Proceedings of the 2003 IEEE International Frequency Control Symposium and PDA Exhibition
Jointly with the 17th European Frequency and Time Forum

Properties and Applications of Singly Rotated $GaPO_4$ Resonators

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Abstract - **The novel piezoelectric crystal gallium orthophosphate ($GaPO_4$) shows very promising properties for resonator applications [1]. Advantages over quartz are temperature stability up to 970 °C, higher electromechanical coupling coefficients and lower damping. Singly rotated Y-cut resonators with different rotating angles are investigated:**
Y-84° resonators show low electromechanical coupling coefficients and Q factors in the order of millions, but also high drive level dependencies (DLD).
Y-15°45' resonators operating at 10 MHz in the third overtone, mounted in HC-52/U crystal holders show in comparison to quartz resonators in the same crystal holder low motional resistances of about 30 Ω and Q factors around 200000. Because of the high coupling coefficients this resonators can be used for VCXO applications with very high pulling ranges up to 1500 ppm. The DLD of this high coupled resonators are very low. Resonators with a cut angle of about Y+27° show no frequency jumps and a very linear frequency dependence on temperature in a temperature range from room temperature up to 600 °C.

Keywords - $GaPO_4$, gallium orthophosphate, resonator, VCXO, OCXO, drive level

I. Introduction

The piezoelectric crystal gallium orthophosphate ($GaPO_4$) belongs to the same point group as quartz (32 or D_3) and possesses similar physical properties. But because of the lack of the α-β phase transition most material properties are stable up to 970 °C, where a phase transition occurs (low quartz -> cristobalite like structure). Other advantages against quartz are the doubled piezoelectric coefficient d_{11} and thus the higher electric mechanical coupling coefficient k. The higher density (3570 kg/m^3) leads to a lower acoustic velocity and thus to a lower thickness of a resonator with the same frequency.

First measurements on $GaPO_4$ resonators were published 1989 [2], and because of the low material quality the results were poor. Much effort has been done to increase the material quality and the manufacture process on $GaPO_4$ resonators. This paper gives an overview about the properties of different singly rotated Y-cut $GaPO_4$ resonators, which have been build and measured since 1990, and their applications.

We gratefully acknowledge EU funding of the GAPOGROWTH project under contract No. G5RD-CT-2002-00709 (GROWTH programme) and of the QxSENS project under contract No. G6RD-CT-2002-00648

II. Physical Properties of $GaPO_4$ Resonators

The most important material properties for resonator applications are coupling, temperature dependence and damping (intrinsic material viscosity). For singly rotated Y-cuts only one of the three modes shows electromechanical coupling. In Fig. 1 the theoretically expected coupling coefficient and the calculated deviation of temperature dependence on resonance frequency (first deviation of frequency on temperature, TCF1) are shown for room temperature (25 °C).

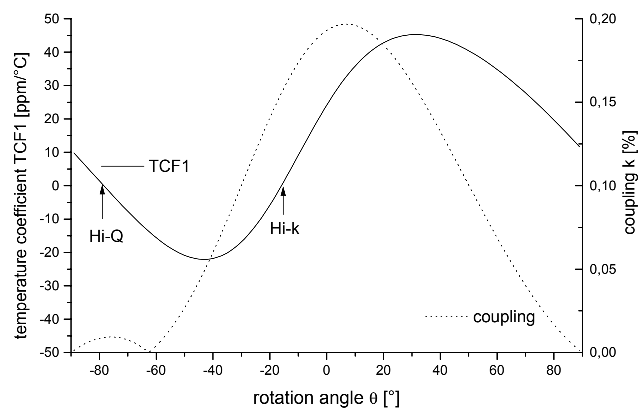

Fig. 1: Temperature coefficient and coupling of single rotated $GaPO_4$ y-cuts

The angle θ (x axes) means the amount of rotation around the crystal x axes of a Y-cut plate made of $GaPO_4$. The coupling coefficient k depends very strongly on θ and vanishes at θ = 90° (z-cut). There are two points of interest, where the temperature coefficient TCF1 vanishes. They are called Hi-Q and Hi-k. The Hi-k cut near y-16.5° has a coupling twice that of the quartz AT cut but the Hi-Q cut in $GaPO_4$ shows only a very low coupling.

