

Extract Temperature Coefficients of LGS for High-Temperature Applications Based on the Finite Element Method [†]

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Abstract

Surface-acoustic-wave (SAW) sensors with Langasite (LGS) substrate have broad prospects in the field of wireless passive temperature sensing in harsh environments. However, there are still challenges in terms of accuracy regarding the material temperature coefficient of LGS and the temperature simulation of heavy mass load electrodes. This paper presents a method for fitting the material temperature coefficient of LGS based on a combination of finite element simulation (FEM) and measured data. Eleven different cuts of LGS SAW resonators were fabricated, and the frequency response of each cut device at 30–800 °C was obtained through experiments. Some of the data were used in the training dataset and the material temperature coefficient of LGS was obtained through comsol simulation fitting. The remaining data were used as a test dataset to verify the accuracy of the results. The results show that the material coefficient obtained using this method has good accuracy in the frequency prediction of thick electrode LGS SAW sensors at different temperatures with different cuts.

Keywords: surface acoustic wave; LGS; temperature–frequency characteristics; FEM simulation; data fitting; material temperature coefficient



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1. Introduction

Surface-acoustic-wave (SAW) sensors have the advantages of a simple structure, miniaturization, and wireless and multi-parameter integration, which give SAW sensors great potential for real-time monitoring of temperature, pressure, and other parameters in harsh environments. Langasite (LGS) is a new type of high-temperature piezoelectric material with a high melting point (1470 °C) and no phase transition from room temperature to melting point, which makes it an attractive material for the preparation of high-temperature SAW sensors. As early as 2013, the first commercial application of LGS SAW sensors above 800 °C emerged [1]. So far, LGS SAW has been able to read signals at up to 1300 °C [2].

In order to better simulate and predict the performance of the LGS SAW sensor at high temperature, considering properties such as its frequency variation, temperature sensitivity, and other indicators, higher requirements are put forward for the material temperature coefficient of LGS. Until now, the widely used temperature coefficient [3–5] has been suitable for scenarios involving temperatures below 300 °C, whereas it does not have good

accuracy for scenarios involving temperatures above 800 °C. In view of this, Nicolay et al. used the numerical calculation method [6] to fit the material temperature coefficient of LGS through the measured data. However, the numerical method for frequency calculation is only suitable for thin and small-density metal electrodes, such as aluminum, whose mass has little impact on frequency; for the large-thickness and high-density platinum electrode devices applied in high-temperature scenarios, the frequency calculation has a certain deviation. In addition, in the previous literature [7–10] on the methods that were commonly used for extracting temperature coefficients before this, the simulations of temperature coefficients were all based on numerical calculations, and the simulations based on the finite element method still need to be studied. Clearly, we need a precise method for predicting the temperature–frequency characteristics of thick-electrode saw devices across the entire range from room temperature to high temperature, as well as the corresponding material parameters.

To achieve this, this work proposes a method based on finite element simulation, which is used to fit the measured data to obtain the appropriate material parameters. And based on the obtained material parameters and the finite element model, we make predictions for other different cuts of LGS saw. We fabricate LGS devices (0, 138.5°, 0°) with 11 different cuts and measure the temperature–frequency curves from room temperature to 800 °C of each cut. Then, we build a three-dimensional (3D) model of the device in COMSOL 6.1, and select some measurement results as the training set to fit the material temperature coefficient of LGS using the simulated annealing algorithm. To prove the accuracy of this method, the remaining measurement results are used as the test set to evaluate the accuracy of the prediction results. The results show that the model established by us and the material parameters obtained through fitting have accuracy in predicting the temperature–frequency characteristics of LGS saws with different cuts.

2. Method

2.1. Device Design

First, we use the coupling-of-modes (COMs) model to design the saw resonator in different cuts. The COM model can take into account the second-order effects caused by electrodes, such as surface acoustic wave reflection, velocity change, and loss attenuation. The basic formula of this model is shown in the equation below:

$$\begin{aligned}\frac{\partial R(x)}{\partial x} &= -jk_E R(x) + jK_R S(x)e^{-2jk_0 x} + j\alpha_R V_t e^{-jk_0 x} \\ \frac{\partial S(x)}{\partial x} &= -jK_S R(x)e^{+2jk_0 x} + jk_E S(x) - j\alpha_S V_t e^{+jk_0 x} \\ \frac{\partial I(x)}{\partial x} &= +2j\alpha_S R(x)e^{+jk_0 x} + 2j\alpha_R S(x)e^{-jk_0 x} - jR_F V_t\end{aligned}\quad (1)$$

