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A Reformulation of the Basis of Crystal Physics

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Abstract

The basis of crystal physics, namely the classification of tensors by rank and according to parity (*i.e.* polar or axial), is closely examined and found to be fundamentally deficient. An appreciation of the importance of a pre-metrical approach that stresses the role of invariant objects leads to a superior description in terms of differential forms. Rank is then replaced by the degree of the form and parity is replaced by a distinction between inner and outer orientation. It is shown how these factors can be used to predict the behaviour of physical properties under active inversion, which is then the operation of fundamental importance.

1. Introduction

Crystal physics classifies tensors by rank and according to parity, that is according to whether they are polar or axial. Conventionally, this last distinction is associated (Nye, 1960; Birss, 1966) with behaviour under coordinate inversion (a conclusion that will be disturbed in what follows) but the important point, for the moment, is that some such distinction must be made if the forms of property tensors are to be predicted correctly for crystals of various symmetries. For example, the most obvious aspect of such predictions is the pattern of nullities generated by the rules contained in the following statement.

($S1$) For centrosymmetrical crystals, polar property tensors of odd rank and axial property tensors of even rank vanish identically.

Such rules embody the general philosophy on which crystal physics rests, namely that a property tensor can only be put into its simplest form after the rank and parity of the tensor have first been determined by inspection, which can, of course, only mean inspection of the experimental situation that the tensor is intended to describe. In practice, other information (*e.g.* derived reflexively or from balance equations) may be used in addition but this does not disturb the basic philosophy of crystal physics which is, in summary, that

($S2$) the form of a property tensor is predicted as a *consequence* of a prior attribution of both its rank and its parity by inspection of the corresponding experimental situation.

(This statement relates, of course, not to the eventual particularized form of the tensor appropriate to an individual crystal symmetry but to the initial form before such particularization has been considered.)

Logically, however, it should be noted that there may be consistency problems if there is any question of using a procedure that alters the rank of a tensor from odd to even (or *vice versa*), because such an alteration would also involve a simultaneous change of parity, to be consistent with ($S1$), and this would contradict the assumption in ($S2$) that rank and parity can be separately[3] determined by inspection. It is therefore necessary to enquire whether such procedures are used in tensor analysis and it is shown, in the next section, that, in fact, they are so used.

2. Existing limitations

2.1. *Associated and other related tensors*

A convenient starting point is to consider an extension of a procedure, familiar in tensor analysis, in which a tensor is used to form *associated* tensors. It will be recalled that this is done by first defining a local inner product between base vectors, $\mathbf{e}_i$, by specifying the corresponding six metrical coefficients $g_{ij} = \mathbf{e}_i . \mathbf{e}_j$. These coefficients may then be used to transform an arbitrary tensor – say a mixed tensor t^i_{jk}, for example – into an associated tensor by the procedure, outlined below, of 'lowering affixes'.

The arbitrary tensor is properly regarded as a set of correspondences between tables of numbers, *e.g.* the t^i_{jk}, and the corresponding bases or coordinate systems used, provided that these correspondences exhibit the correct transformation behaviour, *i.e.* that indicated by the affixes. It may therefore be supposed that experimental measurements have revealed the existence of this correspondence but, equally, there exists another such correspondence in that the correspondence between the metrical coefficients g_{ij} and the $\mathbf{e}_i$ is just the tensor g_{ij} itself, the metrical tensor of the space. Tensor analysis therefore permits the metrical coefficients to be

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used to raise and lower affixes in a way that is sufficiently exemplified by the equation

$$g_{ij}\, t^{j}_{kl} = s_{ikl},$$

in which the affix j is 'lowered' in the mixed tensor t^{j}_{kl} to form the associated tensor s_{ikl} (which is triply covariant).

Since the essence of a tensor is that it is a correspondence between a table of numbers and a basis (*i.e.* originally between t^{j}_{kl} and $\mathbf{e}_i$), the above procedure has automatically produced a second such correspondence (*i.e.* between s_{ikl} and $\mathbf{e}_i$), which clearly cannot be regarded as being a new tensor. However carefully the experimental arrangements are examined, if experiment defines one correspondence, then equally it defines the other. In consequence, it is often stated that it is merely a matter of convenience (in the presence of a metric) as to whether a tensor is expressed in contravariant, covariant or mixed form. Naturally, raising and lowering affixes does not alter the rank of the tensor but the further development outlined below does precisely that.

