Invariant Elastic Constants for Crystals

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1. Introduction. The stress-strain relations, for an elastic solid, in an arbitrary Cartesian frame of reference, are

$$(1) \quad \sigma_{ij} = C_{ijkm} e_{km}, \quad (i, j, k, m = 1, 2, 3),$$

where σ_{ij} are the components of the stress tensor, e_{km} , the strain tensor and C_{ijkm} , the elastic constants. On making an arbitrary orthogonal coordinate transformation from an unprimed to a primed system, the stress-strain relations take the form

$$(2) \quad \sigma'_{pq} = C'_{pqrs} e'_{rs}, \quad (p, q, r, s = 1, 2, 3).$$

The elastic constants in the two frames of reference are connected by the relations

$$(3) \quad C'_{pqrs} = \alpha_{pi} \alpha_{qj} \alpha_{rk} \alpha_{sm} C_{ijkm},$$

where α_{pi} 's are the elements of the transformation matrix.

In general, C_{ijkm} are 81 constants. However, since C_{ijkm} , as we know from the theory of elasticity [1], satisfy the conditions

$$(4) \quad C_{ijkm} = C_{jikm} = C_{ijmk} = C_{kmi j},$$

the number of constants reduces from 81 to 21 which corresponds to the most asymmetric elastic solid, *viz.*, triclinic crystals. For the case of crystals with higher symmetry, the number of constants can be reduced further, the exact number being dependent on the symmetries present in the crystal. This is achieved by setting $C'_{pqrs} = C_{pqrs}$ in (3) and admitting *only those coordinate transformations* for which the atomic arrangement in the crystal will appear exactly the same to observers in those coordinate systems. These are all well known facts.

The relations (1) are form-invariant, but the elastic constants, C_{ijkm} , change their values under arbitrary orthogonal coordinate transformations; also, the number of constants, required to specify the elastic properties of a crystal, changes from coordinate system to coordinate system. These two aspects are not very satisfactory as will be evident from the following consideration.

In the case of isotropic elastic solids, the stress-strain relations in an unprimed and primed systems are, respectively,

$$(5) \quad \sigma_{ij} = \lambda \delta_{ij} e_{rr} + 2\mu e_{ij},$$

$$(6) \quad \sigma'_{pq} = \lambda \delta_{pq} e'_{rr} + 2\mu e'_{pq}.$$

We see that the values of the Lamé constants λ and μ which appear in (5) and (6) do not depend on the choice of the coordinate system.

In a recent paper [3] Thomas has obtained invariant elastic constants λ , μ and α for cubic crystals similar to Lamé constants for isotropic solids. He has proposed the following expression

$$(7) \quad C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \alpha \nu_{ai} \nu_{aj} \nu_{ak} \nu_{al},$$

where ν_{ai} are the components of the unit vectors $\mathbf{v}_a$ ($a = 1, 2, 3$) which represent the crystallographic directions in an arbitrary Cartesian system. (The crystallographic axes represent in direction and magnitude the three non-parallel edges of the unit cell of a crystal. The unit vectors along these three axes are referred to as crystallographic directions, [2].) The stress-strain relations in an unprimed and primed systems are, respectively,

$$(8) \quad \sigma_{ij} = \lambda \delta_{ij} e_{rr} + 2\mu e_{ij} + \alpha e_{km} \nu_{ai} \nu_{aj} \nu_{ak} \nu_{am},$$

$$(9) \quad \sigma'_{pq} = \lambda \delta_{pq} e'_{rr} + 2\mu e'_{pq} + \alpha e'_{rs} \nu'_{ap} \nu'_{aq} \nu'_{ar} \nu'_{as},$$

where ν_{ai} and ν'_{ap} are the components of $\mathbf{v}_a$ in the unprimed and primed systems respectively. It should be emphasized that the *same* elastic constants appear in (8) and (9), whereas the elastic constants which appear in (1) and (2) depend on the choice of axes. The formulation of the stress-strain relations in the form (8) gives the theory of cubic crystals in the elastic domain a status comparable to that of classical or isotropic theory of elasticity. It is, therefore, appropriate to call λ , μ and α the universal constants for the cubic crystals.

In the present paper, a formulation in which the number of elastic constants and their values do not depend on the choice of the coordinate system is proposed, thereby carrying through in the case of all other crystal classes the programme initiated by Thomas for cubic crystals. In §2, we discuss the structure of second (χ^{ij}), third (d^{ijk}) and fourth (C^{ijkl}) rank tensors which represent some property of the crystal, in respect to their dependence on the crystallographic directions and certain scalars. These scalars which characterize some property of the crystal do not change their values under *arbitrary* orthogonal coordinate transformations as the tensor components. The scalars are expressed as the inner product of two tensors, one of which is the tensor property of the crystal (say, C^{ijkl}) and the other the product of the type $\nu_{ai} \nu_{bj} \nu_{ck} \nu_{dl}$. In §3, we obtain expressions for C_{ijkl} in the case of various crystal classes in terms of their *universal constants*. This is achieved by keeping the *coordinates* fixed and transforming only the *vectors* $\mathbf{v}_a$ ($a = 1, 2, 3$) according to the symmetries present in the crystal. In §4, the stress-strain relations for hexagonal crystals are given.

