match no. 8 pp. 3 - 19 1980

THE SYMMETRY OF IMPERFECT CRYSTALS

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(received: March 1980)

Broken symmetry is a usual approach in physics of imperfect crystals. This approach presupposes that the function $\delta\rho(\vec{r})$ which describes the electron density deviation of imperfect crystals from a certain ideal distribution $\rho^{\circ}(\vec{r})$ has Fedorov-Schönflies space symmetry, that is a subgroup $\mathfrak{G}_{\delta\rho} \subset \mathfrak{G}_{\rho^{\circ}}$ of the symmetry group of undisturbed crystal.

In this approach I. M. Lifschitz [1] was the first to develop the theory of the isolated impurity atom in crystal. Since then this theory has been applied to different physical situations: The impurity influence on the electronic spectra of metals [2], on the crystal lattice vibrations [3], on the spin perturbation spectra in ferromagnetics [4], on the dielectric and unelastic relaxation [5] etc.

In every case there was discovered a general law: impurity atom in crystal with the quasicontinuous spectrum of the elementary perturbations brings local perturbation, the latter leading to the appearance of discrete lines out of the band of the ideal crystal, that is so-called quasilocal or resonance levels.

It is expedient to use the broken symmetry approach when the symmetry decrease $\mathfrak{G}_{\rho} \subset \mathfrak{G}_{\rho^{\circ}}$ removes the degeneracy of the physical

states of the system. In general case when there is an additional (unaccidental) degeneracy which is not described by the group $\mathfrak{G}_\rho$ or when additional coordinates (or degrees of freedom) of the physical system are taken into account it is necessary to apply the approaches of the preservation or extension of the abstract symmetry group [6,7].

Let us suppose that the electron density deviation function $\delta\rho(\vec{r})$ has its proper symmetry group $\Omega_{\delta\rho}$ which does not coincide with any of the classical space groups but may have the Fedorov- Schönflies subgroup $\mathfrak{G}_{\delta\rho} \subseteq \Omega_{\delta\rho}$. It follows then from the equation

$$\rho(\vec{r}) = \rho_\circ(\vec{r}) + \delta\rho(\vec{r})$$

that the classical space symmetry group of the imperfect crystal with the electron density distribution $\rho(\vec{r})$ will be

$$\mathfrak{G}_\rho = \mathfrak{G}_{\rho_\circ} \cap \mathfrak{G}_{\delta\rho} \subseteq \mathfrak{G}_{\rho_\circ}, \quad \mathfrak{G}_\rho \times \rho(\vec{r}) \longrightarrow \rho(\vec{r})$$

which means the common part (or intersection) of both groups $\mathfrak{G}_{\rho_\circ}$ and $\Omega_{\delta\rho}$ (see Fig. 1). It constitutes in fact the broken symmetry approach.

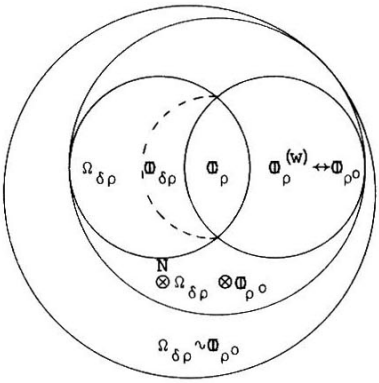

Fig.1 Euler Diagrams show the relation between symmetry groups of imperfect crystal with electron density function $\rho(\vec{r}) = \rho_o(\vec{r}) + \delta\rho(\vec{r})$. In the broken symmetry approach $\Omega_\rho^{(w_q)} = \mathfrak{W}_\rho = \Omega_{\delta\rho} \cap \mathfrak{W}_{\rho o} \subset \mathfrak{W}_{\rho o}$. In the approach of symmetry conservation $\Omega_\rho^{(h)} = \mathfrak{W}_\rho^{(h)} \leftrightarrow \mathfrak{W}_{\rho o}$ $(h = p, q, w_p, w_q)$. In that of symmetry extension $\Omega_\rho = G^C \circledast \mathfrak{W}_\rho^{(h)}$ where the proper symmetry of the function $\rho(\vec{r})$ at the fixed point $\vec{r}$ is characterized by appropriate symmetrizer G^C[6,7]. In every case $\Omega_\rho \subseteq \widetilde{\Omega}_{\delta\rho} \wr \mathfrak{W}_{\rho o}$ or $\Omega_\rho \subseteq \overset{N}{\circledast} \widetilde{\Omega}_{\delta\rho} \circledast \mathfrak{W}_{\rho o}$, $\Omega_{\delta\rho} \subseteq \widetilde{\Omega}_{\delta\rho}$, $\mathfrak{W}_{\rho o} = \mathfrak{W}_{\mathrm{mod}N}$.

