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Calculation model for predicting temperature characteristics of quartz double-layered thickness-shear resonator

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1. Introduction

In recent years, semiconductor manufacturing has progressed to a higher degree of integration and more complex three-dimensional structures, and films such as insulating films have been required to be of high quality at the atomic level. In the atomic layer deposition (ALD) method,1) which is one of the film-forming methods, there is a demand for searching for the optimum temperature, including increasing the temperature, in order to obtain a high-quality film. In order to meet this requirement, the authors have been studying the realization of a thickness-shear resonator for monitoring film formation without temperature dependence by using a double-layered structure in which piezoelectric substrates are directly bonded. In the previous study, the temperature characteristics of the double-layered resonator are not simply weighted by the thickness ratio of the two layers, but the ratio of the electric flux density in each substrate is taken into consideration.2,3) However, in the case of bonding substrates with large anisotropy such as α-quartz crystal, the difference in acoustic impedance is large, so the results suggest that the influence of reflected waves at the bonding boundary cannot be ignored.4)

In this report, a prediction formula for controlling and designing the resonance frequency temperature characteristic of the double-layered resonator considering the influence of the reflected waves at the bonding boundary was examined and compared with experimental results.

2. Calculation model

Consider a double-layered structure in which a substrate with a positive temperature coefficient and a substrate with a negative temperature coefficient are bonded together at an appropriate thickness ratio x as shown in Fig. 1. The resonant frequency change df_{DL} of the double-layered resonator is represented by the following equation using a certain ratio R.

$$df_{\mathrm{DL}} = df_{\#1} \cdot R + df_{\#2} \cdot (1 - R), \tag{1}$$

where $df_{\#1}$ and $df_{\#2}$ are the resonant frequency changes of the #1 and #2 single substrates, respectively, normalized by the resonant frequency at the reference temperature. Model 1 is a model in which R is a simple thickness ratio x.

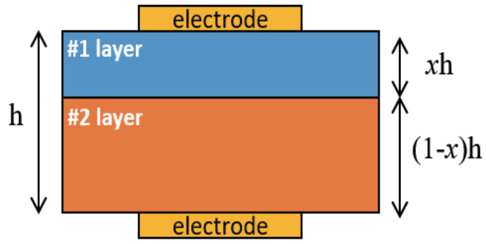

Fig. 1 Concept of double-layered resonator.

Model 2 is a model with the ratio R_{D1} of the electric flux density component [the product of strain and piezoelectric constant ($S'_6 \cdot e'_{26}$)] in each substrate, based on the previous study results for CTGS.3)

$$R_{D1} = \frac{S'_{6@\#1} \cdot e'_{26@\#1}}{S'_{6@\#1} \cdot e'_{26@\#1} + S'_{6@\#2} \cdot e'_{26@\#2}} \tag{2}$$

Here, the strain S' is represented by the sum of the strain in the thickness direction of each substrate.

As the third model to be newly constructed this time, we assumed a formula in which the ratio R_{S1}, which considered the influence of reflection at the bonding boundary, to the total amount of strain in each substrate (Model 3).

$$R_{s1} = \frac{S'_{6@\#1}(A_1)}{S'_{6@\#1}(A_1) + S'_{6@\#2}(A_2)}, \tag{3}$$

$$A_1 = A_0 \{1 + R_{12} \cdot \cos(\Delta \phi_1)\}, \tag{4}$$

$$A_2 = A_0 \{1 + R_{21} \cdot \cos(\Delta \phi_2)\}, \tag{5}$$

$$R_{ij} = \frac{Z_j - Z_i}{Z_j + Z_i}, \tag{6}$$

where A_0 is the standing wave amplitude when there is no reflected wave at the boundary, R_{ij} is the reflection coefficient of the wave incident from medium i to medium j, $\Delta\phi$ is the phase shift due to the propagation path difference, and A_1 and A_2 are amplitudes at #1 and #2 layers, Z_i indicates the acoustic impedance of medium i.

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3. Experiment and Discussion

Taking α-quartz (QZ) as a sample, 129.55°*Y*-cut QZ substrate (#1 layer) with negative temperature characteristics and *Y*-cut (0°*Y*-cut) QZ substrate (#2 layers) with positive temperature characteristics were selected. The designed thickness ratio x was calculated based on Eq. (1) so that the temperature characteristics would be the minimum frequency changes. In the calculations, material constants and temperature coefficients of α-quartz were used from the reference.5) The thickness ratio of the actual sample was x=0.520. Au/Cr cross electrodes with a width of 2 mm were formed on the upper and lower surfaces of the sample. Using an impedance analyzer (HP4294A), the temperature characteristics of the resonance frequency were measured for this sample at 100-300°C.