Employing the g_{ij} to raise and lower affixes does not, of course, exhaust the possibilities of using the g_{ij} to modify the form of tensors, since it is also possible to consider the use of functions of the g_{ij} (such as the determinant, $g = \det g_{ij}$, for example). In addition, tensor components can be labelled in other ways (a simple example being a cyclic relabelling of indices according to $12 \rightarrow 3$, $23 \rightarrow 1$ and $31 \rightarrow 2$). Taken together, these two possibilities allow any arbitrary tensor of first rank, t_i, to be transformed into a tensor of second rank, $t_{jk} = G(t_i)$, by means of a simple linear* transformation G that depends only on the g_{ij}. Moreover, exactly the same argument now applies to this transformation as did to the transformation from tensor to associated tensor: since G depends only on the g_{ij} then t_{jk} clearly cannot be regarded as a new tensor and, if experiment defines the tensor t_i, then equally it defines the tensor t_{jk}.

In an entirely similar way, any (antisymmetrical) tensor of second rank, t_{pq}, can be transformed (by means of a simple linear transformation γ that depends only on the g_{ij}) into a tensor of first rank, $t_r = \gamma(t_{pq})$ and the same conclusion can be drawn about the interchangeability of the tensors t_{pq} and t_r. Indeed, G and γ are but two examples of quite general transformations (Schouten, 1954), valid in n dimensions, that permit any antisymmetrical tensor of rank p to be replaced by an antisymmetrical tensor of rank n-p and again it is true that, if the experimental arrangements define the former, then equally they define the latter as well. Consequently, in three dimensions ($n = 3$), these procedures have exactly the feature envisaged in § 1, that is they alter the rank of a tensor from odd to even (or *vice versa*) and so automatically produce inconsistencies between statements ($S1$) and ($S2$).

* Specifically, $t_{jk} = G(t_i) = G^{i}_{jk}\, t_i$, where $G^{i}_{jk} = g^{-1/2}\, g_{jl}\, g_{km}\, E^{ilm}$ and E^{ilm} is the antisymmetric unit tensor (strictly speaking, relative tensor of weight +1, so that, for example $E^{123} = -E^{213} = +1$ for *all* coordinate systems). Similarly, for the transformation γ, introduced later, $t_r = \gamma(t_{pq}) = \gamma^{pq}_{r}\, t_{pq}$, where $\gamma^{pq}_{r} = g^{-1/2}\, g_{rs}\, E^{pqs}$.

2.2. *Discussion*

Clearly, the inconsistencies alluded to above cannot originate with experiment but must instead arise within the mathematical formalism that is selected to describe experimental conditions (*i.e.* within tensor analysis). A careful consideration of the procedures discussed in § 2.1 reveals that the inconsistencies may be attributed to the way in which a metric can be used within a formalism that de-emphasizes the role of tensors as invariant objects. The two main features involved here are considered in more detail below.

It has already been noted in § 2.1 how a metric permits the transference from one tensor species to another, essentially by adding a second experimental input to the one provided directly by the experimental situation under inspection. Ideally, this dual experimental input should be avoided by working without a metric: more precisely, what is required is a mathematical formulation which can eventually accommodate a metric but in which, for the time being, no metric has been specified – in short, the formulation should be *pre-metrical*. The second feature alluded to above concerns the role of an invariant object.

Vector analysis emphasizes the role of an *invariant object* – the vector – and the task is essentially to find a physical state of affairs that can be represented by this invariant object; by contrast, tensor analysis, whilst recognising the existence of an invariant object – the tensor – regards it as an abstract object that is defined in terms of the behaviour of its components under changes of coordinates. This shift in emphasis from an invariant object to the components thereof (*i.e.* to tables of numbers that transform in a prescribed manner) means that, in physical situations, contact with experiment is automatically made via the components rather than the tensor itself (and this is, of course, implicitly recognised in tensor analysis in the practice of treating different types of tensor components as being essentially on the same footing). Ideally, however, this subordination of the role of an invariant object should be avoided and the question that naturally arises is whether there is available a mathematical formulation (suitable for the purpose) that, first, is pre-metrical in character and, secondly, stresses (rather than de-emphasizes) the role of an invariant object. The answer to this question is that a formulation with these two features was not available historically (*i.e.* when it was required for the satisfactory development of crystal physics) but that it is

now available and is embodied in the calculus of differential forms.

