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The Determination of the Components of a Tensor Characterizing a Crystal

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(2. IV. 64)

Zusammenfassung. Es wird eine Methode entwickelt, welche es gestattet, die Komponenten der Eigenschaftstensoren von Kristallen explizite durch eine Minimalzahl von Konstanten auszudrücken. Die Anwendung auf die Theorie des Deformationspotentials von Ladungsträgern in festen Körpern wird aufgezeigt.

Introduction

In both the classical and quantum mechanical theories of the physical properties of crystalline materials there appear tensors characterizing the body. The explicite knowledge of these tensors is a prerequisite to explain the behaviour of the material.

For example, the hamiltonian density of a ferrodielectric contains among other terms the fourth rank tensor of ferromagnetic coupling, and the sixth rank tensor of magnetoelastic coupling

$$H = \alpha_{iklm} \frac{\partial M_l}{\partial x_i} \frac{\partial M_m}{\partial x_k} + \gamma_{iklmrs} \frac{\partial M_r}{\partial x_i} \frac{\partial M_s}{\partial x_k} \varepsilon_{lm} ,$$

α_{iklm} = tensor of ferromagnetic coupling,
M_r = magnetization,
γ_{iklmrs} = tensor of magnetoelastic coupling,
ε_{lm} = strain tensor.

It is known, that the presence of structural symmetry reduces the number of independent components of a tensor characterizing the body. Furthermore, for various physical reasons the tensor may have an intrinsic symmetry of indices, independently of the symmetry of the body. This, further reduces the number of independent components.

For example, the fourth rank tensor of elastic constants has only three independent components in a cubic crystal. The ferromagnetic tensor α_{iklm} of the same rank has four independent components in a cubic crystal (as will be shown later), its index symmetry being less then that of the tensor of elastic constants.

There is a large number of papers and review articles on tensors in crystals[1]). They all treat the determination of tensor components by a detailed consideration of all symmetry properties of the various crystal classes. This gives rise to very cumbersome and lengthy algebraic manipulations. It is noteworthy that very elegant group theoretical methods exist for the determination of the number of independent tensor components when the body admits a certain group of symmetry[2]). No method is described in the literature, however, which would allow us a systematic determination not only of the number of independent components, but also of the position of these components, as well as of the vanishing components, in the explicite representation of the tensor.

This paper consists of three parts: First, we wish to expose the known group-theoretical method for the determination of the number of independent tensor components in crystals – as a preliminary to the following developments. Second, we shall develop a procedure for the determination of the positions of nonvanishing tensor components, and demonstrate its use on examples of physical interest. Third, we will indicate how to apply the method to deformed crystals, where the deformation diminishes the crystal symmetry, and establish a connection to the deformation potential theory of electrons in crystal lattices.

It is assumed that the reader is familiar with the basic concepts of group representation theory and the generally accepted notations, such as explained in reference[3]). We shall use the term tensor in two senses: either as a geometric entity $\boldsymbol{\alpha}$, which, when expressed in terms of a basis takes the form $\alpha = \alpha_{ik\ldots m}\, e_{ik\ldots m}$, or as the set of components $\alpha_{ik\ldots m}$.

Group Theoretical Determination of the Number of Independent Components of a Tensor

Consider a tensor of rank n, $\alpha_{ik\ldots m}$ $(i, k, \ldots m = 1, 2, 3)$ which describes some physical property of a crystal. Every element g of the point symmetry group G of the crystal can easily be represented by the *three by three* matrix of linear coordinate transformation corresponding to g. The set of these matrices forms the *vector representation* V of G operating in the three-dimensional space R_3 of cartesian coordinates. By definition, a tensor of rank n transforms according to the n-th power (direct product) of the vector representation, V^n. On the other hand, the crystal which has been subjected to the symmetry operation g is physically indistinguishable from the crystal before the operation: therefore the tensor $\boldsymbol{\alpha}$ must not change under g. Each component of α has to be an invariant under V^n,

$$\alpha = V^n(g)\alpha \text{ for all } g \in G.$$

If the tensor α is now looked upon as a vector of 3^n components in the direct product space $(R_3)^n$, which is left invariant by the $3^n \times 3^n$ matrices $V^n(g)$, then α is an *invariant vector*. Any invariant vector may be expressed as a linear combination of a minimum number of linearly independent invariant vectors $\alpha^{(s)}$, whose number r is less, or equal to 3^n:

$$\alpha = \sum_{s=1}^{r} c^{(s)}\, \alpha^{(s)}.$$

The invariant vectors $\alpha^{(s)}$ of the representation V^n have nothing to do with the physical property in question: they are determined uniquely by the symmetry of the crystal and the rank n. Hence all physical information contained in the tensor $\alpha_{ik\ldots m}$ has its site in the coefficients $c^{(s)}$. Their number r is, therefore, the number of independent coefficients characterizing the given tensor.