To obtain the temperature–frequency characteristics of as many modes as possible, we designed a saw resonator with two distinct Rayleigh mode resonant peaks using the COMs model. This was achieved by adjusting the gap between the reflectors and the IDTs, as shown in Figure 1a, changing it from the conventional 0.375λ to 0.5λ , where λ is the wavelength, so that both resonant peaks of the Rayleigh mode could be excited. The simulation results are shown in Figure 1b. Furthermore, since the first two Euler angles of the LGS substrate were fixed, we changed the third Euler angle by rotating the saw pattern on the substrate, as shown in Figure 1c. Since LGS belongs to the trigonal crystals and its third Euler angle is symmetrical about 90°, we chose a total of eleven angles (0, 138.5°, 0°, where $\theta = 14, 20, 27, 35, 44, 55, 63, 70, 80$, and 90) to design the device. It is worth noting that not all the 11 cuts were made in Rayleigh mode, and not all cuts can excite two Rayleigh mode resonant peaks. The special cuts are (0, 138.5°, 0°), (0, 138.5°, 27°), (0, 138.5°, 80°) and

(0, 138.5°, 90°). The first three cuts have only one single Rayleigh peak, while the last cut has only one single pure shear mode peak.

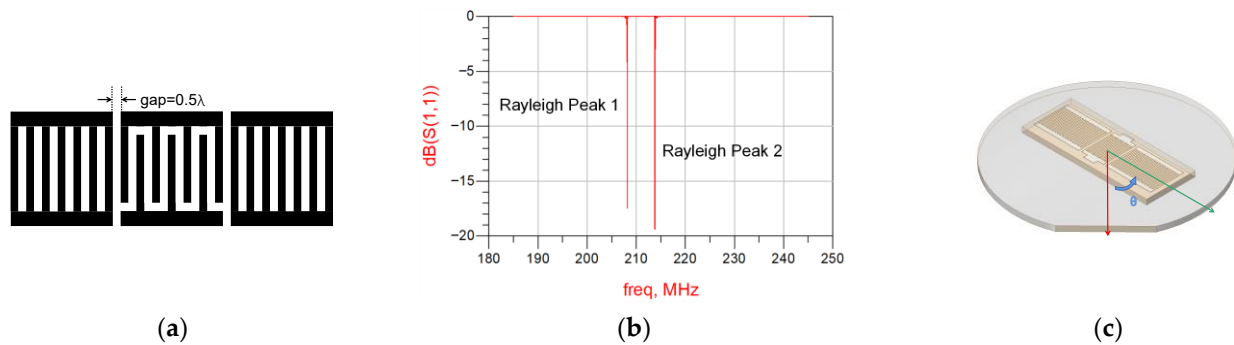


Figure 1. (a) The schematic diagram of the SAW resonator structure; (b) the S11 simulation result of SAW in (0, 138.5°, 55°) using the COM model, which shows two peaks of the Rayleigh mode; (c) the third Euler angle schematic diagram, where θ is the rotation angle of device on the substrate, which is also the third Euler angle.

2.2. Fabrication and Temperature Measurement

The fabrication process of the experimental LGS SAW resonator with Pt-Rh alloy electrodes is described in Figure 2a. The 4-inch (0, 138.5°, θ°) cut LGS wafer was first prepared according to the standard cleaning instructions. After cleaning, the wafer was coated with a negative photoresist, followed by ultraviolet exposure to transfer the pattern from the mask to the wafer after development. Then, a 10 nm adhesive layer Al_2O_3 and a 400 nm Pt-Rh electrode were successively deposited using magnetron sputtering. The film layer was patterned using the lift-off process. Finally, to prevent the agglomeration of Pt-Rh electrodes at high temperature, the entire wafer was deposited with 40 nm Al_2O_3 using magnetron sputtering as the passivation layer.