Other applications, like temperature sensors, need a high temperature dependence of the resonant frequency. Two cuts (extremes of TCF1) are possible: near Y-45° and Y+30°.

The most important properties for resonator applications of quartz and $GaPO_4$ are compared in Table I.

TABLE I
MATERIAL PROPERTIES OF QUARTZ AND $GaPO_4$

Material	Quartz	$GaPO_4$
Point group	**32**	**32**
Phase transition [°C]	**573**	**970**
Piezoelectric constant d_{11} [pC/N]	**2.3**	**4.5**
Main temperature compensated cut	**AT**	**Hi-k, Y-16.5 °**
2nd temperature compensated cut	**BT**	**Hi-Q, Y-78.5 °**
coupling coefficient of AT and Hi-k [%]	**8.8**	**16**
frequency const. of AT and Hi-k [kHz mm]	**1660**	**1270**

A piezoelectric resonator can be represented by a simple series resonant circuit bypassed with a static capacitance C_0 (Fig. 2). The losses are comprised in the motional resistance R_1. C_1 is the motional capacitance and L_1 the motional inductance. Electrodes, enclosure and cable are included in the static capacitance C_0.

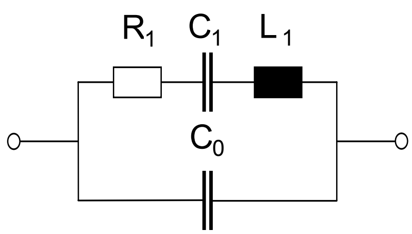

Fig. 2: Simple crystal equivalent circuit

The series resonance frequency f_s can be calculated with (1).

$$f_s = \frac{1}{2\pi\sqrt{L_1 C_1}} \tag{1}$$

The quality factor (Q factor) of the resonator is defined (2):

$$Q = \frac{\omega_s L_1}{R_1} = \frac{1}{\omega_s C_1 R_1} \tag{2}$$

where $\omega_s = 2\pi f_s$.

If the damping constant $\tau_1 = R_1 C_1$ is introduced, then τ_1 is composed of the different damping mechanism [3].

$$\tau_1 = \tau_\alpha + \tau_\phi + \tau_G + \tau_E \tag{3}$$

τ_α...acoustic losses in the material
τ_ϕ...losses due to plate geometry
τ_G...damping because of the surrounding gas
τ_E...electrical resistance of the electrodes

The last term is very small in most cases and the second one τ_ϕ can be made negligible by an adequate size of the resonator with a good energy trapping. If the enclosure is evacuated then the third term diminishes and the crystal's acoustic loss can be measured. This leads for the material quartz to the relation (4):

$$Q \cdot f \approx 16 \cdot 10^{12} \tag{4}$$

This is called the frequency quality product, and it is constant if the resonators are well designed. The best Q factors for the material quartz have been obtained with 5 MHz resonators, which are driven at the 3rd or 5th overtone [3]. An increase of the Q factor can be forced by decreasing R_1, but if the resistance is too low, the oscillator input stage will degrade the loaded Q factor. Too high R_1's prevent the oscillator from starting.

Also important, especially for VCXO applications, is the coupling coefficient k, which can be calculated from the material constants (5) or which can be estimated with the parameters of the electrical equivalent circuit in Fig. 2 (6).

$$k^2 = \frac{e_{eff}^2}{\varepsilon_{eff}\, c_{eff}^D} \quad \text{with} \quad e_{eff} = d_{eff}\, c_{eff} \tag{5}$$

Where c mean the elastic constants, d the piezoelectric constants, e the piezoelectric modulus and ε the dielectric coefficients. All constants depending on the rotation angle θ and temperature are effective combinations of the tensor components.

$$k = \frac{1}{n}\sqrt{\frac{\pi^2 C_1}{8 C_0}} \qquad \text{n...harmonics} \tag{6}$$

The frequency shift of a resonator with a series capacitance C_L is given by (7). Thus the ratio C_1/C_0, which is proportional to the squared coupling, limits the pulling range.

$$\frac{\Delta f}{f} \approx \frac{C_1}{2(C_0 + C_L)} \qquad \text{with } C_1 \ll C_0 \tag{7}$$

III. METHODOLOGY

A network analyzer (HP 4195 A) is used to measure the electrical parameters of the equivalent circuit (Fig. 2). All measurements were made in calibrated state. Most resonators are fixed in a clip fixture. For the estimation of the temperature dependence of the frequency and the pressure dependence of the resistance (with Hi-Q's, not encapsulated) an oven in the vacuum chamber described in [4] was used.

