Proc. 2011 IEEE International Ultrasonics Symposium, Orlando, FL, Oct. 18-21, 2011 (paper P5B-2)

Characterization of Langasite for Application in High Temperature SAW Sensors

S. Sakharov[1], N. Naumenko[2], A. Zabelin[1], S. Zhgoon[3]
[1]Fomos-Materials, Moscow, Russia
[2]Moscow Technical University of Communication and Information
[3]Moscow Power Engineering Institute

***Abstract*—Experimental SAW resonator structures with iridium electrodes were fabricated on Y-cut of langasite with few different propagation directions and their characteristics were measured in a wide temperature interval, up to 700ºC, and compared with simulations. Between two sets of material constants reported by Bungo one set was selected as providing much better agreement with experiments, for the analyzed orientations. Further improvement of simulation accuracy was achieved via after-correction of the calculated temperature characteristics using auxiliary function extracted from experimental data. This approach was used to predict resonator characteristics in orientation with Euler angles (0º, 22º, 90º), in which Bluestein-Gulyaev wave propagates, and provided excellent agreement between experiments and simulations, in a wide temperature interval.**

I. Introduction

Langasite (LGS) is considered as the most promising material for wireless high temperature sensors utilizing SAW resonators. The simulation of such devices usually requires accurate characterization of LGS in a wide range of temperatures, up to 700ºC. The previously reported sets of LGS material constants (for example, [1]-[3]) usually comprise the first- and second-order temperature coefficients. Our preliminary investigation of SAW resonators with W, Pt and Ir electrodes built on different orientations of LGS, in a wide interval of temperatures [4], has revealed that these constants help to predict the temperature behavior of SAW resonators on LGS up to 250ºC. At higher temperatures, simulations diverge with experiments.

In this paper, we report on the results of further experimental and theoretical investigation of few cuts of LGS potentially useful for application in high temperature SAW sensors. Frequency versus temperature characteristics of SAW resonators built on different LGS orientations have been measured and compared with simulations performed with different sets of material constants. This work is aimed at improved characterization of LGS in a wide temperature range, from 25ºC to 700ºC.

II. Experimental Devices and Resonator Characteristics

The experimental structure of SAW resonator utilized for characterization of different LGS cuts has pitch p=6.584 µm and electrode thickness varying between 50 nm and 215 nm, which is between 0.5%λ and 1.5%λ, where λ=2p is the wavelength at synchronous resonance condition. With such period of the resonator structure, center frequencies of test devices between 170 and 210 MHz were obtained, in the analyzed LGS orientations.

As a metal of electrode, iridium (Ir) was used. Compared to other metals, which we investigated previously (W, Pt) [4], Ir has the longest life time and smaller resistance at high temperatures, between 500º and 800ºC. Besides, Ir does not require any sublayer, due to its good adhesiveness to LGS.

Experimental devices were fabricated on Y-cut of LGS with four different propagation directions defined by the Euler angles (0º,90º,0º), (0º,90º,32º), (0º,90º,58º) and (0º,90º,90º). The second and third orientations are non-symmetric, which means certain directivity of SAW radiation, i.e. NSPUDT properties. Orientation (0º, 90º, 32º) was selected due to nearly zero beam steering and sufficiently high electromechanical coupling of SAW. In orientation (0º, 90º, 90º), Bluestein-Gulyaev wave (BGW) propagates, due to the crystal symmetry.

SAW resonators were mounted in nitrated metallic small-size packages commonly used in production of quartz resonators. The package tips were electrically connected to the pads of a SAW resonator by means of conducting silver-based glue *ThreeBond* (Japan) and after-dried during 30 minutes at the temperature 150°C.