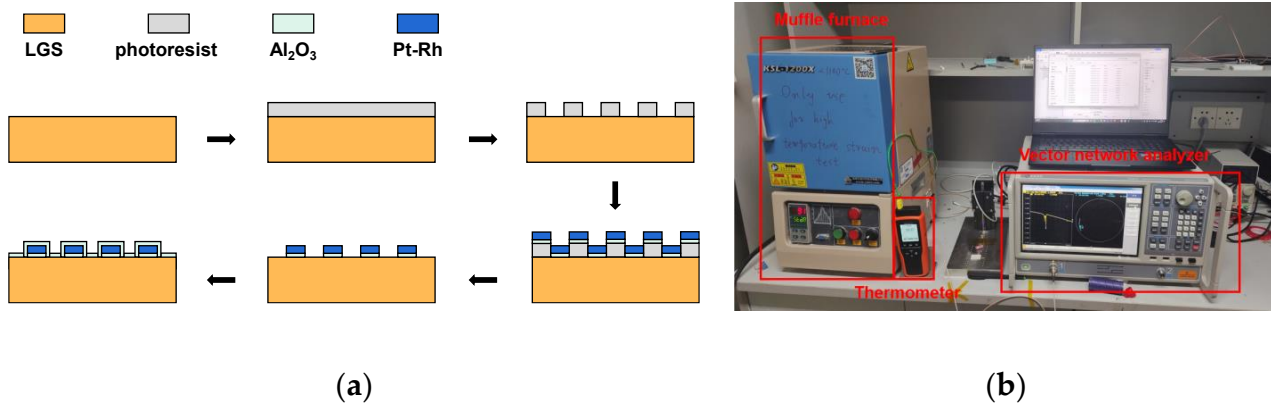


Figure 2. (a) The fabrication process of LGS high-temperature sensors with 11 different cuts; (b) a wired temperature measurement system composed of a Muffle furnace and a vector network analyzer.

The frequency response from room temperature to 800 °C was measured in a high-temperature Muffle furnace. SAW devices were fixed in the Muffle furnace (HEFEIKEJING Type: KSL-1100X-S, Hefei, China) by ceramic fixtures and led out through Pt-Rh alloy wires which connected to the external SMA wires, as shown in Figure 2b. Inside the Muffle furnace, thermocouples (Manufacturer: KAIPUSEN Type: CXCWX-T-K, Jiangsu, China) were placed beside SAW devices to observe the temperature in real time. The S11 parameters were recorded every 100 °C. We waited until the temperature was completely stable before recording each result to ensure the accuracy of the measurement. It is worth noting that

since SAW devices did not experience temperatures as high as 800 °C throughout the entire fabrication process, before the formal measurement, all SAW devices, including all the connections, underwent a pre-test to ensure that all parts of the entire system were stable.

2.3. Data and Fitting Process

As mentioned, among all eleven cuts, with the exception of 0°, 27°, 80° and 90°, there were two distinct Rayleigh peaks in the remaining seven cuts. The relationship between the resonant frequency and temperature is expressed by the fractional frequency change, as shown in the following equation:

$$\text{Fractional Frequency Change} = \frac{f(T_1) - f(T_0)}{f(T_0)} \times 100\% \quad (2)$$

The relationship between frequency or fractional frequency change and temperature can be fitted into a quadratic function, and the measured original data and fitting curves of all eleven different cut devices from room temperature to 800 °C are shown in Figures 3 and 4.

