resonance frequency of the fundamental thickness-shear vibration (n = 1), where the influence of the k_{26} on the resonance frequency is highest, and resonance frequency of the near highest harmonic, where the influence of the k_{26} on the resonance frequency decreases with the order of harmonic. The precision of computation of the frequency-temperature dependencies of the fundamental and harmonic thickness-shear resonance depends on the value of electromechanical coupling factor. The purely elastic case for a laterally-unbounded plate, which corresponds closely to the limiting case of high harmonic resonance frequency-temperature behavior, was assumed for the calculations.

VI. Conclusion

The electromechanical coupling coefficient k_{26} associated with thickness-shear mode resonators is two times greater than that of quartz, increasing the spacing between the series and parallel resonance frequencies of resonators suitable for the frequency range from 1 to 100 MHz. This is important for some types of crystal oscillators and monolithic filters. The large electromechanical coupling coefficient also increases the difference between the temperature dependencies of the fundamental resonance frequency and its harmonics.

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