The drive level dependence with low power (up to 3 dBm only) is measured with the same network analyzer but higher drive levels (up to 20 V_{SS}) are only reached with the frequency synthesizer Agilent 33250A and the vector analyzer ZPV (Rohde & Schwarz). For these experiments the samples were connected direct to the output of the synthesizer to get the maximum power. For the current measurements a 10 Ohm resistance is used in series to the resonator, and the voltage across this resistance is used to calculate the current.

IV. Results

Singly rotated Y-cut resonators with different rotating angles were investigated:

- Y-84° resonators, denoted as Hi-Q, show very high Q factors, obtained with annealed resonators under vacuum conditions [4, 6].
- Resonators with a cut angle of about Y+27° show a high, nearly linear resonant frequency dependency on temperature.
- Y-15°45' resonators operating at 10 MHz in the third overtone mounted in HC-52/U crystal holders show low motional resistances of about 30 Ω, which is low in comparison to quartz resonators with the same holder

A. *Hi-Q Resonators*

All Hi-Q resonators are either mounted in a vacuum chamber without cap or encapsulated in an evacuated HC 49/U package. All resonators are polished, and they have a diameter of 7.4 mm with a thickness of roughly 0.271 mm, to get a resonance frequency in the vicinity of 6 MHz. The design is plano-convex with different curvatures. The electrodes are made of gold (180 nm) with a undercoating of 20 nm Cr.

The Hi-Q cut Y-84° shows a very low electromechanical coupling of 0.61 % (theoretically expected), which is much lower than the coupling factors of other singly rotated temperature compensated cuts. The frequency-temperature behaviour is parabolic with a 2nd order temperature coefficient lower than that of the quartz BT-cut and a turnover point near 80 °C [5]. The most important properties are summarized in Table II.

TABLE II
PROPERTIES OF HI-Q RESONATORS

No.	R_1 [Ω]	C_1 [aF]	f_s [MHz]	Q [10^6]	T_{anneal} [°C]	k [%]	Curv. [mm]
2-3	750	21.0	5.913	1.710	350	0.33	100
4-1	653	22.0	5.800	1.899	370	0.34	150
09	773	34.5	6.793	0.868	250	0.42	250

The measurements on these resonators were done with a low drive level of 16 µW (0.15 mA), at 84 °C, and under vacuum conditions (< 0.1 mbar). C_0 was around 2.4 pF and the 2nd order temperature coefficient was $2.7 \cdot 10^{-8}/°C^2$.

The resistances R_1 in Table II are very high compared to those of standard resonators. This is because of the very low coupling coefficient, which is lower then calculated. But due to the very low dynamical capacitance C_1, the Q factors reach high values up to 2 millions. All resonators are annealed at roughly 360 °C (T_{anneal}), except no. 09, which shows a lower Q factor and a higher R_1. The annealing is necessary to reduce mechanical stress and relax the material. The curvature in Table II defines the energy trapping. If the curvature radius is too high (No. 09) it is not possible to get very high Q factors.

If the drive level is too high, hysteresis effects and nonlinear responses influence the frequency-phase behaviour and the admittance depending on frequency (Fig. 3). In Fig. 3 the drive level dependence (DLD) of the admittance and in Fig. 4 the DLD of the phase is represented.