In this approach one neglects the additional symmetry properties of the function $\rho(\vec{r})$. If such an admission turns out to be too rough for the physical system under consideration it is necessary to construct the direct product of two groups $\widetilde{\Omega}_{\delta\rho} \circledast \mathfrak{W}_{\rho o}$ or the wreath product $\widetilde{\Omega}_{\delta\rho} \wr \mathfrak{W}_{\mathrm{mod}N}$. In the latter case

it is convenient to restrict the space group $\mathfrak{G}_{\rho^\circ} = \mathfrak{G}_{\mathrm{mod}N}$ on modulo N where N is a big figure:

$$\tilde{\Omega}_{\delta\rho} \wr \mathfrak{G}_{\rho^\circ} = (\tilde{\Omega}_{\delta\rho}^{\Phi_1} \otimes \ldots \otimes \tilde{\Omega}_{\delta\rho}^{\Phi_N}) \textcircled{S} \mathfrak{G}_{\mathrm{mod}N} = \overset{N}{\underset{\otimes}{}} \tilde{\Omega}_{\delta\rho} \textcircled{S} \mathfrak{G}_{\mathrm{mod}N}$$

As is known the direct product of two groups is well defined without restrictions, but the wreath product exists only in the case when N- fold direct product $\overset{N}{\underset{\otimes}{}} \tilde{\Omega}_{\delta\rho}$ forms an invariant subgroups of $\tilde{\Omega}_{\delta\rho} \wr \mathfrak{G}_{\rho^\circ}$ which means that $\Phi_i \tilde{\Omega}_{\delta\rho} \Phi_i^{-1} = \tilde{\Omega}_{\delta\rho}$, $\Phi_i \in \mathfrak{G}_{\mathrm{mod}N}$. If necessary the symbol $\textcircled{S}$ of the semidirect product may be replaced by $\textcircled{\otimes}$ to receive an other useful construction free from such a restriction.

Now the symmetry group of the composite function $\rho(\vec{r}) = \delta\rho(\vec{r}) + \rho^\circ(\vec{r})$ may be defined as the maximal subgroup $\Omega_\rho = \Omega_{\delta\rho} \mathfrak{G}_{\rho^\circ}$ of the wreath product $\tilde{\Omega}_{\delta\rho} \wr \mathfrak{G}_{\rho^\circ}$ which preserves the function $\rho(\vec{r})$

$$\Omega_{\delta\rho} \mathfrak{G}_{\rho^\circ}(\delta\rho + \rho^\circ) = \Omega_{\delta\rho} \cdot \delta\rho + \mathfrak{G}_{\rho^\circ} : \rho = \delta\rho + \rho^\circ = \rho, \Omega_\rho \subseteq \tilde{\Omega}_{\delta\rho} \wr \mathfrak{G}_{\rho^\circ} + \Omega_{\delta\rho} \subseteq \tilde{\Omega}_{\delta\rho}$$

Which of the subgroups of wreath product becomes the symmetry group Ω_ρ depends on the model of imperfect crystal under consideration. As a first approximation to Ω_ρ it is convenient to choose a junior group $\Omega_\rho \leftrightarrow \mathfrak{G}_{\rho^\circ}$ isomorphic to $\mathfrak{G}_{\rho^\circ}$ according to the law of conservation of the abstract symmetry group of the isolated physical system, under which the summary symmetry of such a system is never lost: One kind of symmetry is transformed into another [6,7]. The effect of this law can be observed -

- in the phenomenon of crystal structure memory, the statistical preservation of the initial symmetry group at the level of domain structure after a phase transition, etc.