The principal objectives of crystal physics were laid down as a complete programme by Woldemar Voigt in his definitive treatise (Voigt, 1910) on that subject and it was he who modified Neumann's principle from its original form as a compatibility statement (that morphological symmetry must be reflected in physical properties) to the now familiar form of an invariance requirement (that property tensors are invariant under the symmetry group of the crystal). It is only comparatively recently that the calculus of differential forms – sometimes called exterior differential calculus – has been available in textbook presentations (Flanders, 1963; Goldberg, 1963; Spivak, 1965; Lichnerowicz, 1967; Hermann, 1973, 1977) and although it first came into prominence, between about 1945 and 1965, through a number of investigations in the field of differential geometry, in which connection particular mention should be made of the name of Élie Cartan (1945). Historically, therefore, the requisite mathematical formulation (*i.e.* the calculus of differential forms) was not available when the programme of crystal physics was being finalized by Voigt and, although the best formulation available at that time (*i.e.* tensor analysis) was used, this still left within the programme the inconsistencies noted at the end of § 2.1. It will be shown in the next section how these inconsistencies can be removed with the aid of differential forms.

3. Differential forms

3.1. *Mathematical definitions*

In differential geometry, the ordinary three-dimensional space of everyday experience is characterized by three principal properties which, when suitably formulated, lead to the concept of a differentiable manifold, M. The first, since the nearness of points must be meaningful, is topology: M must be a topological space (Porteous, 1969). Secondly, M must have an additional coordinatization structure (Hermann, 1970), that is each point of M must have an immediate neighbourhood that is described by n coordinates (there are then no holes in M!). Thirdly, since differentiability must be well defined for real-valued functions, $F(M)$, on M (*e.g.* temperature or pressure), then the final requirement is for smoothness: coordinate systems in overlapping neighbourhoods must be related to each other (Whitney, 1957) by differentiable coordinate transformations (there are then no sharp edges or corners!). In this way, the formal definition (Choquet-Bruhat, Dewitt-Morette & Dillard-Bleick, 1977) of a differentiable manifold generalizes the concept of a differentiable curve or a surface in a way that makes no reference to a containing space, all necessary constructions being performed intrinsically from within the manifold. In the same way that a differentiable surface has a tangent plane at each point, so there is (Dodson & Poston, 1977), at each point ξ of the manifold M, a tangent space, also of n dimensions, that is denoted by $T_n(M, \xi)$ or, when the context is clear, simply by T_n.

In modern textbooks (Hermann, 1973, 1977; Lichnerowicz, 1967; Goldberg, 1963; Bishop & Crittenden, 1964; Spivak, 1965; Flanders, 1963) the use of coordinates is eliminated altogether in defining differential forms and, in addition, a number of different definitions are possible which, although equivalent from a mathematical point of view, are not always equally suitable for physical applications. For example, an exterior differential p form may be defined as an element of order p of the exterior algebra $T_n^{*\Lambda(p)}$ constructed on the vector space of Pfaffian forms (*i.e.* the space T_n^* of linear functionals on the tangent space T_n). Equivalently (Lichnerowicz, 1967), it may be defined as an element of $[T_n^{\Lambda(p)}]^*$, that is a linear functional defined on the space of order p of the exterior algebra $T_n^{\Lambda(p)}$ constructed on T_n. Finally, and most usefully in the present context, the rules embodied in the construction of an exterior algebra can be made explicit in the definition, so that an exterior differential p form is defined (Hermann, 1973) as a mapping from $(T_n)^p = T_n \times T_n \times \ldots \times T_n$ to $F(M)$ that is multilinear and antisymmetrical in its arguments (*i.e.* in the elements of T_n). It will be seen, in § 3.2, that this concept can be much simplified when considering local conditions in three dimensions. It is, however, important to note at this stage that the above definitions do not involve the manifold being endowed with a metric, *i.e.* there is no necessity to define an inner product in the tangent space, T_n, so that differential forms are defined in a way that is not only coordinate independent but is also metric independent. (Being coordinate independent, there is, of course, no place within this formulation for differences of behaviour under coordinate inversion.)

