Acta Cryst. (1996). A**52**, 198–202

On the Problem of the Description of the Ordered Structures in Binary Solid Solutions with a Hexagonal Crystal Lattice

V. N. Bugaev* and R. V. Chepul'skii

Department of Solid State Theory, Institute for Metal Physics, Ukrainian Academy of Sciences, 252680 Kiev, Ukraine. E-mail: kondr@kondr.kiev.ua

(Received 1 May 1995; accepted 13 September 1995)

Abstract

Within the framework of the static concentration-wave method, by means of the geometrically complete procedure, the list of all types of thermodynamically stable, with respect to macroscopic inhomogeneities (Lifshitz), ordered structures arising from the disordered state of binary substitutional solid solutions with a hexagonal crystal lattice is established, as is the list of corresponding isomorphic interstitial structures based on simple hexagonal and h.c.p. crystal lattices.

1. Introduction

A statistical description of structures with long-range order in solid solutions can be reduced to the setting up of a Fourier series of one-particle distribution functions (Krivoglaz, 1969; Khachaturyan, 1973, 1978, 1983; de Fontaine, 1979). From this, the problem arises of the determination of the wave vectors over which the summation in these series is to be carried out.

Lifshitz (1942), considering [within the Landau (1937) approach] the symmetry aspects of the problem of structural phase transformations of second order, ascertained that only the structures characterized by the basis functions of irreducible representations (of the space symmetry group of the system at the point of the phase transformation), which correspond to the stars of the wave vectors whose symmetry groups contain the symmetry elements (from the crystal class of that space group), intersecting at one point can be thermodynamically stable with respect to the violations of the macroscopic homogeneity (the Lifshitz criterion).† Khachaturyan (1973, 1978, 1983) proved the applicability of the Lifshitz criterion to the case of the structural phase transformations of first order.

The complete list of the Lifshitz superstructures arising as a result of the order–disorder phase transitions in binary solid solutions with cubic (f.c.c. and b.c.c.) crystal lattices was established by Lifshitz (1942), Khachaturyan (1973, 1978, 1983), Gufan & Dmitriev (1982) and Bugaev & Chepul'skii (1995), and with the h.c.p. lattice by Lifshitz (1942), Zhorovkov, Fuks & Panin (1975), Gufan (1982), Sanchez, Gratias & de Fontaine (1982), Solov'eva & Shtern (1990) and Zhorovkov (1993). The case of the hexagonal crystal lattice was considered by Bugaev (1978), in which some (six types) Lifshitz superstructures were found.

The aim of the present paper is to find within the static concentration-wave method (Khachaturyan, 1973, 1978, 1983), by means of the geometrically complete procedure, the full list of the Lifshitz superstructures arising from the disordered state of the binary solid solutions with the simple hexagonal crystal lattice.

The superstructures that can be described on the basis of the simple hexagonal crystal lattice are widely observed in experiment, *e.g.* in the case of interstitial ordered structures at the octahedral interstices† of a h.c.p. crystal lattice (Fromm & Gebhardt, 1976). The results obtained in the present work can also be useful for the investigation of those reconstructive transitions whose mechanism cannot be formulated in terms of atomic displacement and which should be interpreted as a transition between the ordered phases derived from a common disordered hexagonal latent parent structure (see *e.g.* Dmitriev, Rochal, Gufan & Toledano, 1989).

2. The procedure for finding superstructures

It is suitable to represent the function that characterizes the space symmetry of the system under consideration as a series over the functions realizing the irreducible representations of the space symmetry group G_0 of the system at the point of phase transformation (Landau, 1937; Lifshitz, 1942; Landau & Lifshitz, 1980). From this, to every irreducible representation (excluding the unity one) its own long-range-order parameter is matched. Non-zero values of these parameters make the corresponding lowering of the space symmetry of the system available.

---

† The first Brillouin zone points corresponding to such wave vectors are usually termed the high-symmetry or the Lifshitz points and these wave vectors themselves and the superstructures corresponding to them (see §2) are usually termed the Lifshitz vectors and the Lifshitz superstructures, respectively.

† The set of octahedral interstices in a h.c.p. crystal lattice forms the simple hexagonal crystal lattice (from the crystallographic standpoint).

