



## Short Communication

## Extended temperature dependence of elastic constants in cubic crystals

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## ABSTRACT

To extend the theory of the temperature dependence of the elastic constants in cubic crystals beyond the second- and third-order elastic constants, the fourth-order elastic constants, as well as the non-linearity in the thermal expansion temperature dependence, have been taken into account. Theoretical results were represented as temperature functions of the effective elastic constants and compared with experimental data for a number of cubic crystals, such as alkali metal halides, and elements gold and silver. The relations obtained give a more accurate description of the experimental temperature dependences of second-order elastic constants for a number of cubic crystals, including deviations from linear behavior. A good agreement between theoretical estimates and experimental data has been observed.

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## 1. Introduction

For most crystals, the typical temperature behavior of the second-order elastic constants (SOEC) is a decrease as temperature increases with an insignificant dependence at low temperatures. Such temperature dependences, especially at room temperatures, are important for solid-state physics and applications of crystals, in designing effective devices such as sensors and resonators. One more attractive task is the calculation the temperature-stable crystalline cuts for crystals or complex layered structures, where abnormal SOEC temperature dependences arise. Recall that SOEC temperature dependences feature anharmonicity. The study of the temperature dependence of elastic constants for crystals was provided in Refs. [1–13]. In Ref. [1], the temperature dependences of elastic constants for Si, Ge, and fused silica were measured by an ultrasonic method. Existing theories of the SOEC temperature dependences are based on the Debye model, taking into account the anharmonicity of atomic lattice vibrations. For the correct description of the temperature dependences over a wide temperature range, the temperature dependence of the phonon number was included in these considerations. However the relations obtained are too complicated. A simpler theory based on small-amplitude bulk acoustic wave (BAW) propagation in crystals under the influence of finite bias fields, has been derived in Sorokin et al. [14] to explain the linear SOEC temperature dependences in cubic crystals. First-order temperature coefficients of

the elastic constants have been obtained, taking into account the SOEC and third-order elastic constants (TOEC), as well as linear thermal dilatation. A satisfactory agreement between calculated and experimental results for a number of cubic crystals has been achieved. A study of the linear temperature coefficients for trigonal, hexagonal, and tetragonal crystals was reported in [15].

A similar method of calculation has been used in Ref. [16] for the temperature dependence of the resonant frequency in quartz piezoelectric resonators. Nevertheless, such approaches should only be applied in quantifying the linear temperature dependence. Hence extending the relations obtained earlier is necessary to improve concordance between theoretical and experimental data on the SOEC temperature dependences for a broad temperature band.

The main objective of this paper is to expand the theory describing the temperature dependence of the elastic constants in cubic crystals up to non-linear behavior by incorporating the fourth-order elastic constants (FOEC), as well as the non-linearity of the thermal expansion temperature dependence.

## 2. Temperature dependence of elastic constants

In the BAW propagation theory for crystals subjected to temperature changes, geometrical and physical non-linearities in the elastic media must both be taken into account (Aleksandrov et al. [17]). The first leads to the dilatation of crystalline specimen, distorting its shape and, therefore, changing the path of the acoustic wave. The second leads to a weakening in chemical bonds between

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atoms as a result of thermal expansion usually producing a decrease in the macroscopic elastic constants of a crystal. The modified Green–Christoffel equation for elastic waves of small amplitude in a uniformly deformed elastic medium, referred to as the initial (natural) state, can be written as [17]:

$$[\Gamma_{BC}(\bar{\eta}) - \rho_0 v^2 \delta_{BC}] \tilde{U}_B = 0, \quad (1)$$

where  $\Gamma_{BC}(\bar{\eta})$  is the effective Green–Christoffel tensor,  $\delta_{BC}$  the Kröner delta,  $\rho_0$  the density of the crystal in the undisturbed state,  $v$  the phase velocity, and  $\tilde{U}_B$  the BAW polarization unit vector; Latin indices vary from 1 to 3. For a mechanically free sample, the static deformation arising as a result of thermal expansion can be written as:

$$\bar{\eta}_{PQ} = \alpha_{PQ}^* \Delta T, \quad (2)$$

where  $\alpha_{PQ}^*$  is the effective tensor of the temperature expansion, and  $\Delta T$  the temperature variation. Here the effective tensor of the thermal expansion will be used in the form:

$$\alpha_{FC}^* = \alpha_{FC} + \beta_{FC} \Delta T, \quad (3)$$

where  $\alpha_{FC}$  is the linear, and  $\beta_{FC}$  the non-linear coefficients of expansion. We take the effective elastic constants as:

$$C_{ABCD}^* = C_{ABCD} + C_{ABCDPQ} \bar{\eta}_{PQ} + \frac{1}{2} C_{ABCDPQMM} \bar{\eta}_{PQ} \bar{\eta}_{MN} + \dots, \quad (4)$$

where  $C_{ABCD}$ ,  $C_{ABCDEF}$ , and  $C_{ABCDEFGH}$  are the second-, third- and fourth-order elastic constants, respectively. The small difference between isentropic and isothermal elastic constants is neglected. The solutions to Eq. (1) are taken in conventional form as plane elastic waves in the continuum approximation. Taking into account the Green–Christoffel's tensor in the form as obtained earlier [17], and the relations (2)–(4), one can present a new view of the Green–Christoffel tensor:

$$\Gamma_{BC}(\Delta T) = \bar{C}_{FC} C_{ABFD}^* N_A N_D = \bar{C}_{FC} N_A N_D \times \left[ C_{ABFD} + C_{ABFDPQ} \alpha_{PQ}^* \Delta T + \frac{1}{2} C_{ABFDMNPQ} \alpha_{PQ}^* \alpha_{MN}^* (\Delta T)^2 \right]. \quad (5)$$

Here  $N_A$  are the components of the unit vector associated with the direction of wave propagation. Under thermal expansion of a mechanically free crystal, Green's tensor for static finite deformation will be written as:

$$\bar{C}_{FC} = \delta_{FC} + 2\bar{\eta}_{FC} = \delta_{FC} + 2\alpha_{FC}^* \Delta T, \quad (6)$$

where  $\bar{\eta}_{FC}$  is the tensor of static deformations.

Taking into account only the terms proportional to  $(\Delta T)$  and  $(\Delta T)^2$ , one obtains:

$$\Gamma_{BC}(\Delta T) = \{ C_{ABCD} + (2C_{ABPD} \delta_{CQ} + C_{ABCDPQ}) \alpha_{PQ} \Delta T + [(2C_{ABPD} \delta_{CQ} + C_{ABCDPQ}) \beta_{PQ} + (2C_{ABMDPQ} \delta_{CN} + C_{ABCDPQMN}) \alpha_{PQ} \alpha_{MN}] (\Delta T)^2 \} N_A N_D. \quad (7)$$

Solutions of Eq. (1) in the form (7) for chosen BAW modes in certain special directions gives us the temperature dependence of their velocities and then the SOEC temperature coefficients. The symmetry of the TOEC and FOEC for cubic crystals was given in Refs. [18,19].

For example, let us consider a cubic crystal, where the acoustic waves along the propagation direction [100] are excited. In this case, the Green–Christoffel tensor should be written in a diagonal form:

$$\Gamma_{BC}(\Delta T) = \begin{pmatrix} \Gamma_{11}(\Delta T) & 0 & 0 \\ & \Gamma_{22}(\Delta T) & 0 \\ & & \Gamma_{22}(\Delta T) \end{pmatrix}, \quad (8)$$

where

$$\Gamma_{11} = C_{11} + (2C_{11} + C_{111} + 2C_{112}) \alpha_{11} \Delta T + [2\beta_{11} C_{11} + 2\alpha_{11}^2 (C_{111} + 2C_{112}) + \beta_{11} (C_{111} + 2C_{112}) + 1/2 \alpha_{11}^2 (C_{1111} + 4C_{1112} + 2C_{1122} + 2C_{1123})] (\Delta T)^2, \quad (9)$$

$$\Gamma_{22} = C_{44} + (2C_{44} + C_{144} + 2C_{155}) \alpha_{11} \Delta T + [2\beta_{11} C_{44} + 2\alpha_{11}^2 (C_{144} + 2C_{155}) + \beta_{11} (C_{144} + 2C_{155}) + 1/2 \alpha_{11}^2 (C_{1144} + 4C_{1155} + 2C_{1255} + 2C_{1266})] (\Delta T)^2. \quad (10)$$

