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1963

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Abstract

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CRYSTALLOGRAPHY

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MAGNETIC SPACE SYMMETRY OF TENSORS

(Presented by Academician A. V. Shubnikov, February 16, 1963)

In ⁽¹⁾ tensors were considered that are defined on the direct product of the rotation group* $\infty\infty\infty$ by the inversion group $\bar{1}1'$; these tensors are subdivided into four types, depending on according to which of the four irreducible representations of the inversion group they transform. In the same place a method was set forth that makes it possible to find the form of a tensor of any of these types that is invariant with respect to a given point group of magnetic symmetry. Here these ideas are generalized to the space groups of magnetic symmetry—the Shubnikov groups.

Shubnikov groups are subgroups of the so-called magnetic Euclidean group—the direct product of the group of motions by the inversion group $\bar{1}1'$. On this group tensors must also be defined that are invariant with respect to Shubnikov groups. We shall call elements of the magnetic Euclidean group $\{t | R^q IPC(\mathbf{k}, \varphi)\}$ coordinate transformations consisting of the transformation $R^q IPC(\mathbf{k}, \varphi) \in \infty\infty\infty \times \bar{1}1'$ and the subsequent translation of the coordinate system by the vector \mathbf{t} . $C(\mathbf{k}, \varphi)$ is a rotation through an angle φ , in the right-hand screw sense, about an axis determined by the unit vector \mathbf{k} ; I is inversion, R is anti-identity (change of the direction of time reckoning). If before the transformation $\{t | R^q IPC(\mathbf{k}, \varphi)\}$ the Cartesian coordinates** of a certain point were x_k , then after it its coordinates will be $x_{i'} = \{t | R^q IPC(\mathbf{k}, \varphi)\}x_k = (-1)^p c_{i'k} x_k - t_{i'} = (-1)^p c_{i'k} (x_k - t_k)$ ($c_{i'k}$ is the matrix of direction cosines of the rotation $C(\mathbf{k}, \varphi)$), and the direction of time reckoning changes to the opposite one if q is odd. If in some system of Cartesian coordinates the components of a tensor $A_{i_1 \dots i_s}(\mathbf{r})$ are given, then their transformation law is as follows:

$$\begin{aligned} \{t | R^q IPC(\mathbf{k}, \varphi)\} A_{i_1 \dots i_s}(\mathbf{r}) &= A_{i'_1 \dots i'_s}(\mathbf{r}') = \\ &= \chi_\Gamma(R^q IP) c_{i'_1 i_1} \dots c_{i'_s i_s} A_{i_1 \dots i_s}((-1)^p c_{j'j} (r_j - t_j)). \end{aligned} \quad (1)$$

Here $\chi_\Gamma(R^q IP) = \pm 1$ is the character of the element $R^q IP$ in the representation Γ of the group $\bar{1}1'$, according to which the tensor A transforms (see Table 1 of the paper ⁽¹⁾); r_j and t_j are the components of the vectors \mathbf{r} and \mathbf{t} in the old coordinate system.

Since the translational components of the elements of the magnetic Euclidean group act only on the argument \mathbf{r} of the tensor, it is clear that the only nontrivial tensors defined on this group will be tensor-

* In contrast to ⁽¹⁾, here international designations of point and space groups of ordinary and magnetic symmetry are used ^(2,3).

** We specify the coordinate system by an orthonormal vector basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ and by indicating the direction of time reckoning. Since any transformation of the magnetic Euclidean group converts this basis into one that is likewise orthonormal, one may (although, of course, this is not necessary) restrict consideration to Cartesian (orthogonal) coordinate systems and orthogonal tensors.

functions of a point. Therefore such tensors are also introduced into consideration. However, we shall not impose any conditions of continuity, differentiability, etc., on the functions $A_{i_1 \dots i_s}(\mathbf{r})$. Moreover, sometimes, in view of physical applications, it is convenient to assume that the tensors $A(\mathbf{r})$ are nonzero only at isolated points; then they can be interpreted, for example, as sources of force fields localized in a crystal lattice: scalars may describe, say, electric charges, vectors of electric type—electric dipole moments, vectors of magnetic type—magnetic moments, and deviators of even type—quadrupole moments.

Tensors describing the microscopic physical properties of a crystal must, naturally, be invariant with respect to the Shubnikov group of the crystal S_k : if $\{t \mid R^q I^p C(\mathbf{k}, \varphi)\} \in S_k$, then $\{t \mid R^q I^p C(\mathbf{k}, \varphi)\} A_{i_1 \dots i_s}(\mathbf{r}) = A_{i_1 \dots i_s}(\mathbf{r})$. These are the tensors that we shall consider here.

