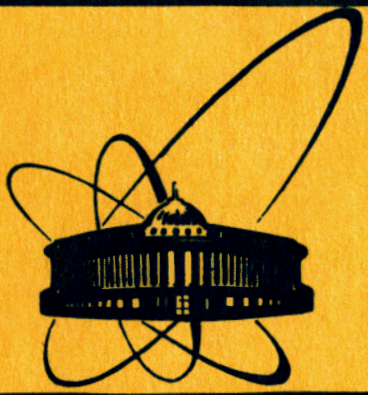

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SYMMETRY ANALYSIS OF TRANSITIONS OF THE ORDER-DISORDER TYPE AND POSSIBLE STRUCTURE DEFORMATIONS

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1. INTRODUCTION

Magnetic phase transitions and those of the order-disorder type are usually followed by structure deformations of crystals. The corresponding displacements of atoms will below be called accompanying displacements. Accurate investigations of the neutron diffraction patterns for determining the structure of magnetic or ordered phases require these displacements to be taken into consideration.

The investigation of the neutron-diffraction patterns is based on the trial-and-error method. In other words, the determination of the crystal structure means to select one variant out of all the possible ones. Therefore, one should be able to find all the possible variants, and for the inclusion of structure deformations, also the accompanying displacements for each variant. It is the central problem of this work. And finally, it will be shown how the analysis of accompanying displacement reduces considerably the number of test variants.

For simplicity all considerations will be made for structures of the type $Me - X$ in hydrides $Nb-H(D)$ and oxides of the type $Me - X$ and $Me - X_2$ in the system $Ta - O$. The ordering occurs for interstitial H, D and O atoms in tetrahedral and octahedral interstices of the Γ_C^v lattice of atoms of the transition metals Nb, Ta. Here we limit ourselves to the analysis of structure deformations of fully ordered interstitial "alloys". Such types of ordering will be considered to be fully ordered, in which the probability of finding the interstitial atoms in interstices is either 0 or 1.

2. POSSIBLE VARIANTS OF ORDERING OF INTERSTITIAL ATOMS

From neutron-diffraction profiles one may easily determine the lattice of a new ordered phase. Following the experimental results of ref.[1] we assume that the ordering leads to the Γ_O^b lattice. Its imbedding into the initial Γ_C^v lattice is shown in Fig.1; it is described by the arm $\vec{k}_1 = \frac{1}{2}\vec{b}_3$ of a six-arm star $\{k_9\}$ (Kovalev[2]).

The lattice type of the ordered phase and the way of its imbedding into the initial one give the transition channel. The transition channel may also be defined by the numbers of

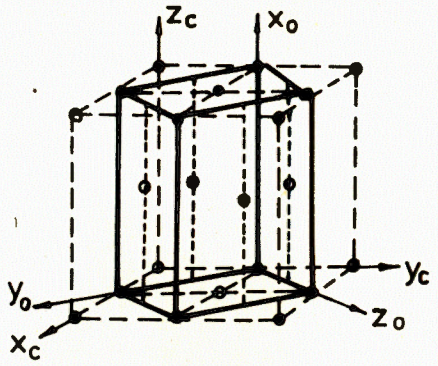

Fig.1. The imbedding of the elementary Γ_O^b cell of the ordered phase into the elementary Γ_C^v cell of the initial phase. The lattice sites which form the orthorhombic lattice are black.

arms $\vec{k}_\ell$ of the star $\{k_n\}$ participating in the transition. Both the definitions of the transition channel are equivalent. The information on the transition channel comes from indices of superstructure relections /3/.

Let us first find the list of test structures of the type Me – X in the case of ordering of H, (D) over tetrahedral interstices of the Γ_C^v lattice and the Me – X and Me – X_2 types in the case of ordering of O over octahedral interstices.

