Acoustical Physics, Vol. 47, No. 4, 2001, pp. 415–418. Translated from Akusticheskiĭ Zhurnal, Vol. 47, No. 4, 2001, pp. 485–488.

Thermal Stabilization of SAW Devices by Metal Films

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Received March 23, 2000

Abstract—The characteristics of surface acoustic waves (SAW) propagating in a structure that consists of a metal layer overlying an YX-cut quartz crystal are numerically analyzed for a wide range of operating temperatures. It is shown that the presence of a metal film of a certain thickness on the surface of an YX-cut quartz crystal considerably improves the thermal stability of the characteristics of SAW propagating in such a structure. *© 2001 MAIK "Nauka/Interperiodica".*

Piezoelectric quartz crystals represent one of the most popular materials used in the SAW technology. These crystals have been extensively studied both theoretically and experimentally and exhibit a high thermal stability of their properties [1]. It was found that some cuts of quartz crystals and some directions in them are characterized by a zero first-order temperature coefficient of delay ($TCD^{(1)}$) of SAW (e.g., the ST,X-cut of the quartz crystal) or by a close-to-zero value of this coefficient (e.g., the AT,X-cut of the quartz crystal [2]). One of the main technical characteristics in the SAW technology is the sensitivity of the thermally stable direction of the crystal to changes in the external temperature. However, in the aforementioned cuts of the quartz crystal, the thermal stability of SAW is observed in only a narrow interval of operating temperatures near room temperature (t_0 = 25°C). The second-order temperature coefficient of delay ($TCD^{(2)}$) of SAW propagating in these crystal cuts is relatively high: $TCD^{(2)} \approx 32 \times 10^{-9}$ 1/°C^2 for the ST,X-cut and $TCD^{(2)} \approx 28.4 \times 10^{-9}$ 1/°C^2 for the AT,X-cut.

This paper presents a theoretical study of the SAW characteristics in a structure consisting of a metal layer overlying an YX-cut quartz substrate in a wide range of operating temperatures t.

As a result of numerical calculations, we determined the materials of the film and the values of the film thickness for which a thermal stabilization of SAW is achieved in a wide temperature range. For example, in the structure consisting of an aluminum film with thickness $h = 0.061\lambda$ (λ is the SAW wavelength) and an YX-cut quartz crystal, the relative variation of the SAW delay time $\Delta\tau/\tau_0$ [3] in the temperature interval from –60 to +60°C was 2.5 times smaller than in the well-known ST,X-cut quartz.

Let us first discuss the conditions for which we perform the numerical analysis of the properties of SAW in a film–substrate system. In the presence of an isotropic metal film of a finite thickness on the surface of a piezoelectric crystal, we will consider the problem on the SAW propagation in the structure that consists of an isotropic layer overlying a piezoelectric substrate. In this case, we use the system of equations of the theory of elasticity in combination with the electrostatic equation [4]:

$$\rho^{(m)}\frac{\partial^2 u_i^{(m)}}{\partial \tau^2} = \frac{\partial T_{ij}^{(m)}}{\partial x_j}; \quad \operatorname{div} D^{(m)} = 0. \qquad (1)$$

Here, T_{ij} is the elastic stress tensor, u_i represents the mechanical displacements, D is the electric displacement vector, $\rho^{(m)}$ represents the densities of the film and substrate materials, τ is time, and x_j are the coordinates. The subscripts are $i, j = 1, 2, 3$; the superscript takes the values $m = 1$ and 2 to indicate the film and substrate materials, respectively.

Using the method described in [4, 5], we developed an algorithm and a program for the numerical calculation of the main characteristics (the velocity V_l, the displacement amplitudes u_i, etc.) of SAW propagating in a structure formed by a metal film and a YX-cut quartz substrate; we carried out numerical analysis of the temperature characteristics ($TCD_l^{(1)}$, $TCD_l^{(2)}$, and $\Delta\tau/\tau_0$) of SAW propagating in these structures for a wide range of operating temperatures. In our calculations, we took into account the following factors: the temperature dependences of the quartz material constants C_{ijkl}, e_{ijk}, and ε_{ij}; the thermal expansion of the crystal [2]; the temperature dependences of the crystal density ρ and the density of the layer material ρ_l; the temperature dependences of the Lamé elastic constants of the isotropic layer; the thermal expansion of the film; the variation of the film thickness h with temperature [3]; and the presence of the initial thermal internal stresses in the layered structure due to the difference between the