The ideas developed in §2 are useful in finding the invariant dielectric constants, piezo-electric and photo-elastic coefficients.

2. Tensors and their structure. We consider an arbitrary Cartesian frame of reference xyz . (The results obtained in §2 can be modified to obtain their validity in coordinate systems which are not necessarily rectangular.) For simplicity, we start with a second rank tensor whose components χ^{ij} represent a physical property, like thermal conductivity, magnetic permeability, electrical susceptibility, of a crystal. Let $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$ denote the crystallographic directions and $\mathbf{v}^1, \mathbf{v}^2, \mathbf{v}^3$ the corresponding reciprocal set satisfying the relations

$$(10) \quad \nu_i^a \nu_a^j = \delta_i^j, \quad \nu_i^a \nu_b^i = \delta_b^a \quad \begin{matrix} (a, b = 1, 2, 3) \\ (i, j = 1, 2, 3) \end{matrix}.$$

We now construct a set of scalars, nine in number, from the tensors χ^{ij} and $\nu_i^a \nu_j^b$ in the form

$$(11) \quad A^{ab} = \nu_i^a \nu_j^b \chi^{ij},$$

where a summation is implied by the repeated indices i and j over the values 1, 2 and 3, and a and b are *not* tensor indices. The fact that A^{ab} are scalars can be verified by making an arbitrary orthogonal coordinate transformation from an unprimed to a primed system.

The relations (11) can be inverted by multiplying both sides by $\nu_a^k \nu_b^m$ and making use of (10) and we obtain

$$(12) \quad \chi^{ij} = \nu_a^i \nu_b^j A^{ab}, \quad (a, b = 1, 2, 3),$$

where there is summation over a and b . This is the unique resolution of χ on the triad $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$. Since we are working in Cartesian frames of reference, there is no distinction between contravariant and covariant indices and hence we write (12) as

$$(13) \quad \chi_{ij} = \nu_{ai} \nu_{bj} A_{ab}.$$

The above idea can be extended to third and fourth rank tensors. In the case of a third rank tensor, a set of 27 scalars are constructed from the tensors d^{ijk} and $\nu_i^a \nu_j^b \nu_k^c$ in the form

$$(14) \quad A^{abc} = \nu_i^a \nu_j^b \nu_k^c d^{ijk}.$$

Inverting (14) we obtain

$$(15) \quad d_{ijk} = \nu_{ai} \nu_{bj} \nu_{ck} A_{abc}.$$

Similarly corresponding to a fourth rank tensor we have 81 scalars and they are constructed from the tensors C^{iklm} and $\nu_i^a \nu_j^b \nu_k^c \nu_l^d$ in the form

$$(16) \quad A^{abcd} = \nu_i^a \nu_j^b \nu_k^c \nu_l^d C^{iklm}.$$

The inverse relation of (16) is

$$(17) \quad C_{ikm} = \nu_{ai}\nu_{bj}\nu_{ck}\nu_{dm}A_{abcd}.$$

3. Invariant elastic constants. We are now interested in the fourth rank tensor whose components C_{ikm} represent the elastic constants of the crystal. Using the conditions (4) in (17), we obtain the same relation

$$(18) \quad C_{ikm} = \nu_{ai}\nu_{bj}\nu_{ck}\nu_{dm}A_{abcd},$$

but with only 21 constants which correspond to the most asymmetric crystal system, *viz.*, the triclinic system for which $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ are not mutually orthogonal. The scalars A_{abcd} in (18) are the 21 invariant elastic constants for the triclinic crystal. It is possible, from (18), to obtain expressions in the case of crystals belonging to other systems by imposing the various point group symmetries on C_{ikm} . This is done by keeping the *coordinates* unchanged and transforming only the *vectors* $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ according to the symmetries present in the crystal; whereas in dealing with the elastic symmetry it has been customary to transform co-ordinates.

Monoclinic system. In monoclinic crystals $\mathbf{v}_1$ and $\mathbf{v}_2$ will be separated by an arbitrary angle (different from 90° or 120°) and the angles between $\mathbf{v}_2$ and $\mathbf{v}_3$, and $\mathbf{v}_3$ and $\mathbf{v}_1$ will be 90° each. Then, $\mathbf{v}_3$ will be a two-fold axis of rotation. A rotation of 180° about $\mathbf{v}_3$ will take $\mathbf{v}_1$ to $-\mathbf{v}_1$ and $\mathbf{v}_2$ to $-\mathbf{v}_2$. The invariance of C_{ikm} in (18) under this change leads to the vanishing of eight constants A_{1333} , A_{2333} , A_{3111} , A_{3222} , A_{1123} , A_{1213} , A_{2231} and A_{2321} . Denoting the remaining constants by λ_1 , λ_2 , $\dots$, λ_{13} , respectively, in order, we obtain