©1996 International Union of Crystallography
Printed in Great Britain – all rights reserved

In the framework of the lattice-gas model, let us describe the space symmetry of the atomic distribution in a binary solid solution by the function $P(\mathbf{R})$, which means the probability of finding the impurity atom* at the corresponding crystal-lattice position with the radius vector $\mathbf{R}$. Let the set of all positions $\mathbf{R}$ form a Bravais lattice and the group G_0 be the space symmetry group of this lattice.† In this case, the irreducible representations of the group G_0 are numerated only by the stars $\mathbf{k}_s$ ($s = 1, 2, \ldots$) of the wave vectors that belong to the first Brillouin zone of the corresponding reciprocal crystal lattice‡ and the basis functions of the irreducible representation corresponding to some star $\mathbf{k}_s \equiv \{\mathbf{k}_{1_s}, \mathbf{k}_{2_s}, \ldots, \mathbf{k}_{l_s}\}$ ($\mathbf{k}_{j_s}$ are the wave vectors belonging to the same star s) are the functions (Lifshitz, 1942; Landau & Lifshitz, 1980)

$$\exp(i\mathbf{k}_{1_s}\mathbf{R}), \exp(i\mathbf{k}_{2_s}\mathbf{R}), \ldots, \exp(i\mathbf{k}_{l_s}\mathbf{R}).$$

Thus, one can write the above-mentioned series in terms of the basis functions of the irreducible representations of the group G_0 in the general form

$$P(\mathbf{R}) = c + \sum_{s\neq 0} \eta_s \sum_{j_s} \gamma_s(j_s) \exp(i\mathbf{k}_{j_s}\mathbf{R}), \qquad (1)$$

where the summation is carried over all stars of the wave vectors from the first Brillouin zone (excluding its center: $s \neq 0$) and over all vectors of these stars; $c = n/N$ is the concentration of the impurity (n and N are the total numbers of the impurity atoms and of the crystal lattice positions, respectively); η_s are the long-range-order parameters; $\gamma_s(j_s)$ are the coefficients that determine the symmetry of the function $P(\mathbf{R})$. In (1), the coefficient corresponding to the 'zero' star is assumed to be equal to c, which makes the equality $P(\mathbf{R}) = c$ (for any $\mathbf{R}$) satisfied in the disordered state of the solid solution, when all parameters of long-range order are equal to zero.

In (1), the designations adopted in the static concentration-wave method (Khachaturyan, 1973, 1978, 1983) are used. Two conditions are used for finding superstructures within this method.

Firstly, for the unambiguous definition of the long-range-order parameters, one must impose the normalization condition (Landau, 1937; Landau & Lifshitz, 1980). It is conveniently chosen in the form:§

Condition 1. In the completely ordered state of the solid solution [when the function $P(\mathbf{R})$ at any $\mathbf{R}$ takes only two values, zero or unity, and $c = c_{\rm st}$, where $c_{\rm st}$ is the stoichiometric concentration of the superstructure], all non-zero long-range-order parameters should be equal to unity.

Secondly, for (1) to describe the structures with long-range order, the following condition, which reflects the conservation of the number of the structural degrees of freedom, should be satisfied:

Condition 2. The number of non-zero long-range-order parameters in series (1) should be fewer by unity than the total number of different values that the function $P(\mathbf{R})$ takes at all positions $\mathbf{R}$ (under the arbitrary allowable values of these long-range-order parameters).

The following procedure is used in this work for finding (within the static concentration-wave method) the complete set of Lifshitz superstructures arising from the disordered state of the solid solutions with a hexagonal crystal lattice.*

On condition that the solution is in a completely ordered state, (1) can be written for some (defined below) sites $\mathbf{R}_m$ for every possible combination of l ($l = 1, 2, \ldots$) Lifshitz stars [with n_s wave vectors in every star s ($s = 1, 2, \ldots, l$)] in the following general form:

$$P_m = c_{\rm st} + \sum_{s=1}^{l} \sum_{j_s=1}^{n_s} \gamma_s(j_s) \exp(i\mathbf{k}_{j_s}\mathbf{R}_m),$$