3.2. *Applicability to fields*

If a crystal is subjected to a physical influence (*e.g.* a magnetic field) which gives rise to a resultant physical effect (*e.g.* magnetic induction), then it is customary to distinguish both of these from the constitutive relationship connecting them by describing the influence and effect as *fields* and the constitutive relationship as a *property*. Following its earlier use in differential geometry, the language of differential forms has increasingly been used (since about 1965) to describe physical fields of various types. For example, it is now customary, in textbook descriptions of electromagnetism (Lovelock & Rund, 1975; Thirring, 1978, 1979;

Hestenes, 1966; Riesz, 1958) and also in research publications (Sternberg, 1978; Israel, 1970; Riesz, 1947; Thirring & Wallner, 1978; Barut 1978), to describe the four electromagnetic field quantities as exterior differential forms defined on a manifold of three (space) or four (space–time) dimensions. By restoring the invariant object, the differential form (*i.e.* a mapping), such an approach avoids the tautology of tensor analysis (in defining a tensor only in terms of the behaviour of its components). Tensors appear only when base vectors, $\mathbf{e}_i$, are introduced, whereupon the four electromagnetic field quantities are all represented by antisymmetrical absolute tensor fields that are singly or doubly covariant.

That the suitability of a formulation in terms of differential forms is not confined to electromagnetism was established as a result of pioneering work carried out by Enzo Tonti in the early 1970's which culminated in a definitive review article (Tonti, 1976) in which he examined the reasons why exterior differential forms arise more generally, *i.e.* within the formal structure of a wide range of physical theories. It turns out that the majority of situations of interest in crystal physics can be described in terms of differential forms* just as in electromagnetism. Moreover, for the present purpose, a further simplification can usefully be effected by considering *local* maps – that is maps that bear the same relationship to differential forms as tensors do to tensor fields and vectors do to vector fields.

In crystal physics, local considerations dominate rather than global ones and it is often only necessary to consider the specification of physical conditions in the vicinity of a single point. The tangent spaces, T_3, can therefore be replaced by a single three-dimensional linear space, **V**, and exterior differential p forms can be replaced by local maps either from $V^{\Lambda(p)}$ or from V^p to R. The latter alternative is more directly useful, simply because the specification of physical conditions in crystal physics always involves (Tonti, 1976) field quantities that are naturally referred to simple p-dimensional geometrical elements, such as, for example, lines, areas and volumes. An appreciation of the importance of numbers read off dials as pointer readings (r), when taken together with an insistence on precision where the labelling of maps is concerned, then leads naturally to the realization that a number of experiments define multilinear and antisymmetrical maps, of degree p, of the form

$$\sigma: \mathbf{V}^p \mapsto R; (\mathbf{u},\ldots,\mathbf{z}) \rightsquigarrow r,$$

where $\mathbf{u},\ldots,\mathbf{z}$ are vectors, *i.e.* elements of the linear space **V**. (These are finite or infinitesimal depending on whether physical conditions are spatially uniform or non-uniform; the two situations are not distinguished notationally.)

Thus, for example, using a search coil in the shape of a parallelogram to determine the magnetic flux, Φ, through it establishes a multilinear map from the ordered pair (**u**, **v**) to Φ where **u** and **v** are spatial vectors that coincide with two adjacent sides of the (**u**, **v**) parallelogram. The order of the pair is immediately determined by the sense of the electrical connections to the measuring instrument, so justifying the statement that the map is also antisymmetrical. When, in general, the experimental arrangements define p vectors $\mathbf{u},\ldots,\mathbf{z}$ taken in a certain order, then the corresponding p-dimensional geometrical element is said to have been thereby equipped with an *inner orientation*. However, there exist other experiments in which the connection between inner orientation and the experimental arrangements is not so direct.