It is proved in representation theory (cf. ref. [2]) that the number r of linearly independent vectors of a representation is equal to the multiplicity of the unit representation in it.

This, in turn, may be calculated by the formula

$$r = \frac{1}{N} \sum_g \chi^n (g) ,$$

where N is the number of elements of the group G, and $\chi(g)$ is the character of the element g in the vector representation, i.e. the trace of $V(g)$. The sum is taken over all elements of the group. The procedure is easily modified[4]) to calculate r in case the tensor $\alpha_{ik\ldots m}$ has a symmetry with respect to the interchange of indices. The latter type of symmetry is not related to crystal symmetry, but follows from physical arguments, for example the conservation of energy.

Determination of the Tensor Components

Having found the number of independent components of a tensor characterizing the crystal, this information is yet unsufficient. For instance, it would be impossible to write down explicitely the Hamiltonian involving this tensor. Certain linear combinations of the independent components form the actual cartesian components of the tensor, and there are in general more nonzero cartesian components then independent ones.

As stated in the preceding section, every tensor may be written as the linear combination of a number of invariant tensors of the same rank. We want to find all invariant tensors of rank n explicitely, in order to write down the components of the given tensor in some coordinate system.

The procedure is based on the following easily proved theorem:
Let α be a tensor of rank n. Introduce the (3^n)-dimensional vector space V^n of the tensor components. Let $D^n(g)$ be the (3^n)-dimensional representation of the point symmetry group G of the crystal, according to which the tensor components transform. If $\boldsymbol{v}$ is any vector of V^n, then

$$\boldsymbol{u} = \sum_g D^n (g)\, \boldsymbol{v} \tag{1}$$

is an invariant vector of the group of matrices $D^n(g)$. (In tensor notation $\boldsymbol{u} = u_{ik\ldots m}\, e_i \times e_k \times \ldots \times e_m$.) Since every invariant vector $\boldsymbol{u}$ represents an invariant tensor of rank n, the problem is thus reduced to the construction of all linearly independent vectors $\boldsymbol{u}$.

The tensor representation under study $D^n(g)$ is always the direct product (possibly symmetrized or antisymmetrized) of $D^{n-1}(g)$ and the vector representation $d(g)$,

$$D^n(g) = D^{n-1}(g) \times d(g) . \tag{2}$$

Suppose first, that the vector representation d is irreducible, as is the case for the groups T, O, T_d, T_h, O_h.

As a first step let us decompose $D^{n-1}(g)$ into its p irreducible components

$$D^{n-1}(g) = \sum_{\mu=1}^{p} d^{\mu}(g) . \tag{3}$$

The irreducible representations $d^{\mu}(g)$ are very simple ones, since the crystallographic point groups have only 1, 2 and 3-dimensional irreducible representations*). Several of the $d^{\mu}(g)$ may be equivalent.

Decomposing V^n in the same manner,

$$V^n = V^{n-1} \times V , \tag{4}$$

we denote the basis of V by e_m $(m = 1, 2, 3)$. According to the decomposition (3), V^{n-1} splits into invariant subspaces V^{μ}, of dimensions 1, 2 or 3. A basis of V^{μ} will be denoted by f_l^{μ} $(\mu = 1, \ldots p;\ l = 1$ or 1, 2 or 1, 2, 3). An arbitrary vector $\boldsymbol{v}$ of V^n will now be written as

$$\boldsymbol{v} = a_{lm}^{\mu} f_l^{\mu} \times e_m , \quad a_{lm}^{\mu} = \text{arbitrary.} \tag{5}$$

It follows

$$D^{n-1}(g) f_l^{\mu} = d_{lk}^{\mu}(g) f_k^{\mu} \text{ (no sum over } \mu). \tag{6}$$