$$m = 1, 2, \ldots, \sum_{s=1}^{l} n_s + 1. \qquad (2)$$

In (2), all long-range-order parameters are put equal to unity, $c = c_{\rm st}$, and the values P_m of the function $P(\mathbf{R})$ at corresponding positions R_m must equal zero or unity, in accordance with condition 1. The set of positions $\{R_m\}$ are chosen in such a way that the main determinant of the set of equalities (2), considered as a set of linear inhomogeneous equations in unknowns $c_{\rm st}$ and $\{\gamma_s(j_s)\}$, is not equal to zero. Solving this set of equations for all possible distributions of zeros and unities over the values of P_m, we find the complete assemblage $\{c_{\rm st}, \{\gamma_s(j_s)\}\}$ of those packages $c_{\rm st}$ and $\{\gamma_s(j_s)\}$ that satisfy condition 1 within the chosen set $\{\mathbf{R}_m\}$. It is obvious that the assemblage of the solutions found in the above-mentioned way must contain (as a subset in general) *all* those packages $c_{\rm st}$ and $\{\gamma_s(j_s)\}$ that make condition 1 satisfied within *all* positions $\{\mathbf{R}\}$.

In the final stage of the procedure, we exclude those packages from $\{c_{\rm st}, \{\gamma_s(j_s)\}\}$ that do not meet conditions 1 and 2 within all positions $\{\mathbf{R}\}$.†

---

[*] For definiteness, let the sort of atom with the least concentration in the binary solid solution be termed the impurity. Therefore, the space distribution of the atoms of the host is described by the function $1 - P(\mathbf{R})$.

[†] As a result, the space symmetry group of any superstructure is a subgroup of the group G_0 (in the lattice-gas model).

[‡] Classification by the number of small representations is therefore absent.

[§] Such a normalization condition provides the coincidence of the definition of the long-range-order parameters in the framework of the static concentration-wave method with their classic definition in terms of the occupation probabilities (see *e.g.* Krivoglaz & Smirnov, 1964).

---

[*] Note that this procedure, without any change, can be used for finding both the Lifshitz and the non-Lifshitz superstructures in binary solid solution based on any Bravais lattice.

[†] Owing to the periodicity of the functions $\exp(i\mathbf{k}_{j_s}\mathbf{R})$ {and, consequently [see (1) and (2)], of the corresponding functions $P(\mathbf{R})$}, it is necessary to check for this purpose (by the direct substitution of corresponding coordinates) only a finite (not usually large) number of positions $\mathbf{R}$, limited by the periods of the function $P(\mathbf{R})$.

Table 1. *Characteristics of the hexagonal superstructures described by the expansion (3) in terms of A, K and H stars*

(*a*)	(*b*)	c_{st}	γ_A	$\gamma_K(1)$	$\gamma_K(2)$	$\gamma_H(1)$	$\gamma_H(2)$	Γ_A	Γ_K	Γ_H	P_i	ν_i	Fig.	(*c*)
1	*AB*	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0	$\frac{1}{4}$	0	0	$c+1/2\eta_A$	1/2		●
											$c-1/2\eta_A$	1/2	2(*a*)	○
2	A_2B	$\frac{1}{3}$	0	$\frac{1}{3}$	$\frac{1}{3}$	0	0	0	$\frac{2}{9}$	0	$c+2/3\eta_K$	1/3		●
											$c-1/3\eta_K$	2/3	2(*b*)	○
3	A_2B	$\frac{1}{3}$	0	$-\frac{1}{6}$	$-\frac{1}{6}$	$\frac{i}{2\times 3^{1/2}}$	$\frac{-i}{2\times 3^{1/2}}$	0	$\frac{1}{18}$	$\frac{1}{6}$	$c+1/6\eta_K+1/2\eta_H$	1/3		●
											$c+1/6\eta_K-1/2\eta_H$	1/3		○
											$c-1/3\eta_K$	1/3	2(*c*)	⊗
4	A_5B	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1}{36}$	$\frac{1}{18}$	$\frac{1}{18}$	$c+1/6\eta_A-1/6\eta_K-1/6\eta_H$	1/3		⊗
											$c-1/6\eta_A-1/6\eta_K+1/6\eta_H$	1/3		○
											$c+1/6\eta_A+1/3\eta_K+1/3\eta_H$	1/6		●
											$c-1/6\eta_A+1/3\eta_K-1/3\eta_H$	1/6	2(*d*)	⊕
5	A_2B	$\frac{1}{3}$	$\frac{1}{3}$	$-\frac{1}{6}$	$-\frac{1}{6}$	$-\frac{1}{6}$	$-\frac{1}{6}$	$\frac{1}{9}$	$\frac{1}{18}$	$\frac{1}{18}$	$c+1/3\eta_A+1/6\eta_K+1/6\eta_H$	1/3		●
											$c-1/3\eta_A+1/6\eta_K-1/6\eta_H$	1/3		○
											$c+1/3\eta_A-1/3\eta_K-1/3\eta_H$	1/6		⊗
											$c-1/3\eta_A-1/3\eta_K+1/3\eta_H$	1/6	2(*e*)	⊕