$$(19) \quad \begin{aligned} C_{ikm} = & \lambda_1 \nu_{1i} \nu_{1j} \nu_{1k} \nu_{1m} + \lambda_2 \nu_{2i} \nu_{2j} \nu_{2k} \nu_{2m} + \lambda_3 \nu_{3i} \nu_{3j} \nu_{3k} \nu_{3m} \\ & + \lambda_4 (\nu_{1i} \nu_{1j} \nu_{2k} \nu_{2m} + \nu_{1k} \nu_{1m} \nu_{2i} \nu_{2j}) \\ & + \lambda_5 (\nu_{1i} \nu_{1k} \nu_{2j} \nu_{2m} + \nu_{1j} \nu_{1m} \nu_{2i} \nu_{2k} + \nu_{1i} \nu_{1m} \nu_{2j} \nu_{2k} + \nu_{1j} \nu_{1k} \nu_{2i} \nu_{2m}) \\ & + \lambda_6 (\nu_{2i} \nu_{2j} \nu_{3k} \nu_{3m} + \nu_{2k} \nu_{2m} \nu_{3i} \nu_{3j}) \\ & + \lambda_7 (\nu_{2i} \nu_{2k} \nu_{3j} \nu_{3m} + \nu_{2j} \nu_{2m} \nu_{3i} \nu_{3k} + \nu_{2i} \nu_{2m} \nu_{3j} \nu_{3k} + \nu_{2j} \nu_{2k} \nu_{3i} \nu_{3m}) \\ & + \lambda_8 (\nu_{3i} \nu_{3j} \nu_{1k} \nu_{1m} + \nu_{3k} \nu_{3m} \nu_{1i} \nu_{1j}) \\ & + \lambda_9 (\nu_{3i} \nu_{3k} \nu_{1j} \nu_{1m} + \nu_{3j} \nu_{3m} \nu_{1i} \nu_{1k} + \nu_{3i} \nu_{3m} \nu_{1j} \nu_{1k} + \nu_{3j} \nu_{3k} \nu_{1i} \nu_{1m}) \\ & + \lambda_{10} (\nu_{1i} \nu_{2j} \nu_{2k} \nu_{2m} + \nu_{2i} \nu_{1j} \nu_{2k} \nu_{2m} + \nu_{2i} \nu_{2j} \nu_{1k} \nu_{2m} + \nu_{2i} \nu_{2j} \nu_{2k} \nu_{1m}) \\ & + \lambda_{11} (\nu_{2i} \nu_{1j} \nu_{1k} \nu_{1m} + \nu_{1i} \nu_{2j} \nu_{1k} \nu_{1m} + \nu_{1i} \nu_{1j} \nu_{2k} \nu_{1m} + \nu_{1i} \nu_{1j} \nu_{1k} \nu_{2m}) \\ & + \lambda_{12} (\nu_{3i} \nu_{3j} \nu_{1k} \nu_{2m} + \nu_{3j} \nu_{3j} \nu_{1m} \nu_{2k} + \nu_{3k} \nu_{3m} \nu_{1i} \nu_{2j} + \nu_{3k} \nu_{3m} \nu_{1j} \nu_{2i}) \\ & + \lambda_{13} (\nu_{3i} \nu_{3k} \nu_{1j} \nu_{2m} + \nu_{3j} \nu_{3k} \nu_{1m} \nu_{2j} + \nu_{3j} \nu_{3m} \nu_{1i} \nu_{2k} + \nu_{3j} \nu_{3m} \nu_{1k} \nu_{2i}) \\ & + \nu_{3i} \nu_{3m} \nu_{1j} \nu_{2k} + \nu_{3i} \nu_{3m} \nu_{1k} \nu_{2j} + \nu_{3j} \nu_{3k} \nu_{1i} \nu_{2m} + \nu_{3j} \nu_{3k} \nu_{1m} \nu_{2i}), \end{aligned}$$

where λ_1 , λ_2 , $\dots$, λ_{13} are the 13 invariant elastic constants for the monoclinic crystal.

Orthorhombic system. In orthorhombic crystals $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ will be mutually orthogonal and each one of them is a two-fold axis of rotation. C_{ijkm} in (18) should be invariant under 180° rotation about each one of $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ individually. These symmetry conditions lead to the vanishing of 12 constants A_{1222} , A_{1333} , A_{2333} , A_{2111} , A_{3111} , A_{3222} , A_{1123} , A_{1213} , A_{2231} , A_{2321} , A_{3312} and A_{3132} . The remaining 9 constants are denoted by λ_1 , λ_2 , $\dots$, λ_9 , respectively, in order, and we have