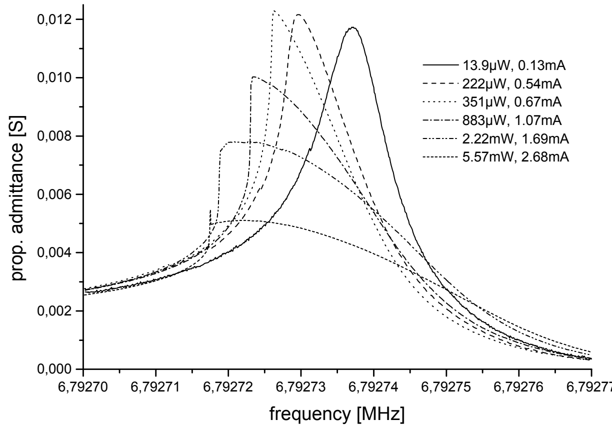

Fig. 3: DLD of "admittance" at room temperature (Hi-Q No. 09)

The measurements signal is the ratio of the voltage across the 10 Ohm series resistance and the output of the synthesizer. This is roughly one tenth of the admittance.

If the Q factor is calculated with the phase steepness (Fig. 4) [5,6] then the result strongly depends on the frequency or phase. This method is very useful to calculate the Q factor in oscillator applications. Usually phase zero is chosen, but this leads to very high Q factors up to infinity if the drive levels are too strong. We attribute the extremely high Q factors, published in the last year [4, 5, 6], to this effect. To prevent this effect, care must be taken, that the response of the frequency phase behaviour is harmonic and continuous.

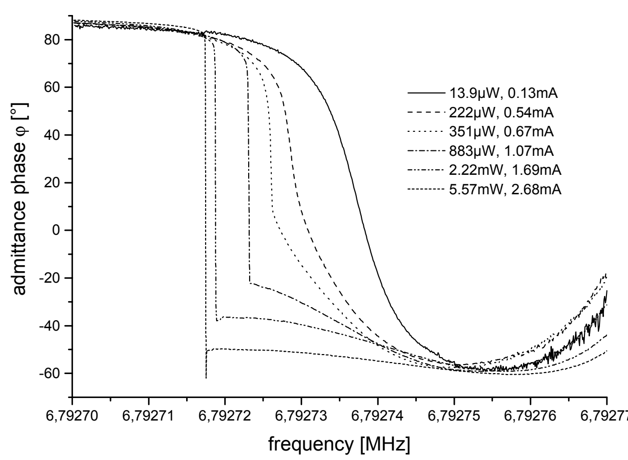

Fig. 4: DLD of phase (steepness) at room temperature (Hi-Q No. 09)

Like for the BT-cut of quartz the frequency of the Hi-Q resonators is decreased with increasing resonator current. The DLD of the Hi-Q resonators is very high. The nonlinear response starts at roughly 20 μW or 0.15 mA. All currents and powers are given in effective values.

The values of the dynamical resistances R_1 are strongly pressure dependent (Fig. 5). Damping values for R_1 can be calculated with (3). The time constant τ_G due to viscous damping in air at 85 °C can be estimated [3] as:

$$\tau_G = \frac{4.12 \cdot 10^{-8}}{\sqrt{f_S}} \sqrt{\rho_G \, \eta_G} \qquad (8)$$

where ρ_G and η_G are the density of the surrounding gas (air) and the viscosity respectively. Fitting of Fig. 5 with a function proportional to the square root of the pressure delivers the function

$$R_1 = \frac{\tau_1}{C_1} = 715\ \Omega + 80.7 \frac{\Omega}{\sqrt{\text{mbar}}} \sqrt{p[\text{mbar}]} \qquad (9)$$

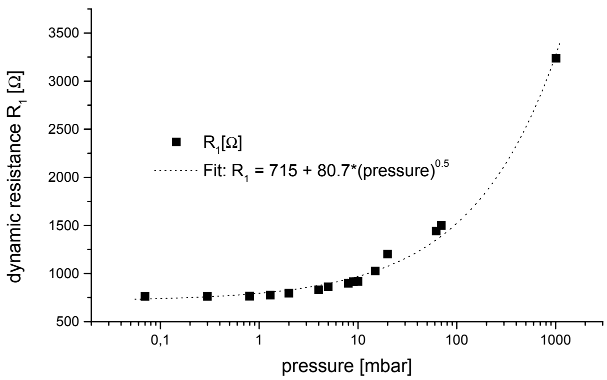

Fig. 5: Dependence on pressure of Hi-Q 2-3 at 85 °C, 0.5 μW

The calculated proportional constant, derived by dividing (8) by C_1, is 114 Ω $\text{mbar}^{-1/2}$. This discrepancy can be attributed to the very simplified model.