(*a*) Number of the superstructure. (*b*) Stoichiometric structural formula. (*c*) Designations of the lattice sites of different types on the corresponding figure.

Table 2. *Characteristics of the hexagonal superstructures described by the expansion (4) in terms of A, M and L stars*

(*a*)	(*b*)	c_{st}	γ_A	$\gamma_M(1)$	$\gamma_M(2)$	$\gamma_M(3)$	$\gamma_L(1)$	$\gamma_L(2)$	$\gamma_L(3)$	Γ_A	Γ_M	Γ_L	P_i	ν_i	Fig.	(*c*)
1	A_3B	$\frac{1}{4}$	0	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0	0	0	0	$\frac{3}{16}$	0	$c+3/4\eta_M$	1/4		●
													$c-1/4\eta_M$	3/4	3(*a*)	○
2	*AB*	$\frac{1}{2}$	0	$\frac{1}{2}$	0	0	0	0	0	0	$\frac{1}{4}$	0	$c+1/2\eta_M$	1/2		●
													$c-1/2\eta_M$	1/2	3(*b*)	○
3	*AB*	$\frac{1}{2}$	0	0	0	0	$\frac{1}{2}$	0	0	0	0	$\frac{1}{4}$	$c+1/2\eta_L$	1/2		●
													$c-1/2\eta_L$	1/2	3(*c*)	○
4	A_3B	$\frac{1}{4}$	0	$\frac{1}{4}$	0	0	0	$\frac{1}{4}$	$\frac{1}{4}$	0	$\frac{1}{16}$	$\frac{1}{8}$	$c+1/4\eta_M+1/2\eta_L$	1/4		●
													$c+1/4\eta_M-1/2\eta_L$	1/4		○
													$c-1/4\eta_M$	1/2	3(*d*)	⊗
5	A_7B	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{64}$	$\frac{3}{64}$	$\frac{3}{64}$	$c+1/8\eta_A+3/8\eta_M+3/8\eta_L$	1/8		●
													$c-1/8\eta_A+3/8\eta_M-3/8\eta_L$	1/8		○
													$c+1/8\eta_A-1/8\eta_M-1/8\eta_L$	3/8		⊗
													$c-1/8\eta_A-1/8\eta_M+1/8\eta_L$	3/8	3(*e*)	⊕
6	A_3B	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	0	0	$\frac{1}{4}$	0	0	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$	$c+1/4\eta_A+1/4\eta_M+1/4\eta_L$	1/4		●
													$c-1/4\eta_A+1/4\eta_M-1/4\eta_L$	1/4		○
													$c+1/4\eta_A-1/4\eta_M-1/4\eta_L$	1/4		⊗
													$c-1/4\eta_A-1/4\eta_M+1/4\eta_L$	1/4	3(*f*)	⊕
7	A_3B_5	$\frac{3}{8}$	$\frac{3}{8}$	$-\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$-\frac{1}{8}$	$\frac{1}{8}$	$\frac{1}{8}$	$\frac{9}{64}$	$\frac{3}{64}$	$\frac{3}{64}$	$c+3/8\eta_A+1/8\eta_M+1/8\eta_L$	3/8		●
													$c-3/8\eta_A+1/8\eta_M-1/8\eta_L$	3/8		○
													$c+3/8\eta_A-3/8\eta_M-3/8\eta_L$	1/8		⊗
													$c-3/8\eta_A-3/8\eta_M+3/8\eta_L$	1/8	3(*g*)	⊕

(*a*), (*b*), (*c*) are the same as in Table 1.