$$\begin{aligned}
 (20) \quad C_{ijkm} = & \lambda_1 \nu_{1i} \nu_{1j} \nu_{1k} \nu_{1m} + \lambda_2 \nu_{2i} \nu_{2j} \nu_{2k} \nu_{2m} + \lambda_3 \nu_{3i} \nu_{3j} \nu_{3k} \nu_{3m} \\
 & + \lambda_4 (\nu_{1i} \nu_{1j} \nu_{2k} \nu_{2m} + \nu_{1k} \nu_{1m} \nu_{2i} \nu_{2j}) \\
 & + \lambda_5 (\nu_{1i} \nu_{1k} \nu_{2j} \nu_{2m} + \nu_{1j} \nu_{1m} \nu_{2i} \nu_{2k} + \nu_{1i} \nu_{1m} \nu_{2j} \nu_{2k} + \nu_{1j} \nu_{1k} \nu_{2i} \nu_{2m}) \\
 & + \lambda_6 (\nu_{2i} \nu_{2j} \nu_{3k} \nu_{3m} + \nu_{2k} \nu_{2m} \nu_{3i} \nu_{3j}) \\
 & + \lambda_7 (\nu_{2i} \nu_{2k} \nu_{3j} \nu_{3m} + \nu_{2j} \nu_{2m} \nu_{3i} \nu_{3k} + \nu_{2i} \nu_{2m} \nu_{3j} \nu_{3k} + \nu_{2j} \nu_{2k} \nu_{3i} \nu_{3m}) \\
 & + \lambda_8 (\nu_{3i} \nu_{3j} \nu_{1k} \nu_{1m} + \nu_{3k} \nu_{3m} \nu_{1i} \nu_{1j}) \\
 & + \lambda_9 (\nu_{3i} \nu_{3k} \nu_{1j} \nu_{1m} + \nu_{3j} \nu_{3m} \nu_{1i} \nu_{1k} + \nu_{3i} \nu_{3m} \nu_{1j} \nu_{1k} + \nu_{3j} \nu_{3k} \nu_{1i} \nu_{1m}),
 \end{aligned}$$

where λ_1 , λ_2 , $\dots$, λ_9 are the 9 invariant elastic constants for the orthorhombic crystal.

Tetragonal system. (i) *Classes 4, $\bar{4}$, and $4/m$.* In the case of tetragonal crystals also $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ are mutually orthogonal and they satisfy the relations

$$(21) \quad \nu_{ai} \nu_{aj} = \delta_{ij}.$$

One of them (say) $\mathbf{v}_3$ is a four-fold axis of rotation. A rotation of 90° about $\mathbf{v}_3$ will take $\mathbf{v}_1$ to $\mathbf{v}_2$ and $\mathbf{v}_2$ to $-\mathbf{v}_1$. Invariance of C_{ijkm} in (18) under this change results in the vanishing of 10 constants A_{1333} , A_{2333} , A_{3111} , A_{3222} , A_{1123} , A_{1213} , A_{2231} , A_{2321} , A_{3312} and A_{3132} . We also obtain the following conditions

$$\begin{aligned}
 (22) \quad A_{1111} &= A_{2222}, & A_{2233} &= A_{3311}, \\
 A_{2323} &= A_{3131}, & A_{1222} &= -A_{2111}.
 \end{aligned}$$

Thus, the number of constants is reduced to 7. Making use of (22) and (21) we obtain

$$\begin{aligned}
 (23) \quad C_{ijkm} = & \lambda_1 \delta_{ij} \delta_{km} + \lambda_2 (\delta_{ij} \delta_{jm} + \delta_{im} \delta_{jk}) + \lambda_3 (\nu_{1i} \nu_{1j} \nu_{1k} \nu_{1m} + \nu_{2i} \nu_{2j} \nu_{2k} \nu_{2m}) \\
 & + \lambda_4 \nu_{3i} \nu_{3j} \nu_{3k} \nu_{3m} + \lambda_5 (\nu_{3i} \nu_{3j} \delta_{km} + \nu_{3k} \nu_{3m} \delta_{ij}) \\
 & + \lambda_6 (\nu_{3i} \nu_{3k} \delta_{jm} + \nu_{3j} \nu_{3m} \delta_{ik} + \nu_{3i} \nu_{3m} \delta_{jk} + \nu_{3j} \nu_{3k} \delta_{im}) \\
 & + \lambda_7 (\nu_{2i} \nu_{1j} \nu_{1k} \nu_{1m} + \nu_{1i} \nu_{2j} \nu_{1k} \nu_{1m} + \nu_{1i} \nu_{1j} \nu_{2k} \nu_{1m} + \nu_{1i} \nu_{1j} \nu_{1k} \nu_{2m} \\
 & - \nu_{1i} \nu_{2j} \nu_{2k} \nu_{2m} - \nu_{2i} \nu_{1j} \nu_{2k} \nu_{2m} - \nu_{2i} \nu_{2j} \nu_{1k} \nu_{2m} - \nu_{2i} \nu_{2j} \nu_{2m} \nu_{1k}),
 \end{aligned}$$

where

$$\begin{aligned}
\lambda_1 &= A_{1122} , & \lambda_2 &= A_{1212} , & \lambda_3 &= (A_{1111} - A_{1122} - 2A_{1212}), \\
(24) \quad \lambda_4 &= (A_{3333} + A_{1122} + 2A_{1212} - 2A_{2233} - 4A_{2323}), \\
\lambda_5 &= (A_{2233} - A_{1122}), & \lambda_6 &= (A_{2323} - A_{1212}), & \lambda_7 &= A_{1222}
\end{aligned}$$

are the invariant elastic constants. It can be shown that (23) is valid for the classes $\bar{4}$ and $4/m$ also.