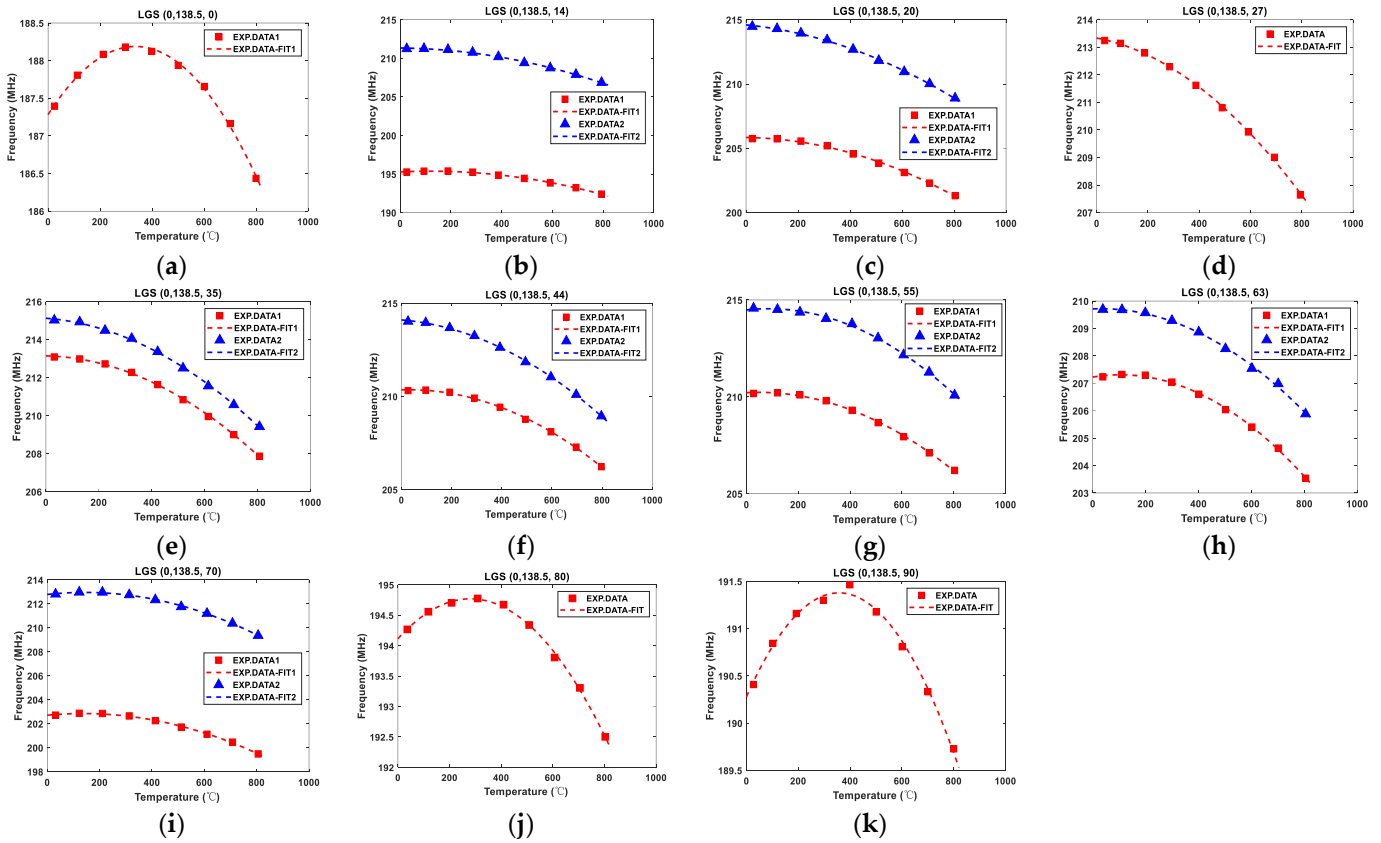


Figure 3. (a–k) The measured frequency of 11 devices from room temperature to 800 °C. The red squares represent the measured resonant peaks at lower frequencies and the red dotted lines represent the fitting curves of the resonant peaks at lower frequencies. The blue triangles represent the measured resonant peaks at higher frequencies and the blue dotted lines represent the fitting curves of the resonant peaks at higher frequencies.