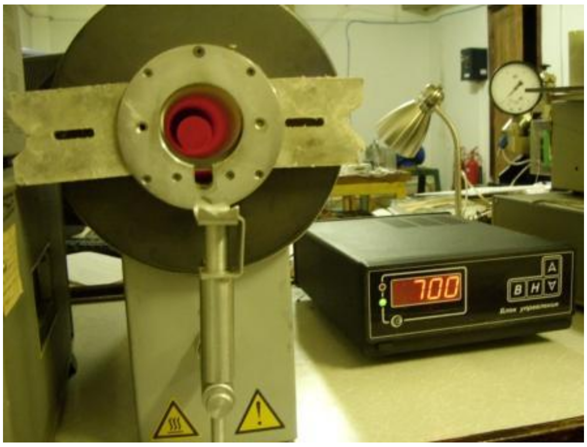

Fig. 1. High-temperature testing equipment

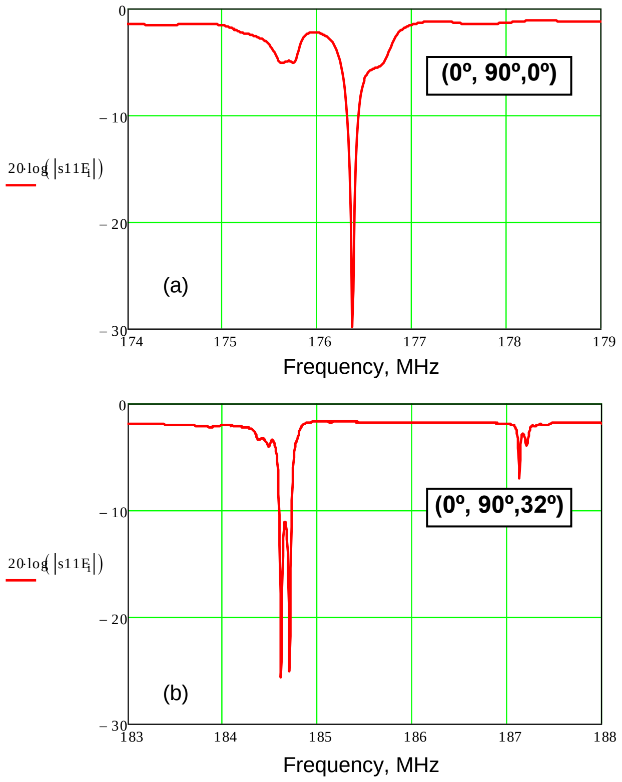

Fig. 2. Typical measured responses S11 of SAW resonators on symmetric and non-symmetric orientations of LGS, with Euler angles (a) (0º, 90º, 0º) and (b) (0º, 90º, 32º).

The measurements of frequency versus temperature characteristics of SAW resonators were made in the interval between 25°C and 700°C with testing equipment, which included analyzer Agilent 8712ET, low-drift tube furnace with temperature-control device and fixture for installing resonators into the furnace (Fig.1). Before the measurements, packaged SAW resonators were welded to Ni-Cr pads of the fixture, then put into the furnace, heated up to the temperature fixed by the temperature-control device and hold about 30 minutes at this temperature. After that S11 frequency response was measured with Agilent analyzer.

The typical frequency responses measured in symmetric and non-symmetric orientations are shown in Fig. 2. In non-symmetric orientations with Euler angles (0º, 90º, 32º) and (0º, 90º, 58º), NSPUDT properties manifest themselves by two resonances of the measured S11 function (Fig. 2b), instead of one resonance observed in symmetric orientations (Fig. 2a).

III. Experimental and Simulated Temperature Characteristics

After the resonator characteristics were measured in the interval between 25°C and 700°C, with decrement 25°C, the experimental resonator frequencies f_R were extracted as functions of temperature. All resonators have shown turnover points characterized by zero TCF, though the value of turnover temperature T_0 is different for each orientation.

Since Ir is a heavy metal, we observed the shift of resonant frequencies with increasing electrode thickness. To exclude the effect of this shift on comparison of simulated and experimental temperature behavior of SAW resonators, the simulated and measured dependences $f_R(T)$ were transformed into relative temperature deviations of frequency, $\Delta f/f_0$, where $\Delta f=f_R(T)-f_0$, and $f_0=f_R(T_0)$ is the resonant frequency at T_0=25º.

All simulations were made with the software *SDA-FEM-SDA* [5], with the upper half-space specified as the air. Electrodes were assumed to be rectangular. Metallization ratio was fixed as η=0.5. The variation of electrode thickness h/p in experimental devices was taken into account. At each temperature varying between 25º and 700ºC, the resonant frequency f_R satisfying condition $[Y(f_R)]^{-1}=0$ was extracted with high accuracy from numerical admittance $Y(f)$, and the function $\Delta f/f_0(T)$ was calculated and compared with measured $\Delta f/f_0(T)$. For non-symmetric orientations characterized by NSPUDT properties, the lower resonance was considered.

Simulations were made with two data sets reported in [1] and [2], shown in the Table 1.