The expression (23) is referred to an arbitrary Cartesian system xyz , with respect to which ν_{ai} are the components of the unit vectors $\mathbf{v}_a$. Suppose we choose x, y, z such that they coincide with $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$, respectively; then we have $\nu_{11} = \nu_{22} = \nu_{33} = 1$ and all others will vanish. For this particular choice of the xyz -system, C_{ijklm} satisfy the relations [2]

$$\begin{aligned}
C_{1111} &= C_{2222} = \lambda_1 + 2\lambda_2 + \lambda_3 , \\
C_{3333} &= \lambda_1 + 2\lambda_2 + \lambda_4 + 2\lambda_5 + 4\lambda_6 , \\
(25) \quad C_{2233} &= C_{3311} = \lambda_1 + \lambda_5 , & C_{1122} &= \lambda_1 , \\
C_{2323} &= C_{3131} = \lambda_2 + \lambda_6 , & C_{1212} &= \lambda_2 , \\
C_{1112} &= -C_{2212} = \lambda_7 .
\end{aligned}$$

(ii) *Classes $4mm, \bar{4}2m, 422, 4/mmm$.* In these classes some additional symmetries are present. For example, in $4mm$ two of the additional symmetries present are the mirror planes formed by $\mathbf{v}_3\mathbf{v}_1$ - and $\mathbf{v}_2\mathbf{v}_3$ -planes, denoted by m next to 4. Invariance of C_{ijklm} in (23) under the change $\mathbf{v}_2$ to $-\mathbf{v}_2$ due to the mirror reflection about $\mathbf{v}_3\mathbf{v}_1$ -plane will make in (23) vanish. We, therefore, have

$$\begin{aligned}
(26) \quad C_{ijklm} &= \lambda_1 \delta_{ij} \delta_{km} + \lambda_2 (\delta_{ik} \delta_{jm} + \delta_{im} \delta_{jk}) + \lambda_3 (\nu_{1i} \nu_{1j} \nu_{1k} \nu_{1m} + \nu_{2i} \nu_{2j} \nu_{2k} \nu_{2m}) \\
&+ \lambda_4 \nu_{3i} \nu_{3j} \nu_{3k} \nu_{3m} + \lambda_5 (\nu_{3i} \nu_{3j} \delta_{km} + \nu_{3k} \nu_{3m} \delta_{ij}) \\
&+ \lambda_6 (\nu_{3i} \nu_{3k} \delta_{jm} + \nu_{3j} \nu_{3m} \delta_{ik} + \nu_{3i} \nu_{3m} \delta_{jk} + \nu_{3j} \nu_{3k} \delta_{im}) .
\end{aligned}$$

It can be shown that (26) holds for all the symmetries in the classes $4mm, \bar{4}2m, 422$ and $4/mmm$. Thus, $\lambda_1, \lambda_2, \dots, \lambda_6$ are the invariant elastic constants for the crystals belonging to the tetragonal classes $4mm, \bar{4}2m, 422$ and $4/mmm$.

Again, C_{ijklm} in (26) can be shown to satisfy conditions similar to (25) when x, y, z , axes coincide with $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$, respectively.

Cubic system. The expression in the case of cubic crystals can be obtained from that corresponding to orthorhombic crystals by imposing the symmetry condition that C_{ijklm} in (20) should be invariant under 120° rotation about an axis which is equally inclined to $\mathbf{v}_1, \mathbf{v}_2$ and $\mathbf{v}_3$. Such an operation will take $\mathbf{v}_1$ to $\mathbf{v}_2$, $\mathbf{v}_2$ to $\mathbf{v}_3$ and $\mathbf{v}_3$ to $\mathbf{v}_1$. This leads to the relations

$$(27) \quad \lambda_1 = \lambda_2 = \lambda_3 , \quad \lambda_4 = \lambda_5 = \lambda_6 , \quad \lambda_7 = \lambda_8 = \lambda_9 .$$

On making use of the relations (21), we have

$$(28) \quad C_{ijkm} = \lambda \delta_{ij} \delta_{km} + \mu (\delta_{ik} \delta_{jm} + \delta_{im} \delta_{jk}) + \alpha \nu_{ai} \nu_{aj} \nu_{ak} \nu_{am},$$

where

$$(29) \quad \lambda = \lambda_4, \quad \mu = \lambda_5, \quad \alpha = \lambda_1 - \lambda_4 - 2\lambda_5$$

are the invariant elastic constants for cubic crystals. The expression (28) agrees with (7) proposed by Thomas.