To construct the group $\Omega_\rho \leftrightarrow \mathbb{D}_{\rho\bullet}$ let us replace the classical transformations $\Phi_i \in \mathbb{D}$ lost after the symmetry decrease $\mathbb{D}_\rho \subset \mathbb{D}_{\rho\bullet}$ by generalized transformations $\Phi_i^{(w_i)} = \langle w_i | \Phi_i \rangle$

$$\mathbb{D}_{\rho\bullet} = \mathbb{D}_\rho \Phi_1 \cup \mathbb{D}_\rho \Phi_2 \cup \ldots \cup \mathbb{D}_\rho \Phi_s \leftrightarrow \mathbb{D}_\rho \Phi_1 \cup \mathbb{D}_\rho \Phi_2^{(w_2)} \cup \ldots \cup \mathbb{D}_\rho \Phi_s^{(w_s)} = \mathbb{D}_\rho^{(w)} = \Omega_\rho$$

The selection of loads w_i to the transformation $\Phi_i (i=2,\ldots,s; \Phi_1 = e)$ is realized according to the algorithms of constructing of color positional groups [6,8]. Let us illustrate this algorithm on the following example.

Fig. 2 represents a unit cell corresponding to the point group G = 4 mm. The positions of the triangles in the regular set of figures are marked by the symbols of operations $g_i \in G$, the white and black colours marking conventionally the physical states of the figures: The black triangle may model a vacancy of impurity atom, for instance. The color positional symmetry group of a system under consideration may be designeted by the symbol $G = 4^{(12)}m^{(12)}m^{(12)}$, showing in the brackets the untrivial cyclic permutation of colours (12) connected with the operations 4 and m: rotation at 90° around the axis 4 is connected with the transition of the positions 1 and 4^3 to the positions 4 and 1 and with the recolouring of the triangles. The remaining positions under operation 4 exchange their positions without recolouring.

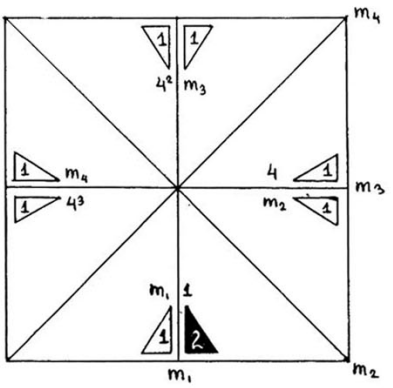

Fig. 2 The point symmetry group $G^{(w)} = 4^{(12)}m^{(12)}m^{(12)}$ of the unit cell containing a vacancy or impurity atom (the blackened triangle) is defined by the positional operators $\langle w_i|g_i\rangle = \langle p_i^{g_1}\ldots p_i^{g_n}|g_i\rangle$, $g_i \in G=4mm, p_i \in P=\{p_1=(1)(2), p_2=(12)\}$ and the multiplication law $\langle w_i|g_i\rangle\langle w_j|g_j\rangle=\langle w_i^{g_j}w_j|g_ig_j\rangle=\langle p_i^{g_jg_1}p_j^{g_1}\ldots p_i^{g_jg_n}p_j^{g_n}|g_ig_j\rangle$[9].

Fig. 3 gives a fragment of a two-dimensional crystal with a constant defect density, unit cells (UC) containing a point defect of the kind of Fig. 2, a being blackened. Let us perform the scaling transformation to the enlarged unit cell (EUC). The translation group T will be in this case the extension of the subgroup T' of T corresponding EUC by means of the finite group $T_{modT'}$ composed of representatives of cosets in the decomposition

$$T=T'\otimes T_{modT'}=T'\otimes\{0,t_1,t_1^2,t_2,t_2^2,t_2^3,t_1t_2,t_1t_2^2,t_1t_2^3,t_1^2t_2,t_1^2t_2^2,t_1^2t_2^3\}.$$