The eigenvalues of the tensor, Eq. (8), are  $\lambda_1 = \rho_0 v_L^2 = \Gamma_{11}(\Delta T)$  for pure longitudinal acoustic wave, and  $\lambda_2 = \lambda_3 = \rho_0 v_S^2 = \Gamma_{22}(\Delta T)$  for pure shear acoustic waves. The directions of the shear wave polarizations are both perpendicular to vector  $\mathbf{N}$ . (9) and (10) can be used to obtain the first- and second-order temperature coefficients for the  $C_{11}$  and  $C_{44}$  elastic constants. To calculate the coefficients for the  $C_{12}$  elastic constant, a BAW propagation along the [110] direction needs to be considered.

We note that in Shrivastava [12] an additional contribution from a phonon-lattice interaction (or phonon pressure) was invoked to explain the anomalous temperature dependence of the  $C_{12}$  elastic constant in NaCl-like structures of alkali halide crystals. The effective elastic constants under isotopic phonon pressure can be written as

$$\begin{aligned} C_{11}^* &= C_{11} - P_{\text{phonon}}, \\ C_{12}^* &= C_{12} + P_{\text{phonon}}, \\ C_{44}^* &= C_{44} - P_{\text{phonon}}. \end{aligned} \quad (11)$$

Hence, the temperature dependence of the elastic constants in the Shrivastava model can be presented as:

$$\begin{aligned} \frac{dC_{11}^*}{dT} &= \frac{dC_{11}}{dT} - \frac{dP_{\text{phonon}}}{dT}, \\ \frac{dC_{12}^*}{dT} &= \frac{dC_{12}}{dT} + \frac{dP_{\text{phonon}}}{dT}, \\ \frac{dC_{44}^*}{dT} &= \frac{dC_{44}}{dT} - \frac{dP_{\text{phonon}}}{dT}, \\ \frac{dP_{\text{phonon}}}{dT} &= (C_{11} + 2C_{12}) \alpha_{11}. \end{aligned} \quad (12)$$

### 3. Comparison of theoretical and experimental results

Assuming that the components of linear and nonlinear elastic constants are the temperature independent parameters, the temperature dependences of effective elastic constants can be calculated exploiting the expressions of the Green–Christoffel's tensor eigenvalues. For example, writing the eigenvalue (9) as:

$$\lambda_1(\Delta T) = C_{11} + TC_{11} \times \Delta T + T^2 C_{11} \times (\Delta T)^2 = C_{11} + \Delta C_{11}, \quad (13)$$

where  $TC_{11} = dC_{11}/dT$ , and  $T^2 C_{11} = d^2 C_{11}/dT^2$  and taking into account the results of BAW propagation along both [100] and [110] directions by following [14], a complete set of expressions for the temperature coefficients for SOEC of cubic crystals is obtained:

$$\begin{aligned} TC_{11} &= (2C_{11} + C_{111} + 2C_{112}) \alpha_{11}, \\ T^2 C_{11} &= (2C_{11} + C_{111} + 2C_{112}) \beta_{11} + (2C_{111} + 4C_{112} + 1/2 C_{1111} + 2C_{1112} + C_{1122} + C_{1123}) \alpha_{11}^2, \\ TC_{44} &= (2C_{44} + C_{144} + 2C_{155}) \alpha_{11}, \\ T^2 C_{44} &= (C_{44} + C_{144} + 2C_{155}) \beta_{11} + (2C_{144} + 4C_{155} + 1/2 C_{1144} + C_{1155} + 2C_{1255} + C_{1266}) \alpha_{11}^2, \\ TC_{12} &= (2C_{12} + C_{123} + 2C_{112}) \alpha_{11}, \\ T^2 C_{12} &= (2C_{12} + C_{123} + 2C_{112}) \beta_{11} + (C_{111} + 4C_{112} + C_{123} + C_{1112} + C_{1122} + 5/2 C_{1123}) \alpha_{11}^2. \end{aligned} \quad (14)$$

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