A tensor $A(\mathbf{r})$ invariant with respect to the group S is, of course, invariant with respect to any of its subgroups, in particular with respect to its translation subgroup T . The elements of the translation subgroup have the form $\{n^k \mathbf{a}_k \mid E\}$, where E is the identity, \mathbf{a}_k ($k = 1, 2, 3$) are the basic vectors of the lattice ⁽⁴⁾, and n^k are integers*. Hence it follows that

$$A_{i_1 \dots i_s}(\mathbf{r} + n^k \mathbf{a}_k) = A_{i_1 \dots i_s}(\mathbf{r}), \quad (2)$$

i.e., the components of such a tensor are periodic functions of a point. The spatial period, or elementary cell, of the tensor $A(\mathbf{r})$ coincides, generally speaking, with the elementary (magnetic) cell of the group S , but may also be smaller. Thus, in 517 groups with “colored” translations ⁽³⁾, along with the ordinary translational elements $\{n^k \mathbf{a}_k \mid E\}$, there are antitranslations of the form $\{\bar{\alpha} + n^k \mathbf{a}_k \mid R\}$. On tensors of even and electric type they act as ordinary translations, since in this case $\chi_T(R) = 1$, and

$$\{\bar{\alpha} + n^k \mathbf{a}_k \mid R\} A_{i_1 \dots i_s}(\mathbf{r}) = A_{i_1 \dots i_s}(\mathbf{r} - \bar{\alpha} - n^k \mathbf{a}_k).$$

Thus the elementary cell of tensors of even and electric types turns out in this case, as was to be expected, to be the “crystal-chemical” cell, half as large in volume as the magnetic one. Conversely, for tensors of magnetic and magneto-electric types $\chi_T(R) = -1$,

$$\{\vec{\alpha} + n^k \mathbf{a}_k \mid R\} \times A_{i_1 \dots i_s}(\mathbf{r}) = -A_{i_1 \dots i_s}(\mathbf{r} - \vec{\alpha} - n^k \mathbf{a}_k),$$

so that the elementary cell for them coincides with the magnetic elementary cell.

In 230 “gray” Shubnikov groups, along with the elements $\{n^k \mathbf{a}_k \mid E\}$, there are also elements $\{n^k \mathbf{a}_k \mid R\}$, in particular the element $\{0 \mid R\}$. This leads to the fact that all tensors of magnetic and magneto-electric types invariant with respect to such groups are identically equal to zero; this follows directly from the fact that $\{0 \mid R\}A_{i_1 \dots i_s}(\mathbf{r}) = -A_{i_1 \dots i_s}(\mathbf{r})$. It is interesting to note that neither inversion I nor anti-inversion RI acts so destructively; thus, although for tensors of electric and magnetic type $\chi_T(RI) = -1$, the action of anti-inversion on them is expressed by the formula $\{0 \mid RI\}A_{i_1 \dots i_s}(\mathbf{r}) = -A_{i_1 \dots i_s}(-\mathbf{r})$ —this by no means yet implies that $A(\mathbf{r}) \equiv 0$.

In what follows we shall assume that the periodicity condition (2) is fulfilled. Therefore it will suffice to consider the action on tensor components of the operations $\{\vec{\alpha} \mid R^q IPC(\mathbf{k}, \varphi)\}$, where $\vec{\alpha} = \alpha^k \mathbf{a}_k$, with $0 \leq \alpha^k < 1$. The number of such operations is equal to the order of the magnetic point group of the crystal M_k . Thus, we consider our tensors within the limits

* n^k are, in essence, the contravariant components of a lattice vector in the basis $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$.

of a single elementary cell of the crystal. Points within one elementary cell are subdivided into points of general and special position. The former are not mapped onto themselves by any operations $\{\vec{\alpha} \mid R^q IPC(\mathbf{k}, \varphi)\}$ except $\{0 \mid E\}$, whereas for the latter, among $\{\vec{\alpha} \mid R^q IPC(\mathbf{k}, \varphi)\}$ there will also be other operations that map the given point onto itself. These operations form the point magnetic group $M(\mathbf{r})$ —the group of magnetic symmetry of the given point of crystalline space.*

If \mathbf{r}_0 is a point of general position, then the components of the tensor $A_{i_1 \dots i_s}(\mathbf{r}_0)$, specified at this point, are not related to one another by any symmetry operations. Therefore the point symmetry of the tensor $A(\mathbf{r}_0)$ for fixed \mathbf{r}_0 of general position is the minimal magnetic point symmetry of the given tensor. For example, if A is a vector of electric type, it is equal to $\infty mm1'$; if A is a vector of magnetic type, $\infty / mm'm'$; if A is a deviator of even type, $mm21'$; if A is a nonsymmetric tensor of the second rank of magnetoelectric type, $\bar{1}$, etc.