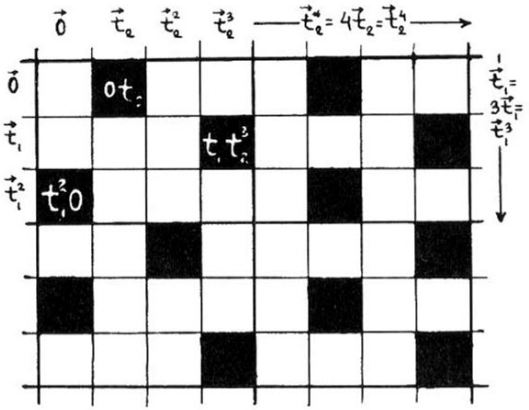

Fig. 3 The translation group $T_{modT'}$ of the finite order corresponding to the enlarged unit cell of two-dimensional crystal with the constant defect density (the blackened unit cells) is defined by the multiplication law of the positional operators $\langle w_i | t_1^{\alpha_i} t_2^{\beta_i} \times w_j | t_1^{\alpha_j} t_2^{\beta_j} \rangle = \langle w_i^{t_1^{\alpha_j} t_2^{\beta_j}} w_j | t_1^{(\alpha_i+\alpha_j)} t_2^{(\beta_i+\beta_j)} \rangle$ and the cyclic boundary conditions $(\vec{t}_1\vec{0})^3 = (\vec{0}\vec{t}_2)^4 = (\vec{t}_1\vec{t}_2)^{12} = \vec{0}\vec{0}$ (modT')

Having defined $T_{modT'}$, we go to the color positional group $T^{(w)}_{modT'}$, combining the transformations $t_1^{\alpha} t_2^{\beta} \in T_{modT'}$, $(\vec{t}_1^3 = \vec{t}_2^4 = \vec{0})$ by the appropriate loads, and from the latter to full translational group $T^{(w)} = T' \otimes T^{(w)}_{modT'}$. The space symmetry group of the model will become then a semi-direct product $\mathfrak{G}^{(w)} = T^{(w)} \circledS G^{(w)}$.

The detailed information on the multiplication law of the positional space operators and their effects on "colour" points can be found in [9]. Without dwelling on it let us point out that the general symmetry groups of imperfect crystals $\mathfrak{D}_{\rho}^{(w)}$ isomorphic to Fedorov-Schönflies group $\mathfrak{D}_{\rho}$ serve as precise positional representation of the latter and in this capacity they answer the basic requirements for the symmetry groups. They present a geometrical description of imperfect crystal structure model, impose restrictions, predict and describe physical properties of the model in point. At last they become classical groups when the defect density approaches zero. Withal the content of appropriate physical theory is not impoverished but on the contrary enriched by the considerations of the internal degrees of freedom of the system and the transition to the non-linear description.

The broken symmetry approach fails for the system properties. The physical properties of the imperfect crystal as a whole system are described more precisely and completely by generalized groups. From the point of view of the generalized symmetry the imperfect crystal is a split object, i.e. a composition of Fedorov and non-Fedorov subspaces with its distant translation ordering defined not globally, but at the level of one or several basic substructures embedded in non-Fedorov space. Fig.1 shows the relations between the symmetry groups of imperfect crystals in the approaches of conservation and extension of the abstract symmetry group.

Let us consider now the phase interpretation of colour groups. According to the well-known relation

$$\rho(\vec{r}) = \frac{1}{v} \Sigma \Sigma \Sigma F(\vec{H}) e^{-2\pi i \vec{H}\cdot\vec{r}}$$ between

the electron density function $\rho(\vec{r})$ and the structure amplitude

$$F(\vec{H}) = \sum_j f_j e^{2\pi i \vec{H}\cdot\vec{r}} = |F(\vec{H})| e^{i\varphi(\vec{H})}$$

the space symmetry group $\mathfrak{G}=TG$ of the physical space $\rho(\vec{r})$ maps homomorphically onto the point symmetry group $G \leftrightarrow \mathfrak{G}/T$ of the Fourier space $F(\vec{H})$ [13,14]. It follows from the equivalency relation $\vec{H}\cdot\hat{g}\vec{r} \leftrightarrow \hat{g}^{-1}\vec{H}\cdot\vec{r}$. According to the Fridel law the symmetry group of F(H) includes the space inversion operators $\bar{1}$ and operators of combined inversion $\bar{1}^* = 1^*\bar{1} = \bar{1}1^*$, the 1^* being the operator of complex conjugation:

$\bar{1}F(\vec{H}) = F(-\vec{H}) = F(\vec{H})$, $\bar{1}^*F(\vec{H}) = F^*(-\vec{H}) = F(\vec{H})$

In symbols: $\mathfrak{G} \times \rho(\vec{r}) \rightarrow \rho(\vec{r})$ $\quad \Phi_i\rho(\vec{r}) = \rho(\phi_i^{-1}\vec{r}) = \rho(\vec{r})$, $\Phi_i \in$

$\downarrow \qquad\qquad \Downarrow$ or

$(\bar{1} \otimes \bar{1}^*) \otimes G \times F(\vec{H}) \rightarrow F(\vec{H})$ $\quad g_iF(\vec{H}) = F(g_i^{-1}\vec{H}) = F(\vec{H})$, $g_i \in G \leftrightarrow \mathfrak{G}/T$

The direct factor $\bar{1} \otimes \bar{1}^*$ presents the properties of the "supersymmetry" of the function $F(\vec{H})$ connected with its proper structure while subgroup G maps symmetry properties of the function $\rho(\vec{r})$ onto the function $F(\vec{H})$.

Let us ascribe to every node of reciprocal lattice the phase $\varphi(\vec{H})$ which corresponds to the node in the Fourier representation.

The symmetry of phase space thus constructed $\{(\varphi(\vec{H}),\vec{H})\}$ will be a colour positional symmetry, corresponding to the systematical extinction conditions of x-ray reflection imposed on F(hkl). The four rules of extinction(l = 4n, 4n + 1, 4n + 2, 4n + 3) for the group $\mathfrak{G}=P4_1$ lead to four ways of ascribing the phases $\varphi(\vec{H})$ to the nodes $\vec{H}$ with equal amplitudes $|F(\vec{H})|$ [15], and to four groups of symmetry $4/m^*$, $4^{(4)}/m^{(2_z^*)}$, $4^{(2_z)}/m^*$, $4^{(4^{-1})}/m^{(2_z^*)}$ of the phase space, coming under one positional group $4^{(1,4,2_z,4^{-1})}/m^{(1^*,2_z^*,1^*,2_z^*)}$. Defining the local systems of reference x, iy at every nodes $\vec{H}$, which are parallel to each other, and constructing the phase vector $\vec{\varphi}(\vec{H})$ of the length of $|F(\vec{H})|$ at an angle of $\varphi(\vec{H})$ to the axis x in every Gaussian plane we get a convenient vector interpretation of the phase space $\{(\vec{\varphi}(\vec{H}),\vec{H})\}$, an analogue of the magnetic crystal structure.

In the vector interpretation the operator 1^* performs the inversion of phases $1^*\varphi(\vec{H}) = -\varphi(\vec{H})$, in the scalar one $1^*(\varphi,\vec{H}) = (\varphi+\pi,\vec{H})$, while combined operators $g^{(p)} = pg$ transform the points $(\varphi,\vec{H})$ of the phase space into the points equivalent ($\cong$) to them under the phase symmetry:

$$pg(\varphi,\vec{H}) = (p\Phi,g\vec{H}) \cong (\varphi,\vec{H}),\quad p\in P \leftrightarrow \bar{G}/H$$
$$P \subset 1^* \otimes \infty\infty,\quad H \lhd \bar{G} = \bar{1} \otimes G,\quad g\in G \leftrightarrow \mathfrak{G}/T$$

To pass from the scalar phase structure to the vector one it is sufficient to replace the points $(\varphi,\vec{H})$ by the points $(\vec{\varphi},\vec{H})$. In

the vector interpretation the phase symmetry group of the example reelives the symbol $4^{(1,4,2_z,4^{-1})}/m^{(2x,2y,2x,2y)}$. Since $1' \overset{\circ}{s}(\vec{r}) = -\overset{\circ}{s}(\vec{r})$ the replacement of the operators $1' \leftrightarrow 1^*$ brings the magnetic and phase symmetry groups to one-to-one correspondence allowing to consider them as physically distinct interpretations of the same abstract colour P- and Wp- symmetry groups. All phase symmetry groups of the Fourier spaces corresponding to 230 Fedorov-Schönflies groups were derived by A. Ju. Papaew, E. H. Ovchinnicova and the author in 1976.