Rhombohedral system. (i) *Classes 3, $\bar{3}$.* In rhombohedral crystals the angle between $\mathbf{v}_1$ and $\mathbf{v}_2$ is 120° and those between $\mathbf{v}_2$ and $\mathbf{v}_3$, and $\mathbf{v}_3$ and $\mathbf{v}_1$ are 90° each. Also $\mathbf{v}_3$ will be a three-fold axis of rotation. In this case $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$ satisfy the relations

$$(30) \quad \nu_{1i} \nu_{1j} + \nu_{2i} \nu_{2j} + \frac{1}{2}(\nu_{1i} \nu_{2j} + \nu_{1j} \nu_{2i}) + \frac{3}{4} \nu_{3i} \nu_{3j} = \frac{3}{4} \delta_{ij}.$$

A rotation of 120° about $\mathbf{v}_3$ will take $\mathbf{v}_1$ to $\mathbf{v}_2$ and $\mathbf{v}_2$ to $-(\mathbf{v}_1 + \mathbf{v}_2)$. The requirement that C_{ijkm} in (18) should be invariant under this symmetry operation yields the relations

$$(31) \quad \begin{aligned} A_{1111} &= A_{2222} = 2A_{1222}, & A_{1222} &= A_{2111}, \\ A_{1122} + 2A_{1212} &= 3A_{1222}, & A_{1333} &= 0, & A_{2333} &= 0, \\ A_{2233} &= A_{3311} = 2A_{3312}, & A_{2323} &= A_{3131} = 2A_{3132}, \\ A_{2231} &= A_{2321}, & A_{1123} &= A_{1213}, \\ A_{3111} &= -A_{3222} = (A_{1123} - A_{2231}). \end{aligned}$$

On making use of (31) together with (30), we have

$$(32) \quad \begin{aligned} C_{ijkm} &= \lambda_1 \delta_{ij} \delta_{km} + \lambda_2 (\delta_{ik} \delta_{jm} + \delta_{im} \delta_{jk}) + \lambda_3 \nu_{3i} \nu_{3j} \nu_{3k} \nu_{3m} \\ &+ \lambda_4 (\nu_{3i} \nu_{3j} \delta_{km} + \nu_{3k} \nu_{3m} \delta_{ij}) \\ &+ \lambda_5 (\nu_{3i} \nu_{3k} \delta_{jm} + \nu_{3j} \nu_{3m} \delta_{ik} + \nu_{3i} \nu_{3m} \delta_{jk} + \nu_{3j} \nu_{3k} \delta_{im}) \\ &+ \lambda_6 [\nu_{3i} (\nu_{1i} \nu_{1k} \nu_{1m} - \nu_{2i} \nu_{2k} \nu_{2m} + \nu_{1i} \nu_{1k} \nu_{2m} + \nu_{1i} \nu_{2k} \nu_{1m} + \nu_{2i} \nu_{1k} \nu_{1m}) \\ &+ \nu_{3j} (\nu_{1i} \nu_{1k} \nu_{1m} - \nu_{2i} \nu_{2k} \nu_{2m} + \nu_{1i} \nu_{1k} \nu_{2m} + \nu_{1i} \nu_{2k} \nu_{1m} + \nu_{2i} \nu_{1k} \nu_{1m}) \\ &+ \nu_{3k} (\nu_{1i} \nu_{1j} \nu_{1m} - \nu_{2i} \nu_{2j} \nu_{2m} + \nu_{1i} \nu_{1j} \nu_{2m} + \nu_{1i} \nu_{2j} \nu_{1m} + \nu_{2i} \nu_{1j} \nu_{1m}) \\ &+ \nu_{3m} (\nu_{1i} \nu_{1j} \nu_{1k} - \nu_{2i} \nu_{2j} \nu_{2k} + \nu_{1i} \nu_{1j} \nu_{2k} + \nu_{1i} \nu_{2j} \nu_{1k} + \nu_{2i} \nu_{1j} \nu_{1k})] \\ &+ \lambda_7 [\nu_{3i} (\nu_{3j} \nu_{2k} \nu_{2m} - \nu_{1i} \nu_{1k} \nu_{1m} + \nu_{2i} \nu_{2k} \nu_{1m} + \nu_{2i} \nu_{1k} \nu_{2m} + \nu_{1i} \nu_{2k} \nu_{2m}) \\ &+ \nu_{3j} (\nu_{2i} \nu_{2k} \nu_{2m} - \nu_{1i} \nu_{1k} \nu_{1m} + \nu_{2i} \nu_{2k} \nu_{1m} + \nu_{2i} \nu_{1k} \nu_{2m} + \nu_{1i} \nu_{2k} \nu_{2m}) \\ &+ \nu_{3k} (\nu_{2i} \nu_{2j} \nu_{2m} - \nu_{1i} \nu_{1j} \nu_{1m} + \nu_{2i} \nu_{2j} \nu_{1m} + \nu_{2i} \nu_{1j} \nu_{2m} + \nu_{1i} \nu_{2j} \nu_{2m}) \\ &+ \nu_{3m} (\nu_{2i} \nu_{2j} \nu_{2k} - \nu_{1i} \nu_{1j} \nu_{1k} + \nu_{2i} \nu_{2j} \nu_{1k} + \nu_{2i} \nu_{1j} \nu_{2k} + \nu_{1i} \nu_{2j} \nu_{2k})], \end{aligned}$$