For example, consider a specification of the number, I, of charged particles (*e.g.* electrons) passing, in unit time, through a (**u**, **v**) parallelogram. Now, the direction of progression through the parallelogram does not, of itself, order the vectors **u** and **v** but instead orders any line passing through the parallelogram. When, in general, a **p**-dimensional geometrical element is involved but the experimental arrangements define an inner orientation for a geometrical element of complementary dimension $(3-p)$ having one point in common with the original element, then that original (p-dimensional) element is said to have been thereby equipped with an *outer orientation*. To pass from an outer to an inner orientation it is necessary to make a comparison with a reference set of three vectors that define a standard orientation or handedness (*i.e.* it does not suffice to consider the experimental arrangements alone). Only after this has been done do these experiments define multilinear and antisymmetrical maps, of degree p, of the form

$$\Sigma: \mathbf{V}^p \mapsto R; (\mathbf{u},\ldots,\mathbf{z}) \rightsquigarrow r',$$

where r' is referred to as a W quantity to distinguish it from the ordinary quantity r (for which the experimental arrangements order the vectors $\mathbf{u},\ldots,\mathbf{z}$ uniquely without any need to use a reference set of vectors to pass from an outer to an inner orientation). This differentiation between ordinary and W quantities (*i.e.* between maps of type σ and those of type Σ) is, in fact, the only satisfactory way of distinguishing between two essentially different types of physical fields–a distinction that is not crucial in considering fields in isolation but which becomes so in considering their interactions, *i.e.* in considering properties.

* Strictly speaking, the majority can be described in terms of *scalar-valued* exterior differential forms. The remainder (*e.g.* vector-valued differential forms) are dealt with by Tonti (1976) in the elegant language of fibre bundles (Steenrod, 1951). However, this is beyond the scope of the present article, in which attention is confined to scalar-valued forms (*i.e.* to cases in which an individual fibre is the one-dimensional vector space, R, of real numbers).

3.3. *Applicability to properties*

Consider a linear physical property of a crystal that relates a physical field described by a map of type σ or Σ and of degree p to another physical field described by a map of type σ or Σ and of degree q. Whilst p and q are together analogous, in a sense, to the tensor rank referred to in statement ($S2$) of § 1, the ordinary or W characters of the two physical fields are not together or separately analogous to parity, *i.e.* to even-ness or odd-ness under coordinate inversion. In fact, parity has now disappeared as being an irrelevant factor for the following reasons. As indicated in § 3.2, the difference between maps of type Σ and of type σ is precisely one of use or non-use of a standard reference orientation. However, in progressing from a consideration of experimental arrangements to the mathematical formulation in terms of differential forms *via* the local maps of type σ and Σ, there is at no stage any requirement to assume a metric or to use coordinates. Thus, since both theory and experiment are metric independent and coordinate independent, it would obviously be incorrect to build in a dependence upon coordinates by linking the standard reference orientiation to the orientation of a coordinate system: coordinates have nothing to do with nature but only with Man's choice of description! It is therefore necessary to stipulate that the reference set of three vectors that defines a standard orientation (or handedness) must be considered to be an object *entirely unconnected* with any specification of a set of base vectors for the linear space **V**. There is then seen to be no scope whatever for making predictions about the physical properties of a crystal on the basis of behaviour under coordinate inversion (*i.e.* passive inversion of the frame of reference). On the other hand, active inversion of the crystal (in the sense of replacing a crystal X by an otherwise identical enantiomorphic companion $\bar{X}$) is very relevant and indeed a knowledge of the effect of active inversion holds out an immediate promise of predicting a pattern of nullities analogous to the one referred to in § 1 in discussing statement ($S1$). From what has been said above, it is therefore clear that the basic philosophy of crystal physics should be not ($S2$) but rather the analogous statement

($S3$) The relationship between a property for X and the same property for $\bar{X}$ is predicted as a consequence of a determination of p and q and a determination of the ordinary or W character of influence and effect by inspection of the corresponding experimental situation.