B. Temperature sensitive resonators

Resonators with a cut angle of about Y+30° or Y-45° show a high resonant frequency dependency on temperature (Fig. 1). More exact calculations, incorporating the temperature dependence of TCF1 up to 600 °C, lead to the cuts Y+27° and Y-47°. Experiments were done with 5 mm diameter resonators in a HC-52/U package and with a thickness of 0.24 mm. The surface was lapped plano-convex with a curvature of 50 mm. Because of the higher temperature region, the electrodes were made out of platinum (200 nm). The advantage against gold is that the temperature dependent coefficients of expansion fit better with $GaPO_4$.

Both cuts were studied, but the Y+27° cut seems to be the better choice because of its nearly linear response and the higher coupling. Theoretical calculations propose a very linear response with sensitivity between 43.5 ppm/°C and 46.0 ppm/°C within a temperature range from room temperature up to 600 °C. In Fig. 6 both cuts are compared and the experimental results of the better cut are shown.

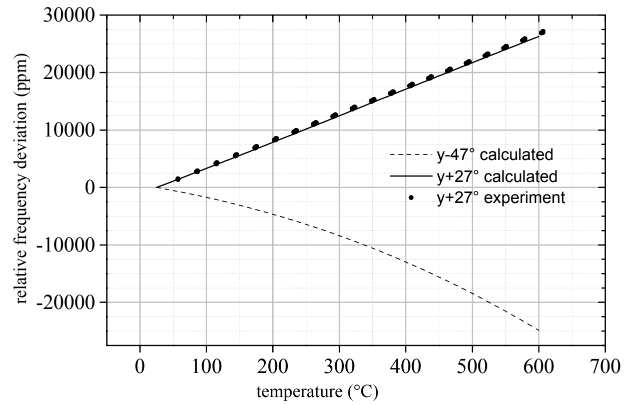

Fig. 6: Temperature dependence of y+27° and y-47° $GaPO_4$ resonators

The experimental data agree very well with the calculations [7]. In Table III the most interesting resonator properties are summarized.

TABLE III
PROPERTIES OF TEMPERATURE SENSITIVE RESONATORS

No.	R_1 [Ω]	C_1 [fF]	f_s [MHz]	Q [10^3]	k [%]	T_{anneal} [°C]
Y+27	60	32.7	5.656	14.3	17.0	700

All electrical parameters are suitable. T_{anneal} is the annealing temperature for the measurement preparation and should be chosen higher than the highest temperature in use. This reduces thermal hysteresis during the warm up and cool down procedure and relaxes mechanical stress.

In the whole temperature range from room temperature up to 600 °C no activity dips or frequency jumps are observed [7].

C. Hi-k Resonators, 10 MHz 3rd Harm., HC-52/U

Hi-k type resonators with the cutting angle near Y-16.5° have also a temperature behaviour on frequency like the BT-cut in quartz (parabolic, 2^{nd} order), but the temperature coefficient TCF2 is only half and the coupling is twice (16 %) that of the AT-cut in quartz. First attempts have shown that it is possible to get very low dynamical resistances of resonators made of $GaPO_4$.

This leads to a new design of 10 MHz resonators vibrating in 3^{rd} harmonics but in a small holder (HC 52/U). Samples with two different designs are measured but the sizes of all resonators were the same (diameter: 6 mm, thickness 0.38 mm, lapped). Type 1 is plano-convex with a curvature of 70 mm and 1 mm bevelled on backside. Type 2 is plano-plano with 1 mm bevelled both sides. The electrodes are made of silver (500 nm). In Table IV are the measurements summarized, which were done with a drive level of 100 μW. Direct measurements of the static capacitance C_0 result in 1.8 pF.