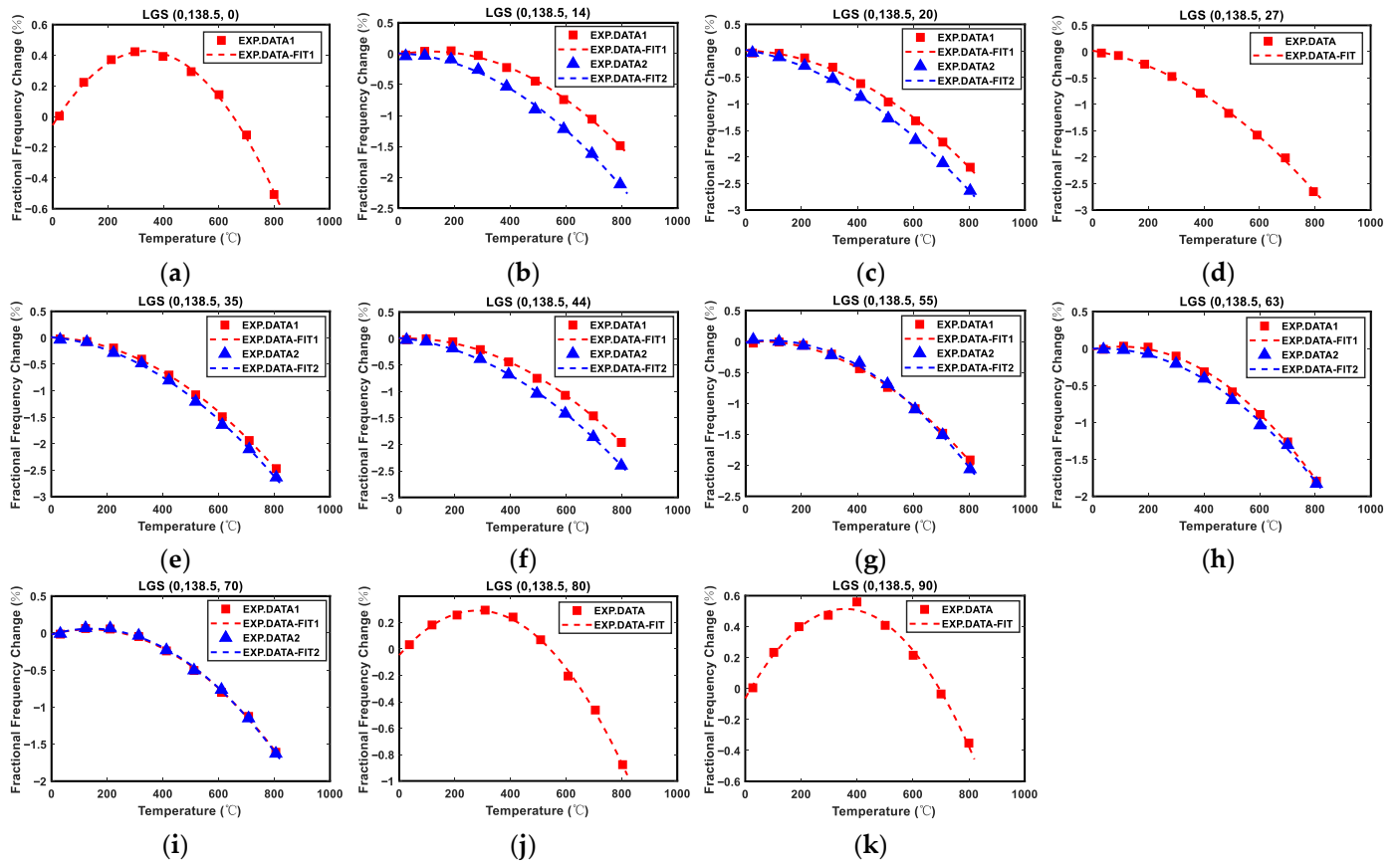


Figure 4. (a–k) The fractional frequency change of 11 devices from room temperature to 800 °C. The red squares represent the measured resonant peaks at lower frequencies, and the red dotted lines represent the fitting curves of the resonant peaks at lower frequencies, the blue triangles represent the measured resonant peaks at higher frequencies, and the blue dotted lines represent the fitting curves of the resonant peaks at higher frequencies.

All the data are classified. Here, the four cuts of 20°, 35°, 55° and 70° are selected as the training sets for LGS material parameters fitting. The remaining seven cuts, 0°, 14°, 27°, 44°, 63°, 80° and 90°, are used as test sets to evaluate the fitting parameters and the accuracy of the model.

The fitting process takes place as follows. First, we establish a 3D model of the SAW device in COMSOL, as shown in Figure 5a. Since all the resonant peaks have been clearly excited during the design of the device, in the finite element solution, only the eigenfrequency solution is needed instead of frequency domain scanning. In COMSOL, the model is solved once every 100 °C, and the obtained eigenfrequency is also fitted as a quadratic function of temperature. Thus, the measured results are compared with the simulation results to obtain an error value. To continuously iterate and obtain more accurate material parameters, we use the simulated annealing algorithm to generate the material parameters for the next simulation. This process is shown in Figure 5b. Specifically, to the material temperature coefficient TC_0 used in the first simulation, a relative value d_{TC} is randomly added or subtracted. The new value TC obtained is then input into the 3D model to be solved, thereby obtaining a new error value Z . This value is compared with the previous error value Z_0 . If Z is smaller, the cycle is further executed based on TC . If Z is larger, it is highly likely that the next round of the cycle will be based on TC_0 , but there is still a certain probability that the next round of the cycle will be based on TC . This is called the Metropolis acceptance criterion. This process is referred to as the classic simulated

annealing algorithm. When the error value keeps decreasing and eventually approaches convergence, the iterative process is stopped.