In seeking to establish the exact nature of this relationship it is important to note that the active operation $X \rightarrow \bar{X}$ inevitably depends, in the last analysis, on some conceptual model of the crystal; it is, in this sense, less precisely defined than the passive operation but its use is nevertheless unavoidable, since the passive operation is without direct physical consequences. The model dependence of active operations can have important repercussions (Post, 1978) for the general case of an arbitrary anti-identity operation [*i.e.* $X \rightarrow \tilde{X}$, with $(\tilde{X}) \equiv X$] but the particular case of $X \rightarrow \bar{X}$ is much easier to deal with by virtue of two special simplifying factors.

Firstly, active spatial inversion is a purely geometrical operation, whereas, more generally, $X \rightarrow \tilde{X}$ may involve physical changes (*e.g.* charge reversal). Secondly, the operation $X \rightarrow \bar{X}$ does not require a metric or a basis for its definition; thus, not only are the fields metric independent and coordinate independent but so also is the anti-identity operation itself, which means that the only possible connection, consistent with $(\bar{X}) \equiv X$, between a property for X and the same property for $\bar{X}$ is a map, T, that is plus or minus the identity* map, *i.e.* $T = \omega I$ with $\omega = \pm 1$. This result is exactly what is needed to establish how ω depends upon p, q and the ordinary or W character of the two physical fields.

Since ω can have only two discrete values, namely $+1$ or -1, it is reasonable to suppose, by analogy with ($S1$), that it is only the odd-ness or even-ness of p and q that is important and, therefore, more specifically, to assume that ω depends upon the following four factors

(i) the odd-ness or even-ness of p
(ii) the odd-ness or even-ness of q
(iii) the σ or Σ character of one field
(iv) the σ or Σ character of the other field.

Changes in these four factors generate 16 possible cases to each of which corresponds a particular value of ω. However, if one of these factors is changed whilst the other three remain unchanged, then either ω changes sign or it does not (no other possibilities being open) but the latter possibility can be ruled out as being contrary to the assumption that ω depends upon the factors (i) to (iv). Sequential use of this result allows the 16 values of ω to be interrelated and thereby expressed in terms of one arbitrarily chosen value (denoted by ω_0) in accordance with a simple table (Table 1). $\sigma\Sigma$ indicates an effect of type σ and an influence of type Σ, and so on. It therefore remains only to evaluate ω_0 but,

* This conclusion cannot be sustained when the anti-identity operation requires a metric for its definition, because it may then be possible to use the metric to decompose T uniquely into constituent parts.

Table 1. *Values of ω in terms of ω_0*

	$(p+q)$ odd	$(p+q)$ even
$\sigma\sigma$ or $\Sigma\Sigma$	$\omega = \omega_0$	$\omega = -\omega_0$
$\sigma\Sigma$ or $\Sigma\sigma$	$\omega = -\omega_0$	$\omega = \omega_0$

before this is done, it is necessary to make one further comment.

It should be noted that Table 1 does not reflect any inherent distinction between influence and effect: if these are interchanged (together, of course, with p and q), then the value predicted for ω is unchanged, which is fully justified* for *within* the crystal no trace remains of any distinction between influence and effect.

3.4. *Evaluation of* ω_0

To evaluate ω_0, the simplest type of property to consider is one for which $p = 1$ and $q = 0$; such a situation arises when some scalar influence, φ, produces a map of type σ that places a directed line segment (**u**) into correspondence with a number (**r**). Now consider a crystal (X) that contains a preferred direction within it; this preferred direction will be reversed for $X \to \bar{X}$, so that the above map cannot be even under $X \to \bar{X}$ and the corresponding value of ω must therefore be -1. A comparison with Table 1 immediately reveals that this gives $\omega_0 = -1$

Alternatively, it is possible to consider a situation in which some scalar influence produces a map of type Σ that places a line segment with outer orientation into correspondence with a number. Now consider a crystal (X) that contains within it a prefixed axis and a preferred direction of circulation around that axis; both remain unchanged for $X \to \bar{X}$, so that the corresponding ω must therefore be $+1$ and this implies, again, that $\omega_0 = -1$.