The coordinates of tetrahedral and octahedral interstices entering into the conventional Γ_C^v cell of the initial disordered phase in the unit reference frame /4/ have the form:

tetrahedral

sites $\underline{1(\frac{1}{4}0\frac{1}{2})}, \underline{2(\frac{1}{2}\frac{1}{4}0)}, \underline{3(0\frac{1}{2}\frac{1}{4})}, 4(\frac{3}{4}0\frac{1}{2}), 5(\frac{1}{2}\frac{3}{4}0), 6(0\frac{1}{2}\frac{3}{4}),$

(12d) $7(\frac{3}{4}0\frac{1}{2}), 8(\frac{1}{2}\frac{3}{4}0), 9(0\frac{1}{2}\frac{3}{4}), \underline{10(\frac{1}{4}\frac{1}{2}0)}, \underline{11(0\frac{1}{4}\frac{1}{2})}, \underline{12(\frac{1}{2}0\frac{1}{4})}.$

octahedral

sites $\underline{1(\frac{1}{2}00)}, \underline{2(0\frac{1}{2}0)}, \underline{3(00\frac{1}{2})},$

(6b) $4(0\frac{1}{2}\frac{1}{2}), 5(\frac{1}{2}0\frac{1}{2}), 6(\frac{1}{2}\frac{1}{2}0).$

The positions in the primitive cell are underlined.

Transitions of the order-disorder type are followed by decreasing symmetry of the crystal, and it is assumed that the groups of symmetry of ordered phases will be subgroups of the initial group O_h^9.

In the given transition channel)as lattice of ordered phases Γ_O^b, arm $\vec{k}_1 = \frac{1}{2}\vec{b}_3$ of the star $\{k_9\}$) as it follows from Tables of ref.5, after ordering there are possible the following groups of symmetry: D_{2h}^{17}, D_{2h}^{18}, D_{2h}^{19}, D_{2h}^{20}, D_{2h}^{21}, D_{2h}^{22}. Besides, there

may appear the phases described by subgroups of the indicated groups with $\vec{k} = 0$.

As a rule, with each symmetry group of a low-symmetric phase one may associate an irreducible representation of the primary group which describes the transition into this phase. Let us find for the groups D_{2h}^{17-22} the corresponding irreducible representations of the group O_h^9. The change of the distribution density function of the interstitial atoms over interstices – $\delta\rho$, which leads to the structure with a lower symmetry of one of the groups D_{2h}^{17-22}, may be written, as it follows from the symmetry analysis /3/, as a superposition of basis functions of the corresponding irreducible representation which will be called the relevant representation. In the general case the relevant representation can be reducible. Then,

$$\delta\rho = \sum_{\nu} \sum_{\vec{k}_\ell, a} c_a^{\vec{k}_\ell, \nu} \phi_a^{\vec{k}_\ell, \nu}, \qquad (1)$$

where ν numbers irreducible representations, $\vec{k}_\ell$ are arms of the star $\{k_n\}$, and a numbers basis functions of an ν-th irreducible representation of groups of the wave vector $G_{\vec{k}_\ell}$. Below we restrict ourselves to one irreducible relevant representation, and therefore the sum over ν in (1) can be omitted. The change of the distribution density $\delta\rho$ should possess the symmetry of the corresponding group of D_{2h}^{17-22} that means that the restriction of the relevant irreducible representation of the initial group O_h^9 on the given subgroup should contain an identity representation (Birman criterion).

In our example the transition occurs along one arm $\vec{k}_1$ of the star $\{k_9\}$, and all the irreducible representations of the group $G_{\vec{k}_1}$ are one-dimensional, hence the expression (1) becomes:

$$\delta\rho = c^{\vec{k}_1} \phi^{\vec{k}_1}. \qquad (1a)$$

In this case by the Birman criterion the restriction of the relevant representation of O_h^9 on the corresponding orthorhombic subgroup should coincide with the identity representation. It is to be noted that because of one-dimensionality of the irreducible representations (IR) participating in the considered transitions only the groups D_{2h}^{17-22} are to be taken as symmetry groups of the ordered phases. Phases described by subgroups of these groups with $\vec{k} = 0$ will be described by several IRs at once. Notice that in the transition "$\Gamma_C^v \to \Gamma_O^b$" there appear the so-called "lost" translations $\vec{t}_n$, which after the transition are no longer lattice. From Fig.1 it is seen that $\vec{t}_n = \vec{a}_1 + \vec{a}_3$, $\vec{a}_2 + \vec{a}_3$, $\vec{a}_3$, $\vec{a}_1 + \vec{a}_2 + \vec{a}_3$, ..., where $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ are the shortest translations of the initial Γ_C^v lattice. This means