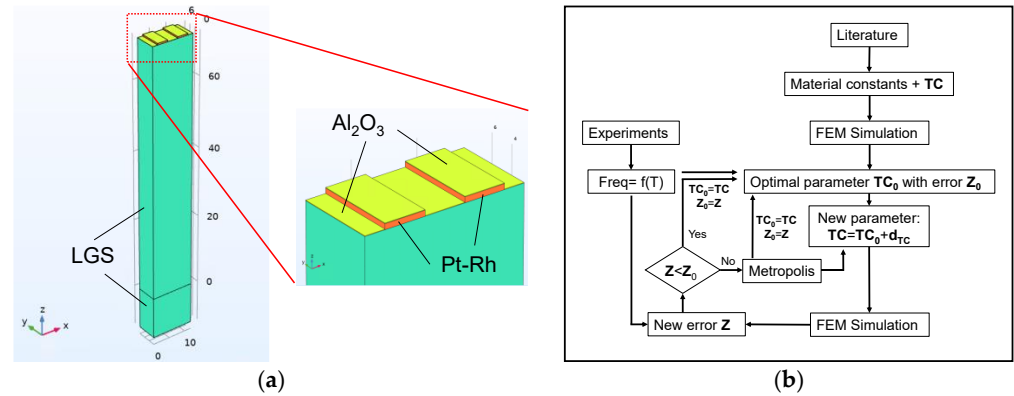


Figure 5. (a) Finite element models for intrinsic frequency simulation at different temperatures; (b) The simulated annealing process for fitting the temperature coefficient of materials of devices.

When fitting, the types of material temperature coefficients to be fitted need to be taken into consideration. For LGS, it has a total of six independent elastic coefficients, two independent piezoelectric coefficients, and two independent dielectric coefficients. The first-order and second-order temperature coefficients of each material coefficient need to be fitted to ensure the minimum error across the entire temperature range. However, for the thermal expansion coefficients of LGS and Pt-Rh, we did not take them into account in our study because the final error obtained by running them in the program was no smaller than that obtained without introducing these parameters. Therefore, ultimately through this process, we obtained a total of 20 new material temperature coefficients for LGS.

3. Results and Discussion

The entire program went through approximately 2000 iterations, taking a total of 65 h, which means each loop took about 120 s. When the process was terminated, we obtained the comparison results between simulation and measurement of the training sets that are shown in Figure 6a–h. For all training sets, the measurement results can be in good agreement with the simulation results.

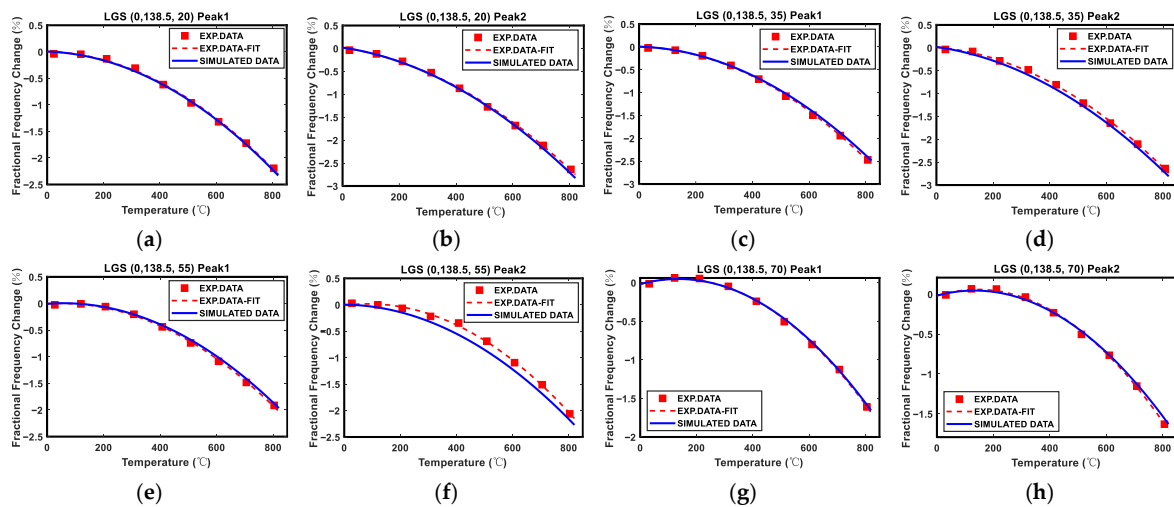


Figure 6. (a–h) The fractional frequency change of 4 devices as the training sets from room temperature to 800 °C. The red squares represent the measured resonant peaks and the red dotted lines represent the fitting curves of the resonant peaks, while the blue solid lines represent the simulation results.