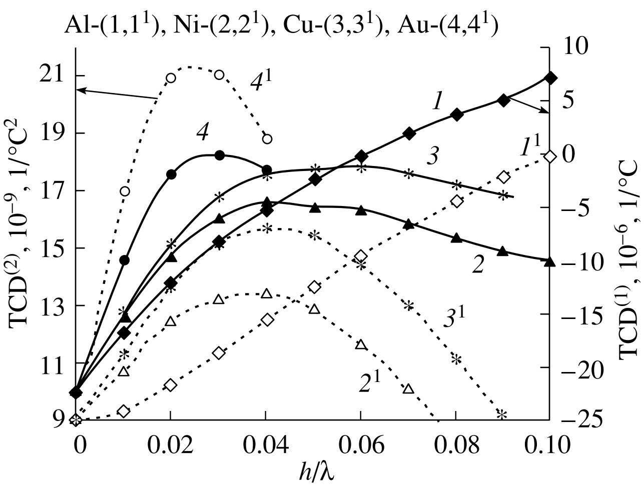

Fig. 1. Dependences of the coefficients $TCD_l^{(1)}$ (solid curves) and $TCD_l^{(2)}$ (dotted curves) of SAW on the relative layer thickness for different metal films on the surface of a YX-cut quartz crystal: (*1*, *1*¹) Al, (*2*, *2*¹) Ni, (*3*, *3*¹) Cu, and (*4*, *4*¹) Au.

coefficients of thermal expansion of the film and substrate materials [6, 7].

The temperature coefficients of delay, $TCD_l^{(1)}$ and $TCD_l^{(2)}$, of SAW propagating in the layered structure can be calculated by the formulas [2, 8]

$$TCD_l^{(1)} = \frac{1}{\tau_0(t_0)}\frac{d\tau_l}{dt}\bigg|_{t_0} = \alpha_{11}^{(1)} - TCV_l^{(1)}, \qquad (2)$$

$$TCD_l^{(2)} = \frac{1}{2}\frac{1}{\tau(t_0)}\frac{d^2\tau_l}{dt^2}, \qquad (3)$$

where τ_l and τ_0 are the SAW delay times in the layered structure at the operating and room temperatures, respectively; $TCV_l^{(1)}$ is the temperature coefficient of velocity for SAW propagating in the layered structure [2]; and $\alpha_{11}^{(1)}$ is the coefficient of thermal expansion of the crystal in the direction of wave propagation.

If the film thickness h is much smaller than the substrate thickness H, we can assume that, as the operating temperature t varies, the substrate length varies in one or another direction and the film length also varies. This process should be accompanied by a variation of the film thickness h [3].

To calculate the dependence of the SAW delay time τ_l on the temperature t in the layered structure, we can use the Taylor series expansion of τ_l near the room temperature t_0:

$$\tau_l(t) = \tau_0(t_0) + \frac{d\tau_l}{dt}\bigg|_{t_0}(t-t_0) + \frac{1}{2}\frac{d^2\tau_l}{dt^2}\bigg|_{t_0}(t-t_0)^2 + \dots . \qquad (4)$$

If we neglect the higher orders in Eq. (4), we can represent the relative variation of the SAW delay time $\Delta\tau/\tau_0 = (\tau_l - \tau_0)/\tau_0$ in the form

$$\frac{\tau_l - \tau_0}{\tau_0} = TCD_l^{(1)}(t-t_0) + TCD_l^{(2)}(t-t_0)^2. \qquad (5)$$

As one can see from Eqs. (2)–(5), to calculate the temperature characteristics of SAW in the layered structure, it is necessary first to solve the system of equations (1) from which one can determine the velocity V_l of SAW in the layered structure for different values of the film thickness and for different operating temperatures t.

According to [8], YX-cut quartz exhibits no thermal stability of the SAW characteristics. For example, at room temperature, the first-order temperature coefficients of delay of SAW take the following values: $TDC^{(1)} = -22 \times 10^{-6}$ 1/°C 1 for a free surface and $TCD_m^{(1)} = -22.3 \times 10^{-6}$ 1/°C for a coated (i.e., covered with an infinitely thin metal film whose mass is negligibly small) surface. A metal film of finite thickness h (with a finite mass) covering the surface of an YX-cut quartz crystal can noticeably change the SAW velocity (making it smaller or greater, depending on the temperature characteristics of the film and substrate materials), and at some value of the thickness h, it can improve the temperature characteristics of SAW propagating in the structure.