Describing the electron density distribution of imperfect crystal by the composite function $\rho(\vec{r}) = \rho^\circ(\vec{r}) + \delta\rho(\vec{r})$ and considering $\delta\rho(\vec{r})$ as a weak perturbation of some ideal distribution $\rho^\circ(\vec{r})$ we can find in the same way the non-classical symmetry groups Ω_ρ of imperfect crystal, $\Omega_\rho \times \rho(\vec{r}) \to \rho(\vec{r})$ and their images in the Fourier space. The adequacy criterium of the crystal deviation model will be of course the correspondence of the observed and calculated intensities of X-ray reflexes.

Let us consider as an example the symmetry of the space modulated phases of Na_2CO_3 crystal. The so-called "incommensurate" modulation in that crystals appears below $T_i = 620^\circ$ K. The temperature dependence $\vec{q}_o(T)$ of the wave vector of the modulation wave is shown at Fig. 4 [16]. In the reference system $\vec{a}^*, \vec{b}^*, \vec{c}^*$ of three dimensional reciprocal lattice T (3) corresponding to the main reflections of the basic crystal structure $\rho^\circ(\vec{r})$ these

reflections have numerical indices (hkl) while the components $\vec{q}_1, \vec{q}_3$ of the wave vector of the harmonic atom displacements wave run continuously all the real values at the segments $0{,}182a^* \geqslant q_1 \geqslant \frac{1}{6}a^*$; $0{,}318\ c^* \leqslant q_3 \leqslant \frac{1}{3}c^*$ with the change of the temperature. The indices $\tilde{h}, \tilde{l}$ of the satellite reflections $(\tilde{h}k\tilde{l})$ describing such a modulation change in the appropriate way. One can achieve the numerical indices (hklm) of those reflections in the reference system of the four-dimensional lattice $T^*(4)$ connected with $T^*(3)$ by the scaling transformation:

$$h\vec{a}^* + k\vec{b}^* + l\vec{c}^* + m\vec{d}^* = (h+mq_1)\vec{a}^* + k\vec{b}^* + (l+mq_3)\vec{c}^* = \tilde{h}\vec{a}^* + k\vec{b}^* + \tilde{l}\vec{c}^*.$$

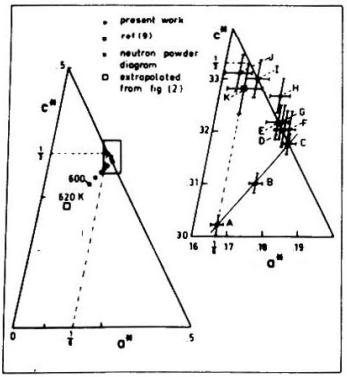

Fig.4 The temperature dependence of the wave vector of the modulated wave for the incommensurate γ_1 (from A to C), γ_2 (C to G), γ_i (G to I) and commensurate (I to K) δ-phases of Na_2CO_3 crystal in the plane $\vec{a}^*, \vec{c}^*$ of the reciprocal lattice. A: 470° K, B: 370° K, C: 300° K, D: 295° K, E: 275° K, F: 235° K, G: 200° K, H: 175° K, I: 120° K, J: 20° K and K: 4,2° K (according to (16)).

The continuous character of the dependence $\vec{q}_o(T)$ gives to the terminus "incommensurate modulation" [17] a general rather physical than geometrical sense. The space modulation is called an "incommensurate" one if $\vec{q}_o(T)$ is continuous at some temperature segment and $\vec{q}_o(T_1) \neq \vec{q}_o(T_2)$ if $T_1 \neq T_2$ irrespective of the fact rational or irrational satellite coordinated of (hkl). The modulation will be "commensurate" if the wave vector $\vec{q}_o(T)$ has the constant rational coordinates $\tilde{h}$, $\tilde{k}$, $\tilde{l}$ in the reference system of $T^*(3)$ - lattice in a certain field of temperature changing.