Table 1

Irreducible representations of the group O_h^9, star $\{k_9\}$

Representation	elements of $G_{\vec{k}_1}$							
	h_1	h_4	h_{13}	h_{16}	h_{25}	h_{28}	h_{37}	h_{40}
τ_1	1	1	1	1	1	1	1	1
τ_2	1	1	1	1	-1	-1	-1	-1
τ_3	1	-1	1	-1	1	-1	1	-1
τ_4	1	-1	1	-1	-1	1	-1	1
τ_5	1	-1	-1	1	1	-1	-1	1
τ_6	1	-1	-1	1	-1	1	1	-1
τ_7	1	1	-1	-1	1	1	-1	-1
τ_8	1	1	-1	-1	-1	-1	1	1

Table 2

The orthorhombic groups D_{2h}^{17-22} as the restriction of the O_h^9 group

orthorhombic groups	elements of the restriction of O_h^9							
	h_1	h_4	h_{13}	h_{16}	h_{25}	h_{28}	h_{37}	h_{40}
D_{2h}^{17}	-	$\vec{t}_n$	-	$\vec{t}_n$	$\vec{t}_n$	-	$\vec{t}_n$	-
D_{2h}^{18}	-	-	$\vec{t}_n$	$\vec{t}_n$	-	-	$\vec{t}_n$	$\vec{t}_n$
D_{2h}^{19}	-	-	-	-	-	-	-	-
D_{2h}^{20}	-	$\vec{t}_n$	$\vec{t}_n$	-	-	$\vec{t}_n$	$\vec{t}_n$	-
D_{2h}^{21}	-	$\vec{t}_n$	$\vec{t}_n$	-	$\vec{t}_n$	-	-	$\vec{t}_n$
D_{2h}^{22}	-	-	-	-	$\vec{t}_n$	$\vec{t}_n$	$\vec{t}_n$	$\vec{t}_n$
$D_{2h}^{17'}$	-	-	$\vec{t}_n$	$\vec{t}_n$	$\vec{t}_n$	$\vec{t}_n$	-	-
$D_{2h}^{18'}$	-	$\vec{t}_n$	-	$\vec{t}_n$	-	$\vec{t}_n$	-	$\vec{t}_n$

that the orthorhombic subgroups D_{2h}^{17-22} are translational subgroups. In this case when choosing the restriction of the O_h^9 representation on a given group one should consider elements not only of the zero block (of the type $\{h_i|0\}$) but also of all the blocks with the lost translations (of the type $\{h_i|\vec{t}_n\}$). The groups as the restriction of O_h^9 are presented in Table 2. An empty place in table 2 signifies that a given element enters into the group D_{2h}^i from the zero block of the O_h^9 group, i.e., in the form $\{h_i|0\}$. If the table box contains $\vec{t}_n$, then this element is taken from a nonzero block, in the form $\{h_i|\vec{t}_n\}$. The groups D_{2h}^{17} and D_{2h}^{18} enter into Table 2 twice. This means that two equivalent choices are possible for the corresponding restrictions. It may be verified that by passing to the orthorhombic coordinate system $x_0 y_0 z_0$ and shifting appropriately the origin, the elements of groups D_{2h}^{17-22} may be represented in the standard Table form. In Table 3 we compare the representations of group O_h^9 to orthorhombic symmetry groups. In this way it is shown over which representation of O_h^9 the transition into a definite orthorhombic structure takes place.

Let us establish now which of the groups D_{2h}^{17-22} may be groups of the ordered phases in the course of ordering of interstitial atoms over tetrahedral and octahedral interstices. To this end, one should define the composition of the permutation representation. By standard formulae [3] we obtain for tetrahedral interstices:

$$d_p^{k_9} = \tau_1^{k_9} \oplus \tau_4^{k_9} \oplus \tau_5^{k_9} \oplus 2\tau_6^{k_9} \oplus \tau_7^{k_9} \qquad (2)$$

for octahedral interstices:

$$d_p^{k_9} = \tau_1^{k_9} \oplus \tau_4^{k_9} \oplus \tau_6^{k_9} . \qquad (3)$$