3. The superstructures in the hexagonal lattice

As a result of the use of the procedure described in §2, we found 12 types of superstructure* in the case of the hexagonal crystal lattice. It was revealed that for all these superstructures the combinations of the Lifshitz stars *A*, *K*, *H* or stars *A*, *M*, *L* (of the reciprocal lattice of the disordered solution with the hexagonal crystal lattice†) can be present only separately in corresponding distribution functions $P_{AKH}(\mathbf{R})$ and $P_{AML}(\mathbf{R})$ obtained through the use of (1):

$$\begin{aligned} P_{AKH}(\mathbf{R}) = c &+ \eta_A\gamma_A \exp(i\pi h_3) \\ &+ \eta_K\big(\gamma_K(1)\exp[i(2\pi/3)(h_1+h_2)] \\ &+ \gamma_K(2)\exp[-i(2\pi/3)(h_1+h_2)]\big) \\ &+ \eta_H\big(\gamma_H(1)\exp\{i\pi[\tfrac{2}{3}(h_1+h_2)+h_3]\} \\ &+ \gamma_H(2)\exp\{-i\pi[\tfrac{2}{3}(h_1+h_2)+h_3]\}\big), \end{aligned} \tag{3}$$

$$\begin{aligned} P_{AML}(\mathbf{R}) = c &+ \eta_A\gamma_A \exp(i\pi h_3) \\ &+ \eta_M\{\gamma_M(1)\exp(i\pi h_1) \\ &+ \gamma_M(2)\exp(i\pi h_2) \\ &+ \gamma_M(3)\exp[i\pi(h_1-h_2)]\} \\ &+ \eta_L\{\gamma_L(1)\exp[i\pi(h_1+h_3)] \\ &+ \gamma_L(2)\exp[i\pi(h_2+h_3)] \\ &+ \gamma_L(3)\exp[i\pi(h_1-h_2+h_3)]\}, \end{aligned} \tag{4}$$

---

*Note that six types of superstructure from the complete list given in the present work are equivalent to the superstructures obtained by Bugaev (1978).

†The standard designations of these stars are quoted, for example, by Kovalev (1965).

where the integers h_1, h_2 and h_3 are the coordinates of the vector $\mathbf{R}$ in the hexagonal basis:

$$\mathbf{R} = h_1\mathbf{a}_1 + h_2\mathbf{a}_2 + h_3\mathbf{a}_3. \qquad (5)$$

In (5), the basis translation vectors $\mathbf{a}_i$ ($i = 1, 2, 3$) have the following orthogonal coordinates (see Fig. 1):

$$\mathbf{a}_1 = (a, 0, 0);\ \mathbf{a}_2 = (-a/2, a \times 3^{1/2}/2, 0);\ \mathbf{a}_3 = (0, 0, c)$$

(a and c are the parameters of the hexagonal crystal lattice).

The stoichiometric compositions of the superstructures, the values of the coefficients in corresponding series (3) and (4) and the references to the pictures for every superstructure are given in Tables 1 and 2, respectively.* See also Figs. 2 and 3. Moreover, the values Γ_s†, defined as

$$\Gamma_s \equiv \sum_{j_s} |\gamma_s(j_s)|^2 \qquad (6)$$

(for every star s), the expression P_i for the one-particle distribution functions for every ith sublattice ($i = 1, 2, \ldots$) that contains N_i sites symmetry equivalent in the ordered state and the values of ν_i, defined as

$$\nu_i \equiv N_i/N, \qquad (7)$$

are also given in the tables. This additional information is sufficient for the determination of the free energy F of corresponding superstructures under the statistical-thermodynamic description. For example, within the mean-field self-consistent approach (Khachaturyan, 1978, 1983; de Fontaine, 1979; Bugaev & Tatarenko, 1989),

$$F = (N/2)\left\{\tilde{V}(0)c^2 + \sum_{s\neq 0}\tilde{V}(\mathbf{k}_s)\Gamma_s\eta_s^2\right\} + Nk_BT\sum_i \nu_i\{P_i\ln P_i + (1-P_i)\ln(1-P_i)\}, \qquad (8)$$

where $\tilde{V}(\mathbf{k}_s)$ is the value of the Fourier transform of the mixing potential corresponding to some star $\mathbf{k}_s$ of the wave vectors, T is the absolute temperature and k_B is the Boltzmann constant.