But such precise reformulation of the terminus is not sufficient for the detailed classification of the space modulated crystal phases. It is necessary to distinguish not only between the discrete, continuous or mixed types of the modulation between their 1-, 2- or 3-dimensional character and the kinds of the phase transitions but also between color space symmetries of the modulated phases. In accordance with the magnetic analogy [18] it is necessary to mark out the remodulation phase transitions which separate the phases with different space modulation $\delta\rho(\vec{r})$ of the initial basic structure $\rho^\circ(\vec{r})$.

Writing down the harmonic perturbance of the basic structure $\rho^\circ(\vec{r})$ as the phase modulation wave $\vec{r}_{lk} = \vec{r}_l + \vec{r}_k + \vec{A}_k \sin(\vec{q}_o \vec{r}_l + \varphi_k)$ [19], where $\vec{r}_{lk}$ is the coordinate of the atom k in the unit cell l, $\vec{A}_k$ is the amplitude, φ_k is the phase of the atom displacement wave, one can construct the phase space $\{(\varphi, \vec{r})\}$ which is the inverse Fourier image of the space $\{(\varphi, \vec{H})\}$. It is possible then to define the color positional groups $\mathfrak{P}_\rho^{(w)} \leftrightarrow \mathfrak{P}_{\rho^\circ}$ in the preservation of the abstract symmetry group approach. The composite

operators of those groups act in the space $\{(\varphi,\vec{r})\}$ in accordance with the positional law:

$$\langle \ldots p_i^{\Phi_k} \ldots | \Phi_i \rangle (\varphi,\vec{r}_{1k}) = (p_i^{\Phi_k}\varphi, \Phi_i\vec{r}), \text{ where } \vec{r}_{1k}=\Phi_{1k}\vec{r}_{11}, \Phi_i, \Phi_{1k} \in \mathfrak{D}_\rho .$$

The complanar or collinear character of the phase modulation may be taken into account by means of direct factors $1^{(2^*_z)}$ or $1^{(\infty x 2^* 2^*)}$. The preservation of the polarization plane of the modulated wave corresponds to the former case, while the rotation of this plane at the fixed point $\vec{r}$ around the axis x with the temperature changing corresponds to the latter. The projection $\vec{\varphi}_x(T)$ of the phase vectors $\vec{\varphi}=\vec{n},\varphi$ onto the axis x are preserved under the action of operator $1^{(\infty x 2^* 2^*)}$, $\vec{n}$ being the normal to the polarization plane x, iy of the wave. In other cases the phase symmetry groups $\mathfrak{D}^{(w)}_{\vec{\varphi}}$ of the space modulated crystals may demand some other factors for the symmetry correction.

Fig. 4 taken from [16] gives the temperature dependence $\vec{q}_o(T)$ of the stationary space modulation wave vector of Na_2CO_3 crystal between 620^o and $4,2^o$ K. At the segment 620^o to 300^o K $\vec{q}_o$ lies at the general point of the plane $\vec{a}^*$, $\vec{c}^*$ at the line $q_i - \alpha q_2 = 0$, while in the interval 300^o to 200^o $\vec{q}_o$ lies at the line $q_1 + q_2 = \frac{1}{2}$. To those temperature dependence of $\vec{q}_o(T)$ there correspond not one [1] but at least two "incommensurate" phases different from the colour symmetry groups $\mathfrak{D}^{(w_p)}_{\gamma_1} = 1^{(2^*_z)} \otimes p_{(b/2)^*} \frac{2^*}{m}\frac{2}{m}\frac{2_1}{m} \otimes P_{a+c} 1\frac{2}{m}1, \mathfrak{D}^{(w_p)}_{\gamma_2} = 1^{(2^*_z)} \otimes p1\frac{2}{m}1 \otimes P_{\vec{a}+\vec{c}} 1\frac{2}{m}1$.

The detailed explanation of this result may be found in [20].

Let us note in the conclusion that the generalized symmetry groups of imperfect crystals allow to generalize the Landau second order phase transition theory [21]. The scaling transformation from the unit cell to the enlarged unit cell, connected with the generalized groups give rise the effective method of numerical calculations in the electron band theory [22,23] and in the lattice dynamics of imperfect crystals [24].

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