Table 3

Relation between the orthorhombic groups and the irreducible representations of the group O_h^9, of the star $\{k_9\}$ (lattice Γ_C^v)

irreducible representation of the group	$\tau_1^{k_9}$	$\tau_2^{k_9}$	$\tau_3^{k_9}$	$\tau_4^{k_9}$	$\tau_5^{k_9}$	$\tau_6^{k_9}$	$\tau_7^{k_9}$	$\tau_8^{k_9}$
orthorhombic group	D_{2h}^{19}	D_{2h}^{22}	$D_{2h}^{18'}$	D_{2h}^{17}	D_{2h}^{20}	D_{2h}^{21}	D_{2h}^{18}	$D_{2h}^{17'}$

From Table 3 and formulae (2), (3) it is seen that in the case of ordering the hydrogen atoms over tetrahedral interstices there are possible ordered phases with symmetry groups: D_{2h}^{17},

D_{2h}^{18}, D_{2h}^{19}, D_{2h}^{20}, and D_{2h}^{21}. In the case of ordering the oxygen atoms over octahedral interstices the symmetry groups of possible ordered phases are D_{2h}^{17}, D_{2h}^{19}, and D_{2h}^{21}.

To get a clear picture of the obtained variants of ordering, i.e., to find which interstices are filled by the interstitial atoms and which of them are empty, it is necessary to calculate permutation modes (concentration waves). The corresponding formulae are given in ref./3/. Results calculated by these formulae are listed in Table 4 and 5. It should be mentioned that the modes obtained describe the change of the probability of finding an interstitial atom in a given interstice. From Tables 4 and 5 it is seen that representations of the star $\{k_9\}$ give no fully ordered structures.

To get fully ordered structures, it is necessary to add the transition over possible representations of the wave vector $\vec{k} = 0$ of the star $\{k_{11}\}$ because this vector does not contradict the cell chosen for the possible ordered phases (the transition over attendant /3/ representations).

We obtain the following composition of the permutation representation with $\vec{k} = 0$ for tetrahedral interstices:

$$d_p^{k_{11}} = \tau_1^{k_{11}} \oplus \tau_5^{k_{11}} \oplus \tau_8^{k_{11}} \qquad (4)$$

for octahedral interstices:

$$d_p^{k_{11}} = \tau_1^{k_{11}} \oplus \tau_5^{k_{11}} . \qquad (5)$$

Table 4

The permutation modes of the irreducible representations of the group O_h^9 for the stars $\{k_9\}$ and $\{k_{11}\}$ (lattice Γ_C^v) and the tetrahedral interstices $\epsilon = \exp(2\pi i/3)$

star	representation	sites of the atoms in elementary cell											
		1	2	3	4	5	6	7	8	9	10	11	12
$\{k_9\}$	τ_1	1	-1	0	-1	-1	0	-1	-1	0	-1	1	0
	τ_4	1	-1	0	1	1	0	-1	-1	0	1	-1	0
	τ_5	0	0	-1	0	0	1	0	0	-1	0	0	1
	τ_6	0	0	1	0	0	1	0	0	1	0	0	1
	τ_6'	1	1	0	1	-1	0	-1	1	0	1	1	0
	τ_7	1	1	0	-1	1	0	-1	1	0	-1	-1	0
$\{k_{11}\}$	τ_5 ψ_1	1	ϵ	ϵ^2	1	ϵ	ϵ^2	1	ϵ	ϵ^2	1	ϵ	ϵ^2
	τ_5 ψ_2	ϵ	1	ϵ^2	ϵ	1	ϵ^2	ϵ	1	ϵ^2	ϵ	1	ϵ^2

Table 5

The permutation modes of the irreducible representations of the group O_h^9, for the stars $\{k_9\}$ and $\{k_{11}\}$ (lattice Γ_C^v) and octahedral interstices (6b); $\epsilon = \exp(2\pi i/3)$

star	representation		sites of atoms					
			1	2	3	4	5	6
$\{k_9\}$	τ_1		0	0	1	0	0	-1
	τ_4		1	-1	0	1	-1	0
	τ_6		1	1	0	1	1	0
$\{k_{11}\}$	τ_5	ψ_1	1	ϵ^2	ϵ	1	ϵ^2	ϵ
		ψ_2	ϵ	ϵ^2	1	ϵ	ϵ^2	1

As the representation $\tau_1^{k_{11}}$ describes the change of concentration of interstitial atoms, which we assume to be given and constant, we will not consider it. The analysis shows that the representation $\tau_8^{k_{11}}$ leads to a symmetry group lower than the orthorhombic groups we have considered, as it should also be rejected.