Fig. 2 shows the measurement results for the first resonance mode. The calculation results of Model 1, Model 2, and Model 3 are also shown. In the previous results for CTGS,3) the calculated results of Model 2 and the experimental values were in good agreement, but the discrepancy was large in the case of the double-layered quartz resonator. Also, the deviation from the experimental value is larger in the result of Model 2 than in the result of Model 1. On the other hand, it matched well with the Model 3 results.

In addition, analysis by the finite element method (FEM) was also performed at three points of 100, 200, and 300°C, and plotted in Fig. 2. It was found that the temperature characteristics analyzed by FEM tended to be similar to the experimental results. For confirmation, the thickness direction distribution of the particle displacement at the center of the resonator calculated by FEM was compared with that calculated by Model 3 considering the amplitude change due to the reflected wave at the bonding boundary obtained by Eqs. (4) and (5). The results were shown in Fig. 3. Both calculation results are almost the same exhibiting a large amplitude on the #1 layer side, where the acoustic impedance is small, and a small amplitude on the #2 layer side. From this result, it can be seen that the magnitude of the particle displacement distribution inside the resonator changes due to the reflection at the bonding boundary, and as a result, Model 3 was validated.

4. Summary

A computational model was constructed to predict the temperature characteristics of a double-layered resonator using α-quartz. It was demonstrated that the temperature characteristics of the double-layered resonator can be expressed not by the electric flux density ratio but by the total strain amount ratio, which takes into account the influence of the reflected wave. We also demonstrated that the particle displacement distribution inside the resonator predicted by this new computational model agrees with that calculated by FEM.

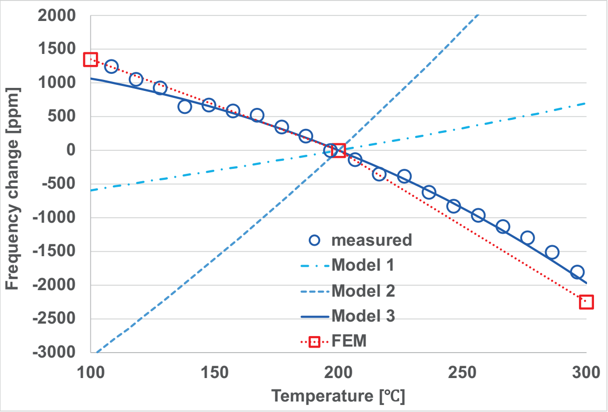

Fig. 2 Comparison of measured resonance frequency temperature characteristics and calculated values for the double-layered resonator (x=0.520).

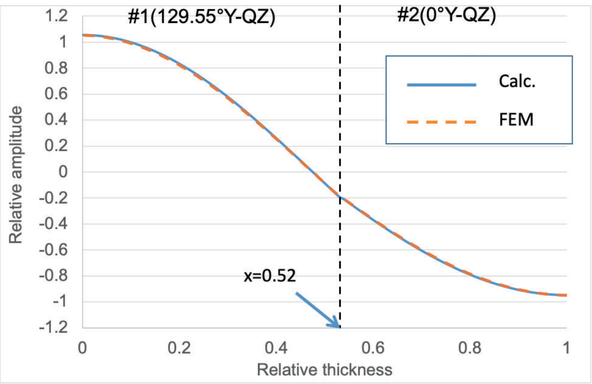

Fig. 3 Comparison of calculated results of particle displacement distribution inside the double-layered resonator.

References

1) S. I. Boyadjiev, V. Georgieva, R. Yordanov, Z. Raicheva, and I. M. Szilágyi, Appl. Surf. Sci., **387**, 1230 (2016).
2) Y. Owada, Y. Ohashi et al, Jpn. J. Appl. Phys, **59**, SKKC03 (2020).
3) Y. Ohashi, Y. Owada et al., Proc. IEEE Trans. UFFC, **69**, 870 (2022).
4) T. Noguchi, Y. Ohashi, et al., JJAP **61**, SG1055 (2022).
5) B. J. James, Proc. IEEE 42nd Freq. Cont. Symp. 146 (1988).