To examine the accuracy of the temperature coefficients of these materials and the accuracy of the finite element simulation method, the remaining seven cuts were simulated using the obtained LGS material temperature coefficients, and the simulation results were compared with the test sets, as shown in Figure 7a–j. Although the cuts in the test sets were not included in advance, the established model can still simulate them quite well.

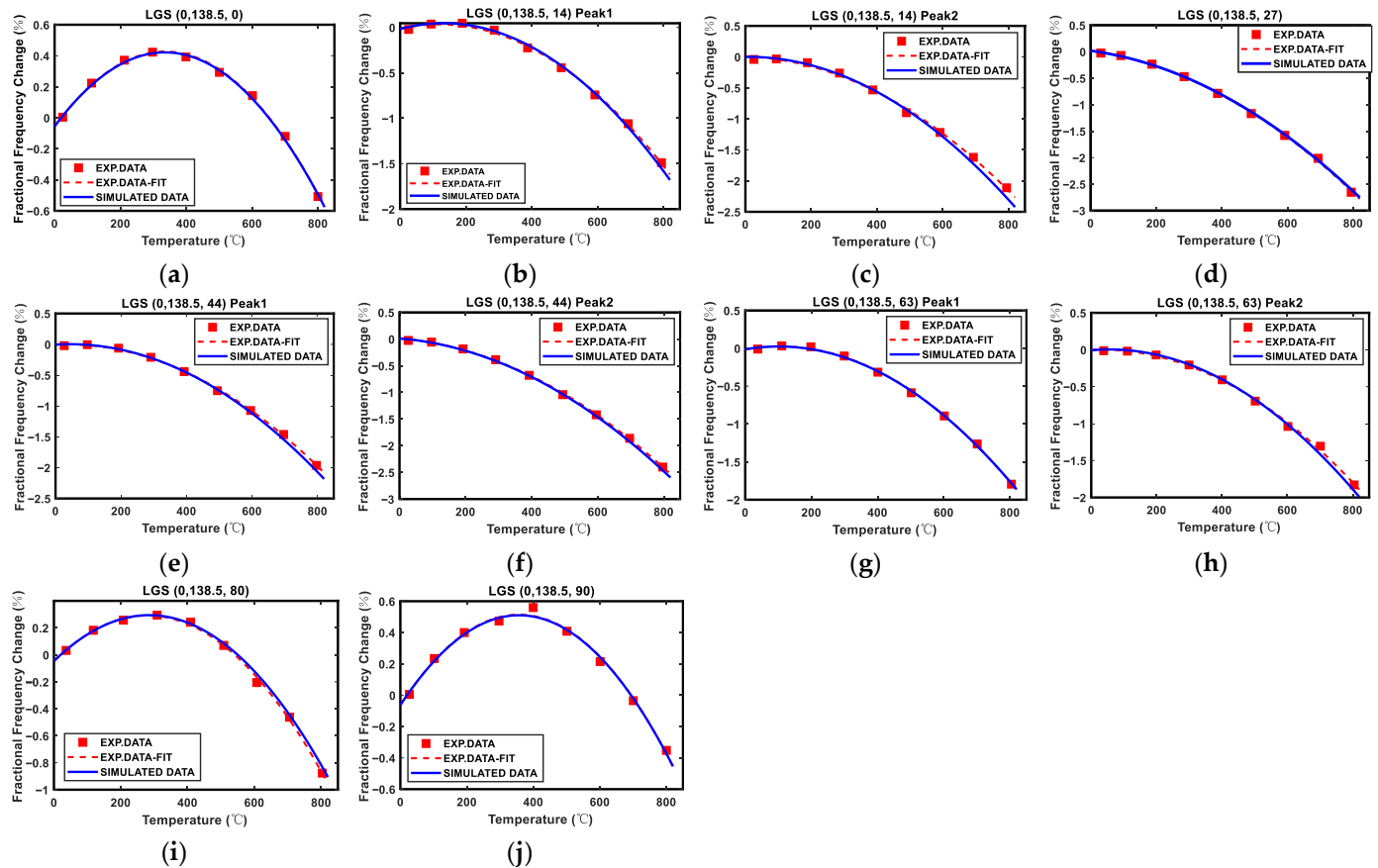


Figure 7. (a–j) The fractional frequency change of 7 devices as the test sets from room temperature to 800 °C. The red squares represent the measured resonant peaks and the red dotted lines represent the fitting curves of the resonant peaks. The blue solid lines represent the simulation results.