Properties of the above type (*i.e.* with $p = 1$ and $q = 0$) are sometimes referred to as spontaneous properties and they constitute a useful device by which ω values may be deduced. To each non-spontaneous physical property there correspond two constituent spontaneous properties, and a comparison of Table 1 with the corresponding table for a spontaneous property reveals that the correct value of ω for the non-spontaneous property can always be obtained by multiplying together the two values for the constituent properties. The use of the word 'device' refers to the fact that the above remains true even if one or both of the two constituent spontaneous properties does not exist: for the purpose of calculating the value of ω appropriate to the non-spontaneous property, *it is as if* all three effects co-existed.

* If the number of physical fields exceeds two, as, for example, in the case of a linear relationship between two influences and two effects, then the justification is not so immediately obvious, as it is necessary to examine the inversion of the whole map connecting all four fields rather than just the parts connecting one influence and effect. In general, it is necessary to consider a number of pairs of what Tonti (1976) calls *variabili di configurazione* and *variabili di sorgente*, that is configuration variables and variables pertaining to the source of change in configuration.

4. Conclusions

The description provided by crystal physics according to which tensors are classified by reference to rank and parity has been shown to be fundamentally deficient. A superior description is in terms of differential forms with rank having been replaced by the degree of the form and parity having been replaced by whether inner or outer orientation is involved. What is then important is not the behaviour of physical properties under passive inversion but the behaviour under active inversion, and Table 1 (with $\omega_0 = -1$) enables this to be predicted from a knowledge of the aforementioned factors.

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Polarization Ratios for Repeatedly Reflected X-ray Beams

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Abstract

The polarization ratio for a repeatedly reflected X-ray beam has been calculated, assuming the Darwin formulism, in the case where the diffracting planes of the crystals are parallel. It is shown that polarization ratios lie closer to unity than those obtained using the kinematic approximation. The integrated intensities and polarization ratios from a double-crystal spectrometer are discussed. The polarization ratio for a graphite monochromator has been measured experimentally and shown to be close to the value predicted by the Darwin theory and significantly different from the kinematic value.

Introduction

The degree of polarization which results from the scattering of an X-ray beam by a crystal depends on the polarization of the incident beam, the degree of perfection of the crystal and on the strength of interaction between the X-ray beam and the crystal, as well as the scattering angle. If the incident beam is unpolarized and the crystal is perfect, the polarization ratio, *i.e.* the ratio of the intensity scattered parallel to the diffraction plane to that scattered perpendicular to the diffraction plane, is $|\cos 2\theta|$, where θ is the Bragg angle. For an ideally mosaic crystal, to which the kinematic theory can be applied, the corresponding ratio will be $\cos^2 2\theta$. However, for a real mosaic crystal, where there is a strong interaction between the incident beam and the crystal, the kinematic theory will not apply and this will be particularly true if the diffracting crystal planes have a large structure factor and the crystal itself is large. Such a situation occurs when the crystal is being used as a monochromator or a focusing device and, in these cases, as has been pointed out by Jennings (1981), extinction theory applies.

Lawrence (1982) has shown that in the case of pyrolytic graphite, a commonly used monochromating material diffracting a large intensity from the (002) planes, the scattering can be described by the Darwin formulism. The reflectivity, R, in the symmetrical Bragg case, assuming no transmitted beam, is given by

$$R = \frac{\sigma + \mu/\gamma - [(\sigma + \mu/\gamma)^2 - \sigma^2]^{1/2}}{\sigma}.$$

σ is the reflectivity per unit length, γ is the direction cosine of the incident and diffracted beams and μ is the linear absorption coefficient. These are the symbols used by Weiss (1966). The reflectivity can be calculated separately for both polarizations, giving $R_{\parallel}$ and $R_{\perp}$ and thus the polarization ratio of the diffracted beam, $R_{\parallel}/R_{\perp}$, is found. The polarization ratio is thus a function of the mosaic spread of the crystal and the polarization ratios calculated in this manner are always greater than $\cos^2 2\theta$.

In this paper, the polarization factor of a repeatedly reflected X-ray beam is calculated and the measurement of the polarization ratio of a graphite crystal described.

Repeatedly reflected beam

The polarization factor for a repeatedly reflected beam has been studied by Vincent (1982). In the special case where the diffracting planes were parallel ($\rho = 0°$ geometry), it was shown that, if the crystals were

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