Using (3), (5) and (6), any invariant vector $\boldsymbol{u}$ of V^n may be expressed as

$$\boldsymbol{u} = \sum_g D^n(g)\, \boldsymbol{v} = \sum_g D^{n-1}(g) \times d(g)\, a_{lm}^{\mu} f_l^{\mu} \times e_m = \sum_g d_{lk}^{\mu}(g)\, d_{mj}(g)\, a_{lm}^{\mu} f_k^{\mu} e_j^{\mu} . \tag{7}$$

At this point the reason becomes evident, why the invariant vector $\boldsymbol{u}$ has been expressed as a group sum of an arbitrary vector $\boldsymbol{v}$. Since d^{μ} and d are irreducible representations, the orthogonality relation**) holds:

$$\sum_g d_{lk}^{\mu}(g)\, d_{mj}(g) = \begin{cases} 0, \text{ if } d^{\mu} \simeq d , \\ \delta_{lm}\, \delta_{kj}\, N/\dim \mu, \text{ if } d^{\mu} \simeq d . \end{cases} \tag{8}$$

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*) Taking spin into account there occurs one four-dimensional representation of the cubic double group O'.

**) The vector representation can always be chosen real, hence $d_{mj} = \bar{d}_{mj}$, where the bar denotes complex conjugate.

In (8), the equivalence relation $d^\mu \simeq d$ means, that the two representations have the same dimension, and their basis can be transformed into each other by a linear transformation. The dimension of the representation d^μ is denoted by $\dim \mu$.

Using the orthogonality relation (8), and setting $N\, a^\mu_{ll}/\dim \mu = a^\mu$ (7) simplifies to

$$\boldsymbol{u} = a^\mu\, f^\mu_k \times e_k \quad (k = 1, 2, 3)\,. \tag{9}$$

The sum over μ includes only those components of D^{n-1}, which are equivalent to the vector representation d.

If d is itself reducible, as is the case for all point groups except T, O, T_d, T_h and O_h, the reduction of d should be effected first:

$$d(g) = \sum_{\nu=1}^{r} h^\nu(g) \quad (r = 2 \text{ or } 3)\,. \tag{10}$$

The three basis vectors of V are also split into groups of 1 and 2, and shall be labeled as

$$e^\nu_k \quad (k = 1 \text{ or } 1, 2)\,,$$

the superscript referring to the irreducible component h^ν.

Correspondingly

$$d(g)\, e^\nu_m = h^\nu_{mj}(g)\, e^\nu_j \text{ (no sum over } \nu)\,. \tag{11}$$

From this follows

$$\boldsymbol{u} = \sum_g d^\mu_{lk}(g)\, h^\nu_{mj}(g)\, a^\mu_{lm}\, f^\mu_k \times e^\nu_j. \tag{12}$$

The orthogonality relation again yields, setting $N a^\mu_{ll}/\dim \nu = a^\mu$,

$$\boldsymbol{u} = a^{\mu\nu}\, f^\mu_k \times e^\nu_k\,. \tag{13}$$

The sum over μ includes only those components of D^{n-1} which are equivalent to the representation h^ν. The latter is the ν-th irreducible component of the vector representation d.

We remark that (13) remains true also if $D^n = D^{n-1} \times d$ is replaced by the more general decomposition

$$D^n = D^{n-m} \times D^m \quad (0 < m < n)\,. \tag{14}$$

In this case f^μ_k and e^ν_k represent basis of equivalent irreducible components of D^{n-m} and D^m, respectively.

Formulas (9) and (13) show, that the invariant tensors of rank n can explicitely be written down, as soon as a basis f^μ_k of the irreducible components of the tensors of rank $n - 1$ is known.

The construction of such a basis is a well-known but tedious procedure in the theory of the decomposition of group representations, and can in general be performed by the method of projection operators. Since we deal with the $(n - 1)$-st power of the vector representation, and furthermore n is usually small, the required basis is more easily constructed building it from the basis of the vector representation.

Pseudovectors

In physical applications pseudovectors (e.g. the magnetic field) are often used, with the consequence that the tensors describing the response of the medium transform with respect to a certain index as a pseudovector. (Pseudoscalars, which are equivalent to totally antisymmetric third rank tensors, play little role in crystal physics.)

Of course, this case may be dealt with entirely within the framework of the methods described, since a pseudovector is equivalent to an antisymmetric tensor of rank two. Whenever a pseudovector index i is encountered, it should be replaced by a pair of indices $j\,k$ according to the convention

$$1 \to 23, \quad 2 \to 31, \quad 3 \to 12,$$

and the resulting entity be taken as changing sign, when j and k are interchanged.