where

$$\begin{aligned}
\lambda_1 &= \frac{3}{8}(5A_{1222} - 4A_{1212}), & \lambda_2 &= \frac{3}{8}(2A_{1212} - A_{1222}), \\
\lambda_3 &= A_{3333} + \frac{3}{8}(5A_{1222} - 4A_{1212}) \\
&\quad + \frac{3}{4}(2A_{1212} - A_{1222}) - \frac{3}{2}A_{2233} - 3A_{2333}, \\
(33) \quad \lambda_4 &= \frac{3}{4}A_{2233} - \frac{3}{8}(5A_{1222} - 4A_{1212}), \\
\lambda_5 &= \frac{3}{4}A_{2323} - \frac{3}{8}(2A_{1212} - A_{1222}), \\
\lambda_6 &= A_{1123}, & \lambda_7 &= A_{2231}
\end{aligned}$$

are the invariant elastic constants for the rhombohedral classes 3 and $\bar{3}$.

Now when xyz -system is so chosen that the z -axis coincides with $\mathbf{v}_3$ and x - and y -axes lie in the $\mathbf{v}_1\mathbf{v}_2$ -plane, it can be shown that C_{ijklm} in (32) satisfy relations [2] similar to (25) for tetragonal classes 4, $\bar{4}$ and $4/m$.

(ii) *Classes 32, 3m, $\bar{3}m$.* For these classes it can be shown, by imposing the additional symmetries, that in (32) $\lambda_6 = -\lambda_7$. Thus, we have

$$\begin{aligned}
(34) \quad C_{ijklm} &= \lambda_1 \delta_{ij} \delta_{km} + \lambda_2 (\delta_{ik} \delta_{jm} + \delta_{im} \delta_{jk}) + \lambda_3 \nu_{3i} \nu_{3j} \nu_{3k} \nu_{3m} \\
&\quad + \lambda_4 (\nu_{3i} \nu_{3j} \delta_{km} + \nu_{3k} \nu_{3m} \delta_{ij}) \\
&\quad + \lambda_5 (\nu_{3i} \nu_{3k} \delta_{jm} + \nu_{3j} \nu_{3m} \delta_{ik} + \nu_{3i} \nu_{3m} \delta_{jk} + \nu_{3j} \nu_{3k} \delta_{im}) \\
&\quad + \lambda_6 [\nu_{3i} (2\nu_{1j} \nu_{1k} \nu_{1m} - 2\nu_{2j} \nu_{2k} \nu_{2m} + \nu_{1j} \nu_{1k} \nu_{2m} + \nu_{1j} \nu_{2k} \nu_{1m} + \nu_{2j} \nu_{1k} \nu_{1m} \\
&\quad - \nu_{2j} \nu_{2k} \nu_{1m} - \nu_{2j} \nu_{1k} \nu_{2m} - \nu_{1j} \nu_{2k} \nu_{2m}) \\
&\quad + \nu_{3j} (2\nu_{1i} \nu_{1k} \nu_{1m} - 2\nu_{2i} \nu_{2k} \nu_{2m} + \nu_{1i} \nu_{1k} \nu_{2m} + \nu_{1i} \nu_{2k} \nu_{1m} \\
&\quad + \nu_{2i} \nu_{1k} \nu_{1m} - \nu_{2i} \nu_{2k} \nu_{1m} - \nu_{2i} \nu_{1k} \nu_{2m} - \nu_{1i} \nu_{2k} \nu_{2m}) \\
&\quad + \nu_{3k} (2\nu_{1i} \nu_{1j} \nu_{1m} - 2\nu_{2i} \nu_{2j} \nu_{2m} + \nu_{1i} \nu_{1j} \nu_{2m} + \nu_{1i} \nu_{2j} \nu_{1m} \\
&\quad + \nu_{2i} \nu_{1j} \nu_{1m} - \nu_{2i} \nu_{2j} \nu_{1m} - \nu_{2i} \nu_{1j} \nu_{2m} - \nu_{1i} \nu_{2j} \nu_{2m}) \\
&\quad + \nu_{3m} (2\nu_{1i} \nu_{1j} \nu_{1k} - 2\nu_{2i} \nu_{2j} \nu_{2k} + \nu_{1i} \nu_{1j} \nu_{2k} + \nu_{1i} \nu_{2j} \nu_{1k} \\
&\quad + \nu_{2i} \nu_{1j} \nu_{1k} - \nu_{2i} \nu_{2j} \nu_{1k} - \nu_{2i} \nu_{1j} \nu_{2k} - \nu_{1i} \nu_{2j} \nu_{2k})].
\end{aligned}$$

Hexagonal system. The relative orientation of $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ in hexagonal crystals is the same as in the rhombohedral crystals, but with the difference that $\mathbf{v}_3$ is a six-fold axis of rotation instead of three-fold. In this case also $\mathbf{v}_1$, $\mathbf{v}_2$, $\mathbf{v}_3$ satisfy the relations (30).