TABLE IV
PROPERTIES OF 10 MHZ RESONATORS, 3RD HARMONICS (HC-52/U)

No.	R_1 [Ω]	C_1 [fF]	f_s [MHz]	Q [10^3]	k [%]	Curv. [mm]
1pf	30	3.70	10.168	157	14.8	flat
2pc	65	0.98	9.852	254	7.6	70
2pc-fm	47	28.0	3.336	36	13.6	70

Fundamental mode data of "2pc" are given in the 3rd line. The resistances are very low compared to quartz (150 – 200 Ω) but the coupling does not reach the theoretical value which means that the design can be improved. The Q factors are high in the 3rd harmonics mode which makes this type of resonators very suitable for small spaced and low power OCXO applications. First results are presented [8] and show good phase noise behaviour. In Fig. 7 the temperature dependence of the frequency is shown. The fitted parabolic constant is a = 2.10^{-8} K^{-2}, which is half of a quartz BT-cut.

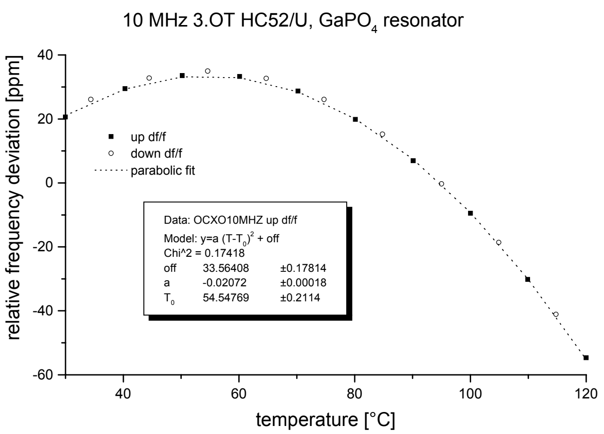

Fig. 7: Temperature dependence of resonator 2pc

D. OTHER TYPES OF HI-K RESONATORS

Resonators with a cut angle of Y-13.64° and a theoretical coupling coefficient of 16.9 % were produced. The turnover temperature was 160 °C. Two designs were investigated:

- big: HC-51/U, 14 mm diameter, plano-convex with 250 mm curvature radius, 0.25 mm thickness, lapped
- small: HC-49/U, 7.4 mm diameter, bevelled (1 mm, 40 mm curvature radius), 0.21 mm thickness, lapped

The measured electrical parameters (drive level 100 µW) are shown in Table V.

TABLE V
PROPERTIES OF TYPICAL HI-K RESONATORS

No.	R_1 [Ω]	C_1 [fF]	f_s [MHz]	Q [10^3]	k [%]	C_0 [pF]
05 small	6.7	71.3	5.994	55.3	16.1	3.4
12 big	1.4	67.9	4.995	335	10.6	7.5

The resistances are very low and the coupling is high as expected. First results with VCXO applications [8] show a pulling range up to 2000 ppm. Also shown is the high Q factor of the bigger resonator in the fundamental mode.

Another very important criterion for oscillator applications is the drive level dependence. In Fig. 8 the DLD for the smaller resonator is represented.

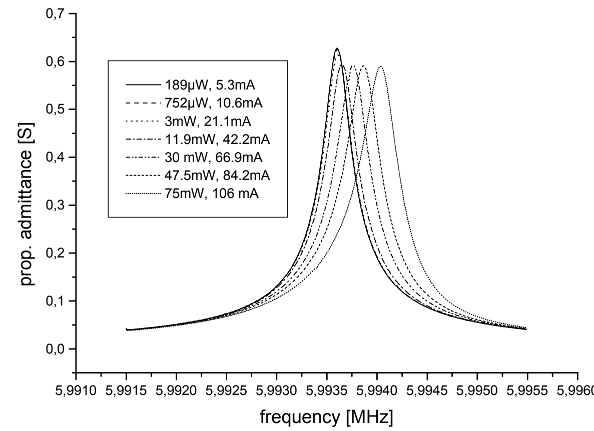

Fig. 8: DLD of Hi-k $GaPO_4$ resonator 05 with a diameter of 7.4 mm

Very high powers cause only a low (positive AT-cut behaviour) frequency shift (amplitude-frequency effect). The form of the curve has only low distortions despite of the high drive levels. Oscillator studies with $GaPO_4$ resonators [8] confirm this results. Similar results are obtained with some types of the Langasite family [9]. A simple theory [10] leads to the conclusion, that the relative frequency shift should be proportional to the squared resonator current I_{eff} (Fig. 9).

$$\frac{\Delta f}{f} = D \cdot I_{eff}^2 \qquad \text{with } I_{eff} \text{ in mA} \tag{10}$$

The proportionality constant D can be derived from Fig. 9 where the DLD for the big and the small resonator is shown against the resonator current squared.