TABLE I

Two sets of material constants of LGS reported by Bungo

Constant	Ref [1]	Ref [2]
c_{11}^E, 10^9 [N/m^2]	189	188.9
c_{12}^E	104	104.2
c_{13}^E	102	101.5
c_{14}^E	14.4	14.42
c_{33}^E	268	268.3
c_{44}^E	53.3	53.3
e_{11} [C/m^2]	-0.438	-0.4371
e_{14}	0.104	0.1039
$\varepsilon_{11}/\varepsilon_0$	19.06	19.05
$\varepsilon_{33}/\varepsilon_0$	51.60	51.81
α_{11}, [ppm/ºC]	5.08	5.046
α_{33}	3.49	3.455
$Tc_{11}^{(1)}$, 10^{-6}	-58.4	-57.54
$Tc_{12}^{(1)}$	-98.7	-98.15
$Tc_{13}^{(1)}$	-82.3	-81.61
$Tc_{14}^{(1)}$	-307.0	-307.5
$Tc_{33}^{(1)}$	-105.0	-104.0
$Tc_{44}^{(1)}$	-58.7	-57.39
$Te_{11}^{(1)}$, 10^{-6}	464.5	469.8
$Te_{14}^{(1)}$	-700.3	-713.8
$T\varepsilon_{11}^{(1)}$, 10^{-6}	135.5	134.5
$T\varepsilon_{33}^{(1)}$	-783.4	-787
$T\alpha_{11}^{(1)}$, 10^{-6}	-	1488
$T\alpha_{33}^{(1)}$	-	2169
$Tc_{11}^{(2)}$, 10^{-9}	-82.7	-82.65
$Tc_{12}^{(2)}$	-51.9	-51.83
$Tc_{13}^{(2)}$	-68.1	-68.10
$Tc_{14}^{(2)}$	95.5	95.34
$Tc_{33}^{(2)}$	-89.7	-89.61
$Tc_{44}^{(2)}$	-103.6	130.5
$Te_{11}^{(2)}$, 10^{-9}	-427.5	-428.5
$Te_{14}^{(2)}$	1600.	1594
$T\varepsilon_{11}^{(2)}$, 10^{-9}	118.0	118
$T\varepsilon_{33}^{(2)}$	661.2	658.6
$T\alpha_{11}^{(2)}$, 10^{-9}	-	-10410
$T\alpha_{33}^{(2)}$	-	-4976

Both data sets were published by Bungo in 1999. Compared to other known material data of LGS, they provide better agreement with experiments at high temperatures.

Though two data sets look very close to each other, in a wide temperature range one of them, reported in [1], provides better agreement with experiments, in the analyzed orientations. It is possible that lower accuracy of data set [2] is explained by too high values of the reported temperature extension coefficients of higher orders. However, if these coefficients are ignored, the data set reported in [1] still provides better agreement with experimental data.

Fig.3,a-d compares the simulated and measured characteristics $\Delta f/f_0(T)$ for few propagation directions on Y-cut of LGS and demonstrates that material data [1] better characterize resonator performance at high temperatures though the difference between the simulated and measured functions, $\delta(T)=(\Delta f/f_0)_{exp}-(\Delta f/f_0)_{sim}$, grows with temperature, for both data sets.

This difference is plotted in Fig. 4 as the *error function* $\delta(T)$, which characterizes inaccuracy of each set of material constants. It was determined at fixed electrode thickness, h=1.5%λ. Though SAW has different nature in symmetric orientations with Euler angles (0º, 90º, 0º) and (0º, 90º, 90º), nearly equal error functions have been obtained for these two cuts when calculations were made with data set [1]. The averaged function derived for this data set (bold line in Fig. 4) is very close to $\delta(T)$ of two symmetric cuts. In non-symmetric orientations with Euler angles (0º, 90º, 32º) and (0º, 90º, 58º) larger deviation of $\delta(T)$ from the averaged function is observed because the temperature behavior of the first resonant frequency can be affected by the variation of beam steering angle with temperature. The effect of anisotropy must be properly taken into account.

The disagreement between the experimental and simulated frequency-temperature characteristics described by the averaged *error function* $\delta(T)$ may be referred to the temperature dependence of Ir constants, which was not taken into account in simulations, or to the higher-order temperature coefficients of LGS density.

Nearly equal error functions $\delta(T)$ obtained for two symmetric orientations allow to assume similar error for arbitrary symmetric LGS cut and use the polynomial approximation of the averaged $\delta(T)$ for *after-correction* of the calculated temperature dependences of resonant frequencies.