If, however, \mathbf{r}_0 is a point of special position, then the point magnetic symmetry $M_A(\mathbf{r}_0)$ of the tensor $A(\mathbf{r}_0)$ for fixed \mathbf{r}_0 is not lower than $M(\mathbf{r}_0)$. It can be

found from (1) as the magnetic symmetry of a material tensor A describing some property of a crystal of symmetry M . In doing so one should use the method set forth in (5), since the sought symmetry of the tensor is often higher than the symmetry of the tensor-function of a scalar parameter.** At some points of special position \mathbf{r}_0 , it follows from symmetry considerations that $A(\mathbf{r}_0) = 0$ (for example, if \mathbf{r}_0 is a center of symmetry and A is a tensor of electric or magnetoelectric type).

Next it is natural to introduce the concept of the spatial magnetic symmetry of a tensor. In accordance with the known definition of the point symmetry of a tensor (6), we shall call the Shubnikov group S_A the group of magnetic spatial symmetry of the tensor $A(\mathbf{r})$, if its components $A_{i_1 \dots i_s}(\mathbf{r})$ are invariant with respect to all transformations belonging to the group S_A , and S_A is the highest group possessing this property. Thus, if $\{\mathbf{t} \mid R^q IPC(\mathbf{k}, \varphi)\} \in S_A$ (and only in this case),

$$\{\mathbf{t} \mid R^q IPC(\mathbf{k}, \varphi)\} A_{i_1 \dots i_s}(\mathbf{r}) = A_{i_1 \dots i_s}(\mathbf{r}). \quad (3)$$

The Shubnikov group S_A of the tensor $A(\mathbf{r})$ is not lower than the Shubnikov group S_k of the crystal, but may be higher than it, even if the tensor $A(\mathbf{r})$ is, by definition, nonzero at points of general position. For example, if S_k is not a “gray” group and A is a tensor of even or electric type, then S_A is in any case not lower than $S_k \times 1'$. However, in contrast to the point symmetry of tensors, one can no longer assert, say, that the Shubnikov group of a tensor of even type is centrosymmetric. If, for example, $S_k = P1$, then, although the point symmetry of such a tensor at each point is $\bar{1}1'$, the spatial symmetry of the whole tensor field is $S_A = P1'$. If, however, the tensor $A(\mathbf{r})$ is nonzero only at one point of the elementary cell, then $S_A = \bar{P}11'$. A further increase of the spatial symmetry of the tensor to $\bar{P}11'$ is due to the fact that the number of points of general position at which the given tensor is (by definition) nonzero is insufficient to reveal all possible dissymmetry of the given tensor field in the given crystalline space.

* If the origin is placed at the given point, all these operations, of course, are written in the form $\{0 \mid R^q IPC(\mathbf{k}, \varphi)\}$, but with another choice of origin the same operations may have the form $\{\bar{\alpha} \mid R^q IPC(\mathbf{k}, \varphi)\}$, where $\bar{\alpha} \neq 0$.

** In (5) the two symmetries differ as the symmetry of a tensor and the symmetry of a physical property, respectively.

Let us consider, in conclusion, the averaging of the tensor $A(\mathbf{r})$ over an elementary cell. The averaged tensor

$$\bar{A}_{i_1 \dots i_s} = V^{-1} \int_V A_{i_1 \dots i_s}(\mathbf{r}) dV$$

(or

$$\bar{A}_{i_1 \dots i_s} = V^{-1} \sum_n A_{i_1 \dots i_s}(\mathbf{r}_n),$$

if $A(\mathbf{r})$ differs from zero only at the points \mathbf{r}_n) proves to be a material tensor of the crystal; if, for example, $A(\mathbf{r})$ describes dipole moments distributed in a crystal lattice, then \bar{A} is the dipole moment per unit volume of the crystal, i.e., the vector of spontaneous polarization. The tensor \bar{A} , since it does not depend on the coordinates, is characterized by the point group of magnetic symmetry $M_{\bar{A}}$, corresponding to the Shubnikov group* S_A .

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Received
6 II 1963

CITED LITERATURE

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* More precisely, $M_{\bar{A}}$ is the factor group of the group S_A with respect to the subgroup of translations T : $M_{\bar{A}} = S_A/T$.

Note: Figure translations are in progress. See original paper for figures.

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