Figure 1 shows the calculated dependences of $TCD_l^{(1)}$ and $TCD_l^{(2)}$ of SAW on the ratio h/λ for different film materials: aluminum (Al), gold (Au), copper (Cu), and nickel (Ni) at room temperature. One can see that, when the surface of a YX-cut quartz crystal is covered with an aluminum layer of thickness $h = 0.061\lambda$, the value of $TCD_l^{(1)}$ becomes zero (curve *1*). The corresponding value of $TCD_l^{(2)}$ is 14.8×10^{-9} 1/°C² (curve *1*¹). A nickel layer (curve *2*) of thickness $h/\lambda = 0.045$ reduces the absolute value of $TCD^{(1)}$ to -4.5×10^{-6} 1/°C but does not compensate it totally (i.e., to zero); the corresponding value of $TCD_l^{(2)}$ is 13×10^{-9} 1/°C² (curve *2*¹). A copper layer (curve *3*) with $h/\lambda = 0.05$ provides an almost total compensation of $TCD^{(1)}$; in this case, $TCD_l^{(2)} = 15.5 \times 10^{-9}$ 1/°C² (curve *3*¹). A gold layer provides a compensation of $TCD^{(1)}$ at $h/\lambda = 0.028$

(curve *4*); in this case, $TCD_l^{(2)} = 21 \times 10^{-9}$ 1/°C² (curve *4*¹).

It can be shown that, for a free surface of an YX-cut quartz crystal, the calculated dependence of the relative variation of the delay time $\Delta\tau/\tau_0$ given by Eq. (5) on the temperature *t* (within the interval –60 to +60°C) is linear, and the value of the relative variation of the delay time varies over wide limits. For example, at t = –60°C, we have $\Delta\tau/\tau_0 = 1942 \times 10^{-6}$ and, at t = +60°C, $\Delta\tau/\tau_0 = -767 \times 10^{-6}$.

Figure 2 presents the calculated temperature dependences of the relative variation of the delay time $\Delta\tau/\tau_0$ of SAW and the temperature dependences of $TCD_l^{(1)}$ (*t* varies from –60 to +60°C) for different materials of the film covering the surface of the YX-cut quartz crystal. All dotted lines in the figure represent $TCD_l^{(1)}$, and all solid lines represent $\Delta\tau/\tau_0$ of SAW. From Fig. 2, one can see that the aluminum film ($h/\lambda = 0.061$) provides a thermal stabilization of the YX-cut quartz crystal ($TCD_l^{(1)} = 0$) at room temperature (curve *1*¹). In addition, in such a structure, the range of variation of the quantity $\Delta\tau/\tau_0$ (curve *1*) within the temperature interval from –60 to +60°C is much smaller (at t = –60°C, we have $\Delta\tau/\tau_0 = 81 \times 10^{-6}$ and, at t = +60°C, $\Delta\tau/\tau_0 = 21 \times 10^{-6}$) than in the case of a free surface of YX-cut quartz. From Fig. 2 it also follows that gold films with h/λ = 0.028 (curves *2*, *2*¹), nickel films with h/λ = 0.045 (curves *4*, *4*¹), and copper films with h/λ = 0.05 (curves *3*, *3*¹), when deposited on the surface of an YX-cut quartz crystal, also provide a thermal stabilization of SAW in the crystal and reduce the value of $\Delta\tau/\tau_0$ of SAW in a wide temperature range from –60 to +60°C.

In contrast to a free YX-cut quartz crystal, the presence of a metal film of a certain thickness on its surface leads to a thermal stabilization of the characteristics of SAW propagating in the resulting layered structure. For example, in the structure consisting of an aluminum film with h/λ = 0.061 and a YX-cut quartz substrate, we obtain $TCD_l^{(1)} = 0.03 \times 10^{-6}$, 1/°C and $TCD_l^{(2)} = 14.87 \times 10^{-9}$ 1/°C². The corresponding values of other parameters are as follows: velocity V_l = 3.162 km/s, power flux angle [9] pfa = 0°, anisotropy coefficient γ = 0.62, and electromechanical coupling coefficient [9] K^2 = 0.185%.

When the crystal surface is loaded with a film of a finite thickness, not only the temperature characteristics but also the velocity of SAW propagating in this structure undergo some changes. It is of interest to consider the changes that occur in the SAW velocity when the surface of the YX-cut quartz crystal is covered with a metal film of finite thickness.