We now perform a rotation of 60° about $\mathbf{v}_3$. This rotation will take $\mathbf{v}_1$ to $(\mathbf{v}_1 + \mathbf{v}_2)$ and $\mathbf{v}_2$ to $-\mathbf{v}_1$. On making this change in (18), we obtain the conditions

$$\begin{aligned}
A_{1111} &= A_{2222} = 2A_{2111}, & A_{1222} &= A_{2111}, \\
A_{1122} + 2A_{1212} &= 3A_{2111}, & A_{2233} &= A_{3311} = 2A_{3312},
\end{aligned}$$

$$\begin{aligned}
(35) \quad & A_{2323} = A_{3131} = 2A_{3132}, \quad A_{1333} = 0, \quad A_{2333} = 0, \\
& A_{3111} = 0, \quad A_{3222} = 0, \quad A_{1123} = 0, \\
& A_{1213} = 0, \quad A_{2231} = 0, \quad A_{2321} = 0.
\end{aligned}$$

Conditions (35) together with (30) give us

$$\begin{aligned}
(36) \quad & C_{ijkm} = \lambda_1 \delta_{ij} \delta_{km} + \lambda_2 (\delta_{ik} \delta_{jm} + \delta_{im} \delta_{jk}) + \lambda_3 \nu_{3i} \nu_{3j} \nu_{3k} \nu_{3m} \\
& + \lambda_4 (\nu_{3i} \nu_{3j} \delta_{km} + \nu_{3k} \nu_{3m} \delta_{ij}) \\
& + \lambda_5 (\nu_{3i} \nu_{3k} \delta_{jm} + \nu_{3j} \nu_{3m} \delta_{ik} + \nu_{3i} \nu_{3m} \delta_{jk} + \nu_{3j} \nu_{3k} \delta_{im}),
\end{aligned}$$

where

$$\begin{aligned}
(37) \quad & \lambda_1 = \frac{3}{8}(5A_{2111} - 4A_{1212}), \quad \lambda_2 = \frac{3}{8}(2A_{1212} - A_{2111}), \\
& \lambda_3 = [A_{3333} + \frac{3}{8}(5A_{2111} - 4A_{1212}) + \frac{3}{4}(2A_{1212} - A_{2111}) - \frac{3}{2}A_{2233} - 3A_{2323}], \\
& \lambda_4 = \frac{3}{4}A_{2233} - \frac{3}{8}(5A_{2111} - 4A_{1212}), \\
& \lambda_5 = \frac{3}{4}A_{2323} - \frac{3}{8}(2A_{1212} - A_{2111}).
\end{aligned}$$

Again, for the particular choice of the xyz -system such that z -axis coincides with $\mathbf{v}_3$, and x - and y -axes lie in the $\mathbf{v}_1\mathbf{v}_2$ -plane, C_{ijkm} satisfy the conditions

$$\begin{aligned}
(38) \quad & C_{1111} = C_{2222} = \lambda_1 + 2\lambda_2, \\
& C_{3333} = \lambda_1 + 2\lambda_2 + \lambda_3 + 2\lambda_4 + 4\lambda_5, \\
& C_{1122} = \lambda_1, \quad C_{2233} = C_{3311} = \lambda_1 + \lambda_4, \\
& C_{2323} = C_{3131} = \lambda_2 + \lambda_5, \\
& C_{1212} = \lambda_2 = \frac{1}{2}(C_{1111} - C_{1122})
\end{aligned}$$

as given in [2].

4. Stress-strain relations. The stress-strain relations can be obtained in various cases by substituting the corresponding expressions for C_{ijkm} in (1). For example, in the case of a hexagonal crystal these relations are

$$\begin{aligned}
(39) \quad & \sigma_{ij} = \lambda_1 \delta_{ij} e_{rr} + 2\lambda_2 e_{ij} + \lambda_3 \nu_{3i} \nu_{3j} \nu_{3k} \nu_{3m} e_{km} + \lambda_4 (\nu_{3i} \nu_{3j} e_{rr} + \delta_{ij} \nu_{3k} \nu_{3m} e_{km}) \\
& + \lambda_5 (\nu_{3i} \nu_{3k} e_{kj} + \nu_{3j} \nu_{3m} e_{im} + \nu_{3i} \nu_{3m} e_{jm} + \nu_{3j} \nu_{3k} e_{ki}).
\end{aligned}$$

The problem of wave propagation in crystals using relations of the type (39) is under study.

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