Permutation modes for the allowed representation $\tau_5^{k_{11}}$ are presented in the second part of Table 4 and 5.

Mixing the permutation modes of the representation $\tau_5^{k_{11}}$ with coefficients $c_1 = c_2 = c$ and complementing them with modes of the representation $\tau_i^{k_9}$, we obtain six variants of the fully ordered structures in the case of tetrahedral interstices and three variants for octahedral interstices (Figs. 2 and 3). Two of them are described by one symmetry group D_{2h}^{21}.

3. POSSIBLE STRUCTURE DEFORMATIONS

For each of the obtained variants of ordering we shall carry out the symmetry analysis of possible structure deformations. The problem may be formulated as follows. The symmetry group of an ordered phase is known. One should find the displacements of metal atoms that do not contradict the symmetry of an ordered state. For this purpose it is sufficient to accomplish a standard group-theoretical analysis of possible displacements and to select the required ones. There are possible two variants: displacements leading to a structure with the same symmetry

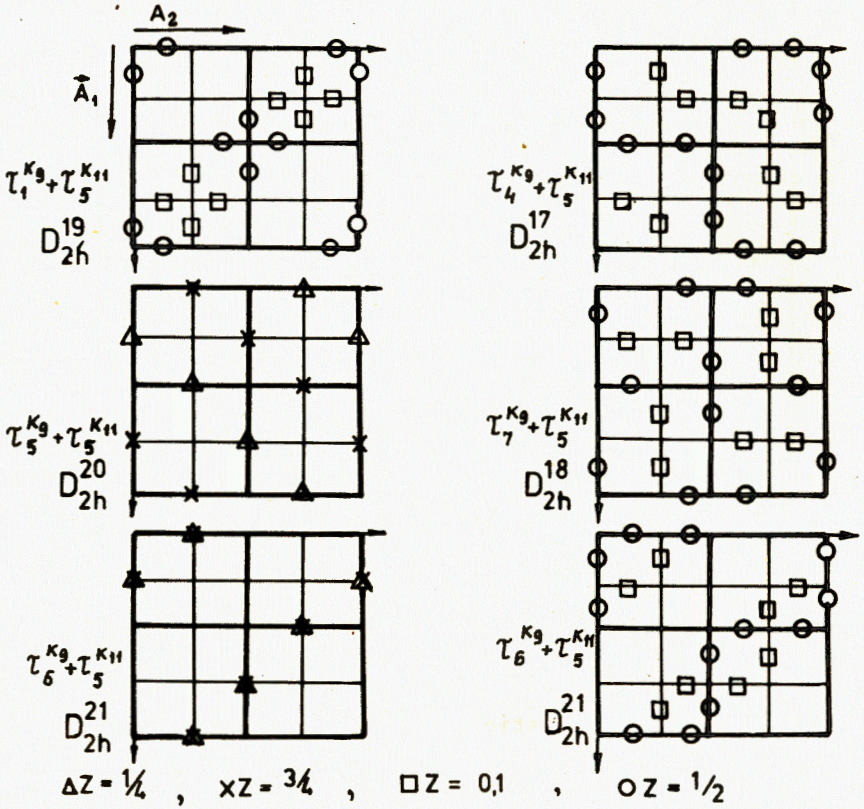

Fig.2. The possible orthorhombic structures as a result of ordering of interstitial atoms over the tetrahedral interstices. Only the "fully" sites in the ordered physe are pointed.