If one is reluctant to make this transcription, pseudovectors as well as vectors may be used from the outset. The method described, and in particular, (9) and (13) hold true, irrespective whether the basis vectors e_i^ν, f_k^μ span the true or pseudovector space. The only difference arises in the decomposition of the pseudovector space V_p, and its powers, with respect to the group G. The decomposition of V_p is identical with that of the antisymmetric square of V:

$$V_p = \{V^2\}\,. \tag{15}$$

However, even this difference disappears if G is a proper group, i.e. does not contain reflections on symmetry planes, the inversion, or the combination of both.

Index Symmetry

Index symmetry of tensors may be classified according to two criteria. First, by specifying the permutation group P, the elements of which are allowed permutations of a set of the indices. Second, by specifying the effect of the permutation of indices upon the tensor components. It is useful to introduce a linear operator $\boldsymbol{p}$ on the tensor space with basis $e_{i\,k\ldots m}$, corresponding to every permutation p of P, so defined that

$$\boldsymbol{p}\,\alpha_{i\,k\ldots m}\,e_{i\,k\ldots m} = \alpha_{i\,k\ldots m}\,e_{p(i\,k\ldots m)} = \alpha_{p(i\,k\ldots m)}\,e_{(i\,k\ldots m)}\,, \tag{16}$$

$$p(i\,k\ldots m) = \text{permutation of the indices } i\,k\ldots m\,.$$

Thus we obtain a representation of P in the space of n-th rank tensors.

While in general the tensor components are transformed into linear combinations of each other by $\boldsymbol{p}$, for physical applications only three special cases are of importance: either the tensor components are invariant, or they change sign under odd permutations and are invariant under even permutations, or, lastly, their transformation properties are irrelevant. The tensor is denoted symmetric, antisymmetric, or general, respectively.

It follows, that the components of the symmetric tensor transform according to the one-dimensional unit representation τ_1, while those of the antisymmetric tensor according to the alternating one-dimensional representation τ_2.

On the other hand, the permutation group P may be the group S_n of all permutations of the n indices, or a subgroup of S_n. For instance, the tensor α_{iklm} of the introduction is symmetrical with respect to the simultaneous interchange of the two pairs of indices $(i\ k)$ and $(l\ m)$, hence transforms according to the unit representation of the group of two elements

$$P = [e, (i\ k)(l\ m)]\ ,^*)$$

a subgroup of S_4, but not equal to S_2.

Consider first the problem of *symmetrization*. If τ_1 is contained s-times in the tensor representation of P, the invariant vectors of the symmetric tensor α will all be contained in the s-dimensional subspace L^s, which transforms by τ_1^s. Hence all that is needed to single out the invariant vectors $\boldsymbol{u}$ of G and P among the invariant vectors of G, is to construct a projection operator P which projects any vector on L^s. Then,

$$\boldsymbol{w} = \boldsymbol{P}\,\boldsymbol{u}\ . \tag{17}$$

The reader will easily verify, that the required projection operator P is the sum of all permutations contained in the group P, divided by the number of permutations N_p:

$$\boldsymbol{P} = (N_p)^{-1} \sum_p \boldsymbol{p}\ . \tag{18}$$

In many instances, the application of this projection operator to the invariant vectors $\boldsymbol{u}$ of the crystal symmetry group will reproduce $\boldsymbol{u}$. In this case the permutational symmetry does not give any new relation between the tensor components not yet deduced from crystal symmetry.

It is evident, that one may proceed also in the reverse order: having determined the invariant vectors of P, their projection upon the invariant subspace of G will also yield $\boldsymbol{w}$. The *first* procedure is more convenient and rapid, especially if the crystal symmetry is high.

The *antisymmetrization* problem can be solved similarly. If τ_2 is contained a-times in the tensor representation of P, the vectors of the antisymmetric tensor α, invariant under G and alternant under P will be obtained by projection of the invariant vectors $\boldsymbol{u}$ of G upon the space L^a, transforming under τ_2^a. The projection operator for this purpose is

$$\boldsymbol{A} = (N_p)^{-1} \sum_P (-1)^\delta \boldsymbol{p}\ , \qquad \delta = \begin{cases} 0 \text{ for even permutations} \\ 1 \text{ for odd permutations.} \end{cases} \tag{19}$$

As a rule, to reduce the labor involved, one should carry out the proper symmetrization or antisymmetrization as soon as in the process of buildup of the basis, all indices upon which the permutations are allowed, appear. For instance, if the tensor is written as $\alpha_{ikl}\, e_i \times e_k \times e_l$, the permutation $p = (i\ k\ l)$ will produce

$$\boldsymbol{p}\ \alpha_{ikl}\, e_i \times e_k \times e_l = \alpha_{ikl}\, e_l \times e_i \times e_k\ .$$

Relations of this type immediately simplify the basis.