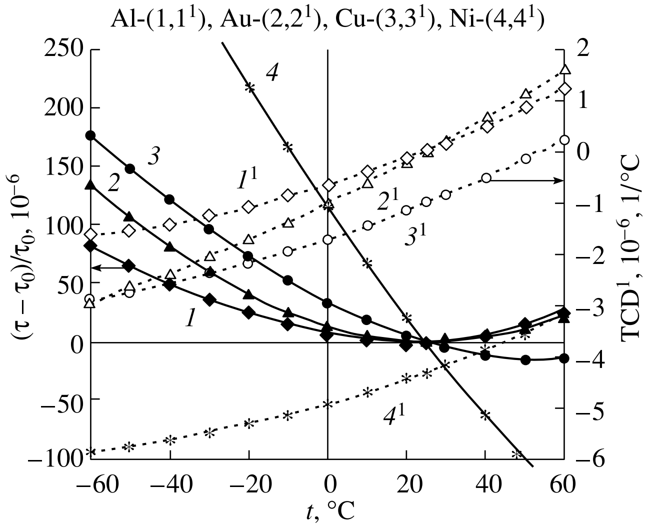

Fig. 2. Temperature dependences of the relative variation of the delay time $\Delta\tau/\tau_0$ (solid curves) and the coefficient $TCD_l^{(1)}$ (dotted curves) of SAW for different films deposited on the surface of a YX-cut quartz crystal: (*1*, *1*¹) Al film with h/λ = 0.061, (*2*, *2*¹) Au with h/λ = 0.028, (*3*, *3*¹) Cu with h/λ = 0.05, and (*4*, *4*¹) Ni with h/λ = 0.045.

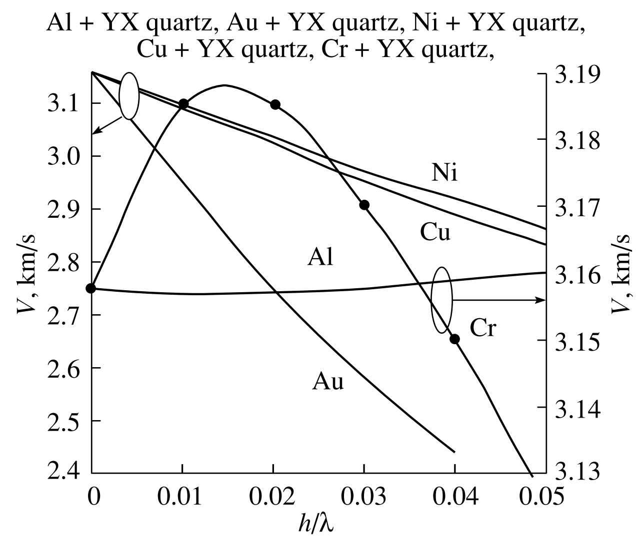

Fig. 3. Dependences of the SAW velocity on the relative layer thickness in the structures: Al film + YX-cut SiO_2; Au film + YX-cut SiO_2; Ni film + YX-cut SiO_2; Cu film + YX-cut SiO_2; and Cr film + YX-cut SiO_2.

Figure 3 presents the dependences of the SAW velocity on the ratio h/λ in the structures: Al film + YX-cut quartz, Au film + YX-cut quartz, Ni film + YX-cut quartz, Cu film + YX-cut quartz, and Cr film + YX-cut quartz. One can see that, unlike Al and Cr films, the copper (Cu), nickel (Ni), and, especially, gold (Au) films effectively reduce the velocity of SAW in the film–crystal structure. For example, in the presence of a gold film whose thickness is equal to 0.01λ, the SAW velocity in the structure decreases from 3.1605 to 2.945 km/s. This result is explained by the fact that the velocity of the slow shear bulk wave in gold is much lower than the velocity of the shear bulk wave in YX-cut quartz. We note that, if the velocity of the shear bulk wave in the film material is much higher than in the substrate, only one surface acoustic wave can exist in the layered structure. The existence of this wave is possible only in a limited range of values of h/λ [4]. When the velocity of the shear bulk wave in the layer material is close to that in the substrate material, the dependence of the SAW velocity in the layered structure on the ratio h/λ can exhibit an anomalous behavior, i.e., local maximums and minimums [10]. This effect is observed in the case of chromium film (see Fig. 3).

The crystal cut and the direction of the SAW propagation are usually described by three Eulerian angles (ϕ, θ, Ψ) [4]. Numerical calculations showed that a thermal stabilization of SAW by thin metal films is possible not only for YX-cut quartz (with the Eulerian angles (0°, 90°, 0°)), but also for other orientations of the quartz crystal, namely, the orientations with the second Eulerian angle θ falling either within the interval 10°–40° or 90°–120° (while the two other angles are $\phi = \Psi = 0°$).

Thus, our numerical experiment shows how a thin metal (Al, Au, Cu, or Ni) film covering the surface of an YX-cut quartz crystal affects the main characteristics of SAW. For different metal films covering the surface of a YX-cut quartz crystal, we determined the thickness values with which it is possible to considerably improve the thermal stability of SAW propagating in such structures in a wide temperature range.

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Translated by E. Golyamina