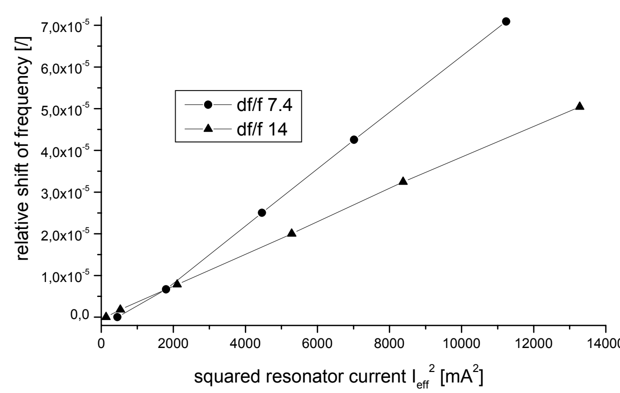

Fig. 9: DLD of the big (14 mm) and the small (7.4 mm) $GaPO_4$ resonators

Table VI shows a comparison of typical D values. The SC-cut values are the lowest which can be obtained for quartz.

TABLE VI
COMPARISSON OF DLD

	big $GaPO_4$	small $GaPO_4$	AT quartz	SC quartz
D [ppb/mA^2]	**3.7**	**7.3**	**200 – 300**	**4 – 10**

V. DISCUSSION

Most resonators show lower coupling coefficients than theoretically expected. This is due to the vibrating area being smaller than the metallized electrode area. An adequate design (less curvature) can increase the vibrating volume and thus decrease the resistance or improve the DLD. But, if the curvature is too low, the energy trapping will be weak, thus the resistance increases. For a better design theoretical studies should be performed.

$GaPO_4$ Hi-k resonators show a very low DLD compared to quartz but Hi-Q resonators show a very strong DLD. One reason could be the very low coupling, but in quartz the SC-cut with low DLD has a lower coupling than the AT-cut with strong DLD. The low DLD and the very low resistance of the big Hi-k cuts made of $GaPO_4$ make this material a good choice for highly stable frequency standards.

Compared to quartz $GaPO_4$ Hi-k resonators have lower resistances with the same design. The Q-frequency product for 7.4 mm Hi-Q resonators working in fundamental mode is $11 \cdot 10^{12}$ Hz, significantly higher quartz resonator with similar design and the same mode and in the order of the maximum $Q \cdot f$ product of the best quartz resonators ($16 \cdot 10^{12}$ Hz).

VI. CONCLUSIONS

Table VII gives an overview of possible applications.

TABLE VII
$GaPO_4$ RESONATORS AND POSSIBLE APPLICATIONS

type	cut	significant properties	possible applications
Hi-Q	**Y-84°**	**high Q and high DLD**	**OCXO, pressure sensor**
TC1	**Y+27°**	**lin. temp. coefficient, no activity dips**	**precise, wide range temperature sensor**
10 MHz 3rd harmonics	**Y-16.5°**	**low R_1, high Q**	**small OCXO**
small Hi-k	**Y-13.6°**	**low R_1, high C_1/C_0**	**wide range VCXO**
big Hi-k	**Y-13.6°**	**very low R_1 and DLD**	**frequency standards**

$GaPO_4$ crystals have promising properties for resonator applications. Compared to quartz $GaPO_4$ has no $\alpha-\beta$ phase transition, which makes a highly linear temperature sensor with high resolution in a wide range possible. It is possible to anneal $GaPO_4$ resonators at temperatures up to 900 °C, which should lead to ultra low aging rates.

The most interesting application next time will be resonators in the "Warner" design with 14 mm diameter and working in the 3rd or 5th harmonic at 5 MHz. This should give very high Q factors with adequate resistances for oscillator applications. Because of the low DLD harder driven resonators should lead to ultra low phase noise.

ACKNOWLEDGMENT

We would like to thank Mr. Bernd Neubig for helpful discussions.

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