*) The identity element of the permutation group is denoted by e.

Examples of Physical Interest

To illustrate the method, let us determine the components of fourth rank tensors of various index symmetries in a crystal of point symmetry O. Among these tensors there is the tensor α_{iklm} of ferromagnetic coupling, which is symmetric with respect to the simultaneous interchange of the two pairs of indices $(i\,k)$ and $(l\,m)$.

The vector representation V of O is irreducible. Choosing the basis e_1, e_2, e_3 for V it is immediate to write down the decomposition of V^2 with respect to the group O:

$$V^2 = A + E + F_2 + F_1 = (\Gamma_1 + \Gamma_{12} + \Gamma_{15'} + \Gamma_{25'}) \tag{20}$$

and the basis*) for the four irreducible components, distinguished by a superscript, is

$$A:\ f_1^1 = e_i \times e_i\,.$$

$$E:\ f_1^2 = e_1 \times e_1 + \varepsilon\, e_2 \times e_2 + \varepsilon^2\, e_3 \times e_3\,,$$
$$f_2^2 = e_1 \times e_1 + \varepsilon^2\, e_2 \times e_2 + \varepsilon\, e_3 \times e_3\,, \qquad \varepsilon = \exp(2\pi\, i/3)\,. \tag{21}$$

$$F_2:\ f_1^3 = e_2 \times e_3 + e_3 \times e_2\,, \qquad F_1:\ f_1^4 = e_3 \times e_2 - e_2 \times e_3\,,$$
$$f_2^3 = e_3 \times e_1 + e_1 \times e_3\,, \qquad f_2^4 = e_3 \times e_1 - e_1 \times e_3\,,$$
$$f_3^3 = e_1 \times e_2 + e_2 \times e_1\,. \qquad f_3^4 = e_1 \times e_2 - e_2 \times e_1\,.$$

Consider the following possibilities of index symmetry:

a) Tensor invariant under the permutation group S_2, which contains the two elements e, $(i\,k)$.

b) Tensor invariant under the permutation group $S_2 \times S_2$, which contains the four elements e, $(i\,k)$, $(l\,m)$, $(i\,k)(l\,m)$.

c) Tensor is invariant under the permutation group P, which contains the two elements e, $(i\,k)(l\,m)$.

d) Tensor is invariant under the permutation group S_2, which contains the two elements e, $(i\,k)$, and is alternant under the permutation group S_2, which contains the two elements e, $(l\,m)$.

e) No index symmetry.

Let us consider these five cases in turn.

a) Since S_2 involves only two indices, the symmetrization can be carried out applying

$$\boldsymbol{P}_a = {}^1/_2\,[e + (i\,k)]$$

to the basis of V^2. One finds

$$\boldsymbol{P}_a\,(A + E + F_2) = A + E + F_2 \equiv [V^2]\,,$$

$$\boldsymbol{P}_a\,F_1 = 0\,.$$

*) In spite of the previous footnote we have chosen complex basis vectors for E, because they have simpler appearence than their real linear combinations. As a consequence, vectors of $E \times E$ have to be expressed with help of the basis $f_k^1 \times \bar{f}_i^1$.

Since the required tensor transforms according to

$$[V^2] \times V^2 ,$$

formula (13) will be applied, and yields

$$\boldsymbol{u} = a^{11} f_k^1 \times f_k^1 + a^{22} f_k^2 \times \bar{f}_k^2 + a^{33} f_k^3 \times f_k^3 . \tag{22}$$

Hence the tensor has three independent components. Inserting the vectors f_k^i from (21) into (22), one finds any required tensor component $\alpha_{i\,k\,l\,m}$, expressed in terms of a^{11}, a^{22} and a^{33} as the coefficient of $e_i \times e_k \times e_l \times e_m$ in $\boldsymbol{u}$.

b) The tensor transforms according to

$$[V^2] \times [V^2] ,$$

since symmetry is present with respect to both index pairs.