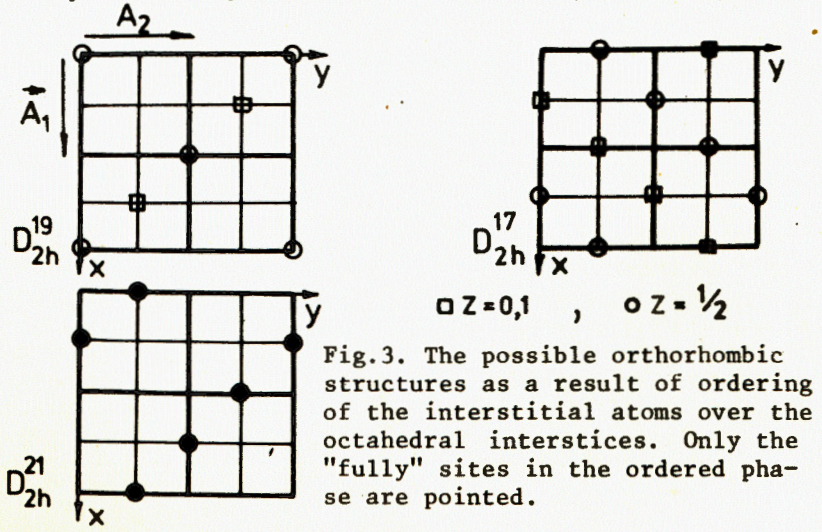

Fig.3. The possible orthorhombic structures as a result of ordering of the interstitial atoms over the octahedral interstices. Only the "fully" sites in the ordered phase are pointed.

group as the ordered phase - in the same transition channel, or the transition in a structure with a higher symmetry, with the wave vector $\vec{k} = 0$.

Metal atoms form the Γ_C^v lattice (positions 2a). The primitive cell of a discordered phase contains only one metal atom with the coordinates (0,0,0).

The composition of the mechanical representation on metal atoms for the star $\{k_9\}$ is as follows

$$d_m^{k_9} = r_4^{k_9} \oplus r_6^{k_9} \oplus r_8^{k_9} . \quad (6)$$

Let us compare it with the permutation representation (2) on tetrahedral interstices. It is seen that the representations $r_4^{k_9}$ and $r_6^{k_9}$ enter both into $d_m^{k_9}$ and into $d_p^{k_9}$. This means that the ordering of interstitial atoms over these representations may be followed by displacements of the metal atoms which are described by the modes of representations $r_4^{k_9}$ and $r_6^{k_9}$. The representations $r_1^{k_9}$, $r_5^{k_9}$ and $r_7^{k_9}$ from the permutation representation (2) do not enter into the mechanical representation (6). Therefore, deformations for the ordering variants over representations $r_1^{k_9}$, $r_5^{k_9}$, $r_7^{k_9}$, if possible, should be described by modes with $\vec{k} = 0$ (the star $\{k_{11}\}$). From the comparison of the permutation representation (3) for octahedral interstices with the mechanical representation (6) it is seen that the types of ordering over $r_4^{k_9}$ and $r_6^{k_9}$, like in the case of tetrahedral interstices, may be accompanied by the displacements of metal atoms with the same symmetry. The ordered structure $D_{2h}^{19}(r_1^{k_9} \oplus r_5^{k_9})$ can be followed only by the deformation of the Me sublattice caused by the wave vector $\vec{k} = 0$. The mechanical representation on atoms for the star $\{k_{11}\}$ coincides with the representation $r_{10}^{k_{11}}$.

$$d_m^{k_{11}} = r_{10}^{k_{11}} . \quad (7)$$

To get a clear picture of possible displacements of the metal atoms, one should find displacement modes (basis functions) for $\vec{k} = 0$ and arm $\vec{k}_1$ of the star $\{k_9\}$. These modes are listed in Table 6, and the atom displacements are shown in Fig.4. As follows from the symmetry analysis, any combination of mixing coefficients of the basis vectors of the three-dimensional irreducible representation $r_{10}^{k_{11}}$ leads to structure deformations, symmetry of which is lower than the orthorhombic one. Consequently, the types of ordering with symmetry D_{2h}^{18}, D_{2h}^{19} and D_{2h}^{20} cannot be accompanied by displacements of the lattice atoms.