Such approach was applied to orientation with Euler angles (0º, 22º, 90º), which is known to combine high electromechanical coupling of BGW with nearly zero temperature coefficient of frequency (TCF), in resonator structures [6]. The results of simulation are compared with the measured $\Delta f/f_0$, in Fig. 5. Excellent agreement between simulation and experiment has been obtained with the method described above.

The experimental performance of resonators on orientation with Euler angles (0º, 22º, 90º) was found to be noticeably degraded if propagation direction is not properly aligned with X+90º direction of LGS. The degradation looks as splitting of one resonance into two or even three resonances and reduced Q-factors compared to Y-cut (Fig. 6). The nature of this effect is studied theoretically in [7].

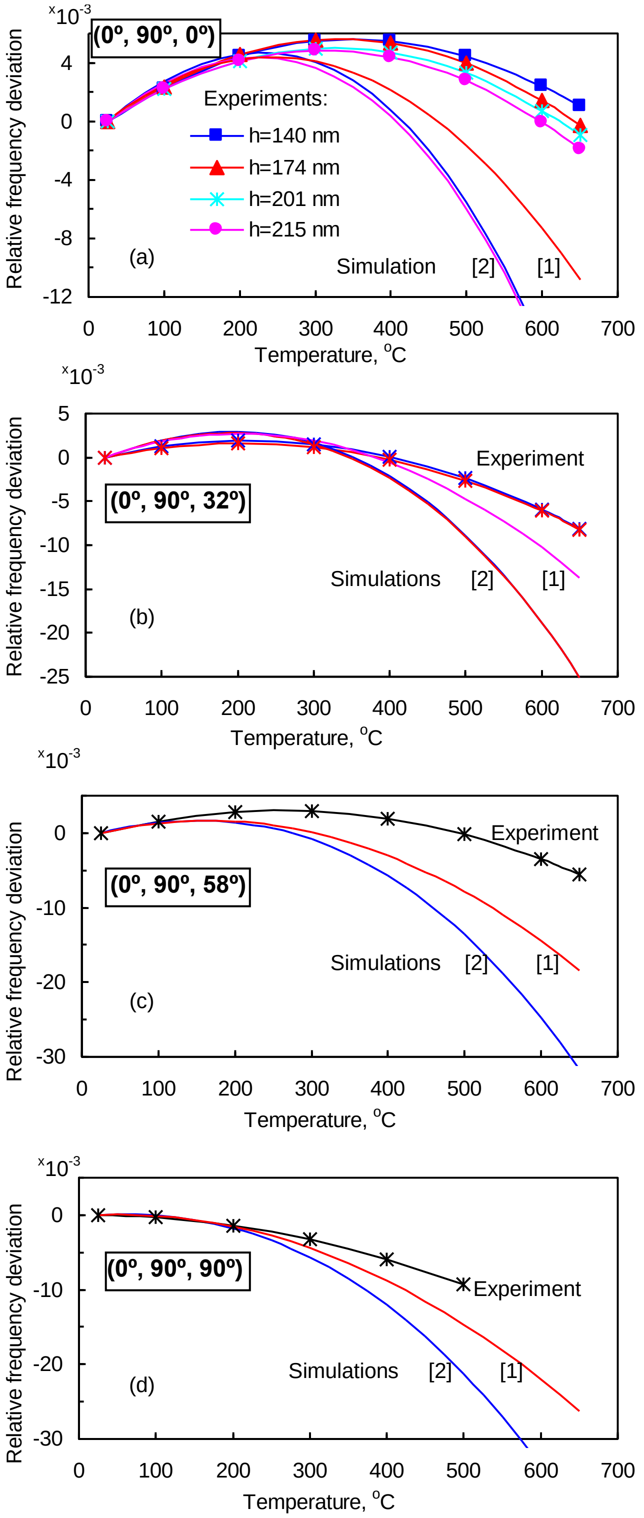

Fig. 3. Measured and simulated deviation of resonant frequency $\Delta f/f_0$ with temperature, for few propagation directions belonging to Y-cut of LGS: (a) (0º,90º,0º), (b) (0º,90º,32º), (c) (0º,90º,58º), (d) (0º,90º,90º). Simulations with two data sets are compared.