Formula (13) yields the same result (22), as in case *a*), hence the tensor components obey the same relations as found under *a*).

c) and e). All four indices are involved in the symmetry group P, therefore the symmetrization can only be carried out, after the invariant vectors of V^4 have been constructed. For this purpose one applies (13) to $V^2 \times V^2$, and finds

$$\boldsymbol{u} = a^{11} f_k^1 \times f_k^1 + a^{22} f_k^2 \times \bar{f}_k^2 + a^{33} f_k^3 \times f_k^3 + a^{44} f_k^4 \times f_k^4 . \tag{23}$$

At this stage problem *e*) is solved: with no index symmetry present the tensor has four independent components, which can be evaluated inserting (21) into (23), and writing out the coefficients of $e_i \times e_k \times e_l \times e_m$. To render the tensor symmetric under P, i.e. the simultaneous interchange of two index pairs, one applies the projection operator (18)

$$\boldsymbol{P}_c = {}^1/_2 \, [e + (i\ k)\ (l\ m)]$$

to $\boldsymbol{u}$. However, one immediately finds that $\boldsymbol{u}$ is already invariant under $\boldsymbol{P}_c$, hence the problems c) and e) have the same solution.

d) To achieve alternation of the tensor with respect to S_2, the projection operator

$$\boldsymbol{A} = {}^1/_2 \, [e - (l\ m)]$$

is applied, and yields

$$\boldsymbol{A}\,(A + E + F_2) = 0 ,$$

$$\boldsymbol{A}\,F_1 = F_1 \equiv \{V^2\} .$$

Using (13) on $[V^2] \times \{V^2\}$, one obtains zero for the invariant vector: consequently all tensor components are zero.

Tensor Properties of Elastically Deformed Crystals

In the introduction we have given an example of a tensor which refers to a deformed crystal. Since the symmetry changes upon deformation, the question arises, how to apply the methods outlined here to elastically deformed crystals?

This question has particular importance in relation to the theory of the deformation potential of solids. This entity, introduced by BARDEEN [5]), represents the effect of the deformation of the body upon the potential, in which the charge carriers in metals or semiconductors move.

It is possible, by group theoretical arguments, to make important statements about this potential, and its eigenvalues.

Let us investigate first the classical energy density H of the deformed crystal, expressed linearly in terms of the components of the strain tensor ε_{ik}:

$$H = \gamma_{ik}\,\varepsilon_{ik}\,. \tag{24}$$

We exclude the case $\gamma_{ik} \equiv 0$, which holds if the state of minimum energy of the body is the undeformed one. In that case H is quadratic in ε_{ik}.

It is clear, that ε_{ik} is not a tensor characterizing the physical properties of the body, but represents the result of external and internal forces. The only invariance properties of ε_{ik} relate to the symmetry group of the deformed crystal, which, in general, consists only of the identity and the inversion. The tensor γ_{ik}, however, describes the properties of the undeformed crystal. In fact, γ_{ik} may be considered as

$$\left.\frac{\delta H}{\delta \varepsilon_{ik}}\right|_{\varepsilon_{ik}\,=\,0}\,,$$

and transforms as the symmetrized square of the vector representation.

The same holds true, if $\hat{H}$ is the Hamiltonian operator of a system which can be described by a one-component wave-function, for example an s-electron, neglecting spin effects.

It should be noted, that $H\,d^3x$ is a scalar, and therefore invariant under coordinate transformations. Since the *Jacobian* $|\,\partial x_i/\partial x_k'\,|$ of all symmetry transformations considered here equals unity, H itself is also invariant.

Thus in the classical as well as in the non-degenerate (s-type) quantum mechanical case the results of the preceding sections may be applied without change. Hence the number of independent components of the tensor γ_{ik} is equal to the multiplicity of the unit representation of the symmetry group G of the undeformed crystal, contained in V^2.