Finally, the common LGS material parameters in the literature [3,4,6] were introduced into the finite element simulation model. The obtained simulation results were compared with the simulation results obtained from our training and the measured results. The results are shown in Figure 8. Due to the overly large number of results, only the fractional frequency changes in the low-frequency resonant peak in each cut at 800 °C were selected for comparison. It can be seen that the simulation results obtained in this paper have the best agreement with the measured results. The LGS material parameters and temperature coefficients obtained in the model described in this paper are shown in Table 1. The basic material parameters of LGS are obtained from the literature [6]. It should be pointed out that during the fitting process, if the density of the material is also fitted as a temperature-related variable, the final simulation results obtained will never correspond well to the measured results. This might be related to the establishment of our model. We will continue to pay attention to this point in subsequent research.

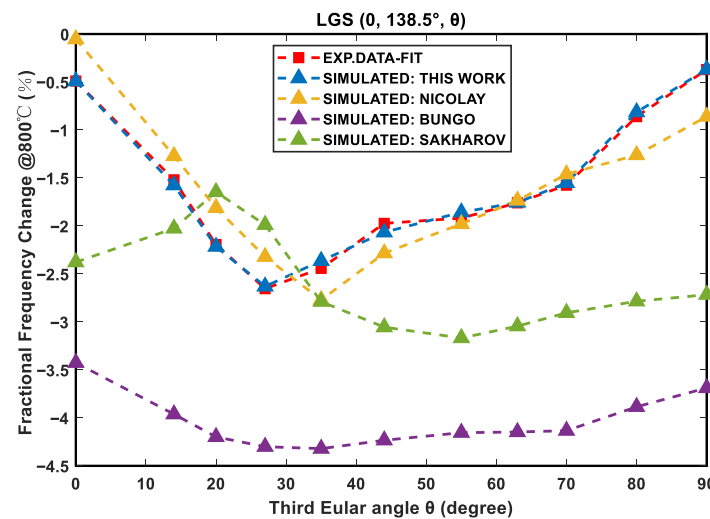


Figure 8. The fractional frequency change simulation results obtained by substituting the material temperature coefficients from different studies into the model at different cuts at 800 °C are compared with the measured results.

Table 1. LGS material parameters and temperature coefficients obtained by fitting.

	Material Constants [6] @ 20 °C	First Order (ppm/°C)	Second Order (ppb/°C)
c_{11} ($\times 10^{10}$ N/m ²)	18.89	−83.5	−38
c_{12} ($\times 10^{10}$ N/m ²)	10.42	−126.3	−23
c_{13} ($\times 10^{10}$ N/m ²)	10.15	−89.9	−78.4
c_{14} ($\times 10^{10}$ N/m ²)	1.44	−277.5	25.6
c_{33} ($\times 10^{10}$ N/m ²)	26.83	−107.3	−24.2
c_{44} ($\times 10^{10}$ N/m ²)	5.33	−42.4	−64.1
e_{11}	−0.4371	617.8	−356.9
e_{14}	0.1039	−866.3	1789.5
ϵ_{11}/ϵ_0	19.05	134.5	118
ϵ_{33}/ϵ_0	51.81	−787	685.6
ρ	5743		

4. Conclusions

We have developed a method that combines 3D finite elements with measured data and extracts the material temperature coefficient of the LGS SAW temperature sensor under thick or large-mass-load electrodes through the simulated annealing algorithm to accurately simulate the performance of LGS SAW temperature sensors in different cuts with high precision and a wide application range. This method precisely models the thick-electrode SAW resonator, taking into account the influence of the mass load on each resonant peak, which is ignored by the numerical calculation method. Through the optimized simulated annealing process, a more accurate material temperature coefficient of LGS is obtained. The measured data in each crystal cut indicate that the simulation results using the temperature coefficients we obtained are highly consistent with the actual frequency–temperature characteristics. Compared with the material coefficients of other studies, our method was almost twice as accurate for some cuts. Overall, the proposed method provides an effective model and precise LGS temperature coefficient for the design, calibration, and optimization of SAW temperature sensors in extreme environments.

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