The above results lead to an important conclusion which may be of a practical use. The study of hydrids requires to find structures from the results of investigations of the neutron

Table 6

The modes of displacements of metal atoms (2a) for the irreducible representations of the group O_h^9, stars $\{k_9\}$, $\{k_{11}\}$, (lattice Γ_C^v).

star	representation		sites of atoms 1	2
$\{k_9\}$	τ_4		$(1\bar{1}0)$	$(\bar{1}10)$
	τ_6		(110)	$(\bar{1}\bar{1}0)$
	τ_8		(001)	$(00\bar{1})$
$\{k_{11}\}$	τ_{10}	ψ_1	(100)	$(\bar{1}00)$
		ψ_2	(010)	$(0\bar{1}0)$
		ψ_3	(001)	$(00\bar{1})$

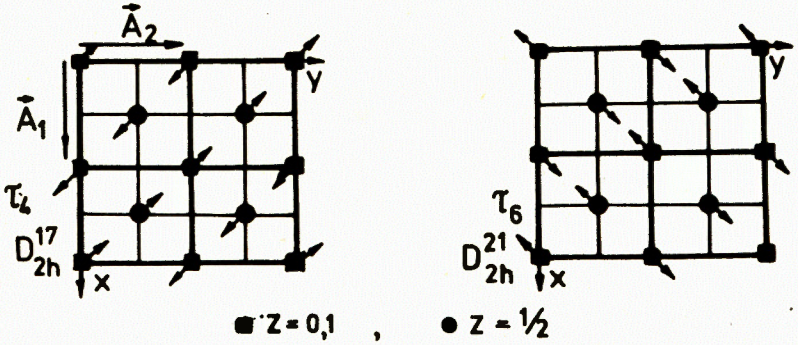

Fig.4. The models of the displacements of metal atoms attendant to the ordering of the interstitial atoms.

difraction patterns. The main difficulty is small values of the intensities of superstructure reflections which provide information on the type of ordering. The reliability of the obtained results depends considerably on the choice of test variants. There are attendant displacements with $\vec{k} = 0$ and $\vec{k} \neq 0$. This means that in the first case the appearance of displacements of metal atoms will influence the intensities of initial (non-ordered) reflections, and in no way the superstructure reflections. In the second case the atom displacements

will contribute to the superstructure reflections, and this contribution may appear to be more essential than that from ordering of the hydrogen atoms. Consider, for instance, the finding of the structure in hydrides Nb–H and Ta–H with the concentration of hydrogen atoms with $c = \frac{1}{6}$ (i.e., one hydrogen atom per six interstices). Superstructure reflections point to the transition channel with arm $\vec{k}_1$ of the star $\{k_9\}$ (Fig.1). In this channel we have found six variants of the ordered structure (Fig.2). Only two variants correspond to the given concentration – these are structures of the type Me–X $D_{2h}^{20}(r_5^{k_9} \oplus r_5^{k_{11}})$ and $D_{2h}^{21}(r_6^{k_9} \oplus r_5^{k_{11}})$. And just one variant – D_{2h}^{21} may be followed, as has been shown above, by displacements of atoms which can be described by modes with the wave vector $\vec{k}_1$. Therefore, if on diffraction patterns one finds the superstructure reflections with suitable large intensities corresponding to the vector $\vec{k}_1$, then one may retain one of two variants namely, D_{2h}^{21}. If such reflections are absent, one should retain D_{2h}^{20} as a test variant. In ref.[6] the group D_{2h}^{20} was proposed. So, the symmetry analysis of the accompanying displacements provides a further information which allows a considerable reduction of the list of test variants. In this paper we have considered, like in the most works devoted to accompanying displacements, the deformation of the metal sublattice in ordering the interstitial atoms over interstices. The coordinates of interstices are defined by coordinates of their centres. One may raise the following question not yet discussed in the literature: Does the ordering of interstitial atoms lead to the displacement of centres of interstices? In other words, does the crystal deformation arising in the course of ordering produce the shift of centres of interstices? If it leads to the shift, then how it can be detected experimentally.