This allows us to write down the change in crystal energy, or in the energy of the electron due to the strain. We shall limit ourselves to $\boldsymbol{k} = 0$ electron wave vectors. This change, ΔE is the linear invariant formed from the two tensors γ_{ik} and ε_{ik}. It is convenient to express the tensor ε with help of a basis

$$\boldsymbol{\varepsilon} = \varepsilon_{ik}\,e_i \times e_k\,,$$

obeying the orthogonality relations

$$e_i \cdot e_k = \delta_{ik} . \tag{25}$$

Thus

$$(e_i \times e_k) \cdot (e_j \times e_l) = \delta_{ij}\, \delta_{kl} . \tag{26}$$

The tensor γ_{ik}, being an invariant tensor, has already been expressed in the form (13),

$$\boldsymbol{u} = \gamma^{\mu\nu}\, e_l^{\mu} \times e_l^{\nu} ,$$

hence

$$\Delta E = \gamma_{ik}\, \varepsilon_{ik} = \boldsymbol{u} \cdot \boldsymbol{\varepsilon} = \gamma^{\mu\nu}\, \varepsilon_{ik}\, (e_l^{\mu} \times e_l^{\nu}) \cdot (e_i \times e_k) . \tag{27}$$

For example, if the vector representation is irreducible, as for the groups T, O, T_d, T_h and O_h, one has the identities

$$e_l^{\mu} \equiv e_l^{\nu} \equiv e_l , \tag{28}$$

and therefore

$$\Delta E = \gamma\, \varepsilon_{ik}\, (e_l \times e_l) \cdot (e_i \times e_k) = \gamma\, \varepsilon_{ll} . \tag{29}$$

This familiar result expresses the fact, that the energy shift of the electrons depends only on the dilatation.

The situation is different, if the electron is in an m-fold degenerate state. In the Hamiltonian

$$\hat{H} = \hat{\gamma}_{ik}\, \varepsilon_{ik} \tag{30}$$

$\hat{\gamma}_{ik}$ is now a tensor operator, which acts on the electron wave functions. The latter transform according to some tensor or spinor representation of the group G. The presence of deformation will split the degeneracy of the state, the extent of which can be determined by well known methods. To fix the ideas, suppose that the splitting is complete. The changes in the eigenvalue of the energy, ΔE_m, will be determined by the solution of a secular equation of degree m. Invariants of order m, formed from the matrix elements of $\hat{\gamma}_{ik}$, and the components of the strain tensor, will appear in ΔE_m.

To construct the invariants of order m of the strain tensor with respect to the given group G, it is sufficient to remark, that they may be obtained as linear invariants of the m-fold product $\varepsilon_{ij} \ldots \varepsilon_{kl}$. For instance, if the charge carrier state is twofold split by the deformation, as is the case for holes in the $\boldsymbol{k} = 0$ state in the lower valence band of germanium, one has to calculate the invariants of

$$I = \gamma_{iklm}\, \varepsilon_{ik}\, \varepsilon_{lm} . \tag{31}$$

The invariant vector of γ_{iklm} with respect to the appropriate symmetry group O has already been determined in example b), equation (23), hence I is the sum of three invariants

$$I = \boldsymbol{u} \cdot \boldsymbol{\varepsilon}\, \boldsymbol{\varepsilon} = (a^{11}\, f_k^1 \times f_k^1 + a^{22}\, f_k^2 \times f_k^2 + a^{33}\, f_k^3 \times f_k^3) \cdot \varepsilon_{ik}\, \varepsilon_{lm}\, (e_i \times e_k \times e_l \times e_m) =$$
$$= I_1 + I_2 + I_3 , \tag{32}$$

where

$$I_1 = a^{11} (\varepsilon_{ii})^2 ,$$

$$I_2 = a^{22} [(\varepsilon_{11} - \varepsilon_{22})^2 + (\varepsilon_{11} - \varepsilon_{33})^2 + (\varepsilon_{22} - \varepsilon_{33})^2] , \tag{33}$$

$$I_3 = a^{33} [\varepsilon_{12}^2 + \varepsilon_{13}^2 + \varepsilon_{23}^2] .$$

The required eigenvalues will be algebraic functions (in this case involving square roots only) of the three invariants, will contain the three deformation potential constants a^{11}, a^{22} and a^{33}, and may be written as

$$\Delta E_m = \Delta E_m (I_1, I_2, I_3) , \quad m = 1, 2 . \tag{34}$$

The exact form of ΔE_m can only be determined by actually solving the secular equation[6]).

It should be born in mind, that these considerations refer to wave functions with $\boldsymbol{k} = 0$. We wish merely to remark that in order to treat the effect of the deformation on $\boldsymbol{k} \neq 0$ wave functions of the electron, one has to construct combined invariants out of the components of $\boldsymbol{k}$ and the deformation tensor.

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