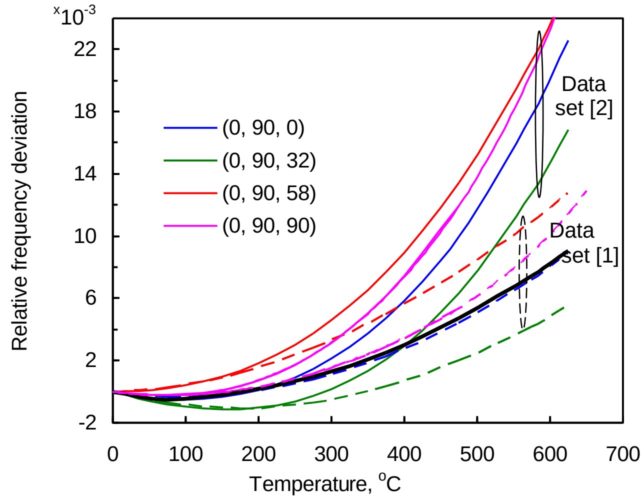

Fig. 4. Error in simulations of temperature deviation of frequency with two data sets, estimated as difference between simulated and measured $\Delta f/f_0$, in four orientations: (0º, 90º, 0º), (0º, 90º, 32º) , (0º, 90º, 58) , (0º, 90º, 90º). The average *error function* $\delta(T)$ has been determined for data set [1] (bold line).

The method of *after-correction* described above enables precise simulation of temperature characteristics of SAW resonators on LGS in a wide range of temperatures, up to 700°C, and can be applied to simultaneous optimization of LGS orientation and Ir thickness, to provide zero or required value of TCF, at fixed electrode thickness.

IV. Conclusion

The material constants reported in [1] were found to characterize the performance of SAW resonator on different cuts of LGS most adequately, in a wide temperature range from 25º to 700ºC. Though even with this data some difference between experimental and simulated temperature deviation of resonant frequency still exists, the agreement between simulation and experiment can be improved via after-correction of simulated dependences using the auxiliary *error function*. Such function was determined from comparison of simulated and measured characteristics of resonators built on Y-cut of LGS, with different propagation directions and then applied to predict the temperature behavior of resonator on LGS orientation with Euler angles (0º, 22º, 90º). Excellent agreement between simulation and experiment has been obtained.

Acknowledgment

This research has been performed under the SAWHOT coordinated project (partially funded by the Ministry of Education and Science of the Russian Federation).

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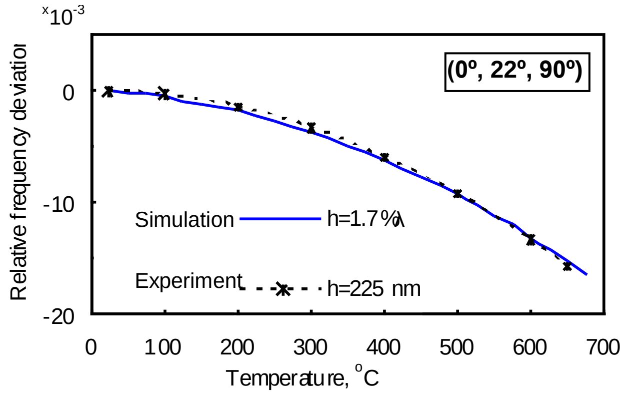

Fig. 5. Measured and simulated deviation of resonant frequency $\Delta f/f_0$ with temperature, for LGS cut (0º, 22º, 90º). Simulation was made with data set [1] and then corrected using the average *error function* $\delta(T)$ shown in Fig.4.

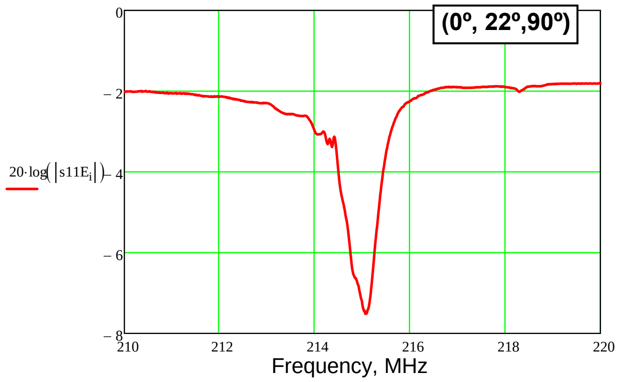

Fig. 6. Typical measured responses S11 of SAW resonators on LGS cut with Euler angles (0º, 22º, 90º).

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