Let us show that the symmetry analysis of the displacements of centres of interstices is essential in interpreting the nature of superstructure reflections. The analysis of displacements of interstices is analogous to the analysis of metal displacements. The mechanical representation for positions (12d) has the form:

$$d_m^{k_9} = 3r_1^{k_9} \oplus 2r_2^{k_9} \oplus 2r_3^{k_9} \oplus 3r_4^{k_9} \oplus r_5^{k_9} \oplus 2r_6^{k_9} \oplus 3r_7^{k_9} \oplus 2r_8^{k_9} . \qquad (8)$$

The mechanical representation for interstices (6b) is of the form:

$$d_m^{k_9} = 2r_1^{k_0} \oplus r_3^{k_9} \oplus r_4^{k_9} \oplus r_5^{k_9} \oplus r_6^{k_9} \oplus 2r_7^{k_9} \oplus r_8^{k_9} . \qquad (9)$$

From the analysis of expressions (8) it is seen that the mechanical representation on the position (12d) contains, in addition to r_4^{k9}, also r_8^{k9} which according to Table 3 describes the transition to the phase D_{2h}^{17}. The permutation representation (2) on the position (12d) contains the representation r_4^{k9} which describes the ordered phase D_{2h}^{17}. The groups D_{2h}^{17} and $D_{2h}^{17'}$ differ only by imbedding into the initial cell O_h^9.

If in some sample the phase "D_{2h}^{17}" is realized, there arises the problem of interpreting the nature of superstructure reflections. These effects may be caused either by ordering or by displacement of interstices without ordering the hydrogen atoms over these interstices. The simultaneous appearance of ordering and displacement will reduce symmetry of the new phase to the symmetry of intersection of groups D_{2h}^{17} and $D_{2h}^{17'}$. Such a transition will be described by two different representations. The inclusion of displacements accompanying the ordering (over r_4^{k9}) does not solve the problem. As follows from (9) and (3), an analogous situation holds also for the position (6d).

If in some compound there will appear the phase D_{2h}^{22} (the position (12d)) or $D_{2h}^{18,20}$ (the position (6d)), then, as can be seen from (8), (2) and (9), (3), respectively, attempts to find neutron diffraction patterns as a result of ordering will be wrong a priori. The appearance of superstructure reflections in these phases is only due to the displacement of interstices.

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Симметрийный анализ переходов типа порядок-беспорядок и возможных структурных искажений

В работе рассмотрены фазовые переходы порядок-беспорядок для структур типа Me–H в гидридах Nb–H(D) с упорядочением H(D) по тетраэдрическим пустотам ГЦК решетки и окислов типа Me–X и $Me–X_2$ / Ta- O/ с упорядочением O по октаэдрическим пустотам. Предполагается, что концентрация атомов внедрения является заданной и постоянной. Из экспериментальных данных следует, что в окончательном виде получается структура с ромбической решеткой Γ_O^b. Методом симметрийного анализа получены все допустимые модели упорядоченной структуры с этой решеткой. Рассмотрены также все возможные структурные деформации, которые могут быть связаны с соответствующими моделями упорядочения. Симметрийный анализ дает как возможные смещения металла, так и смещения центров междоузлий, по которым происходит упорядочение атомов внедрения, не противоречащее симметрии упорядоченной фазы. Из симметрийного анализа следует существование таких окончательных структур, для которых возникает проблема интерпретации природы сверхструктурных рефлексов на нейтронограмме, а именно, возникают ли они за счет упорядочения атомов внедрения по межузлиям ГЦК решетки или за счет смещения центров межузлий без упорядочения.

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Symmetry Analysis of Transitions of the Order-Disorder Type and Possible Structure Deformations

There are considered the order-disorder phase transitions for structures of the type Me–H in hydrides Nb–H(D), with ordering of H(D) over tetrahedral interstices of the Γ_C^v lattice and oxides of the type Me–X and $Me–X_2$ in the system Ta–O, with ordering of O over octahedral interstices. The concentration of interstitial atoms is assumed to be given and constant. Following the experimental data there is assumed the orthorhombic Γ_O^b lattice of the final structure. By the method of the symmetry analysis there are calculated all possible models of ordered structures with this lattice. There are considered the possible structure deformations consistent with any variants of ordering of the interstitial atoms. The symmetry analysis gives both the displacements of the metal atoms and the displacements of centres of interstices, which may be connected with all models of structure regarded as a result of the order-disorder phase transition. From the symmetry analysis such final structures follow for which there arises the problem of interpreting the nature of superstructure reflections in neutron diffraction patterns: are they a result of the ordering of the interstitial atoms over the interstices or a result of the displacements of centres of this interstices without ordering.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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