Notice in conclusion that, for every substitutional superstructure in a binary solid solution based on a Bravais lattice, one can put in correspondence the isomorphic interstitial superstructure (see, for example, Khachaturyan, 1973, 1978, 1983) in which the interstitial atoms are distributed only with one interstitial (Bravais) sublattice isomorphically to the corresponding

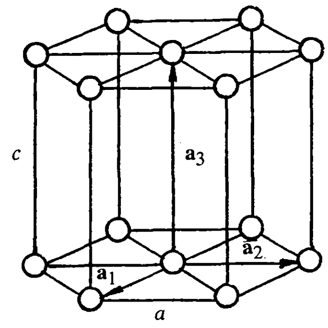

Fig. 1. Hexagonal crystal lattice.

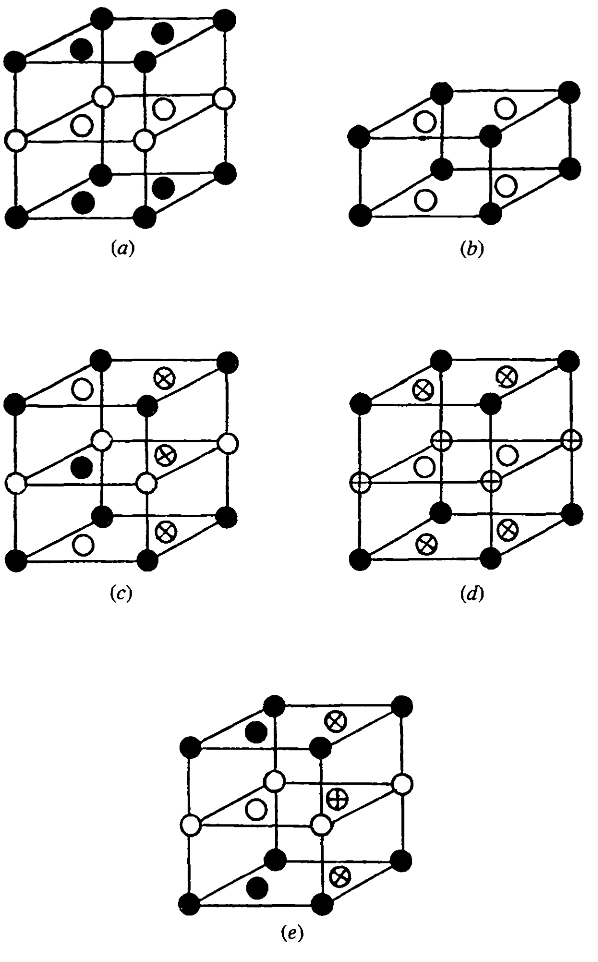

Fig. 2. Superstructures determined in Table 1.

---

* The characteristics are quoted only for the superstructures with the stoichiometric compositions $c_{\rm st} < 0.5$. The anti-isostructures with the stoichiometric compositions $1 - c_{\rm st}$ can be described by the change of the signs of all coefficients $\gamma_s(j_s)$, corresponding to every superstructure from Tables 1 and 2.

† Note that it is easy to find from (1) and (6) that the sum of the values of Γ_s over all stars (with corresponding non-zero long-range-order parameters) is determined by the stoichiometric composition $c_{\rm st}$ of the superstructure only:

$$\sum_s \Gamma_s = c_{\rm st}(1 - c_{\rm st}).$$

substitutional superstructure.* The stoichiometric composition $c_{\mathrm{st}}^{\mathrm{int}}$ of the interstitial superstructure can be obtained from the stoichiometric composition c_{st} of the isomorphic substitutional superstructure by the use of the following relation:

$$c_{\mathrm{st}}^{\mathrm{int}} = c_{\mathrm{st}}/(1 + c_{\mathrm{st}}), \tag{9}$$

i.e. one can connect the definite interstitial superstructure with the stoichiometric formula $A_{n+m}X_m$ to any given substitutional superstructure – A_nB_m (A, B are the designations of the atoms at the sites, X is the designation of the interstitials). Thus, for all substitutional superstructures quoted in Tables 1 and 2 (with the structural stoichiometric formulae AB, AB_2, AB_3, AB_5, AB_7 and A_3B_5), one can match up the interstitial superstructures (with the formulae A_2X, A_3X, A_4X, A_6X, A_8X and A_8X_3, respectively), based on the simple hexagonal or h.c.p. crystal lattices.

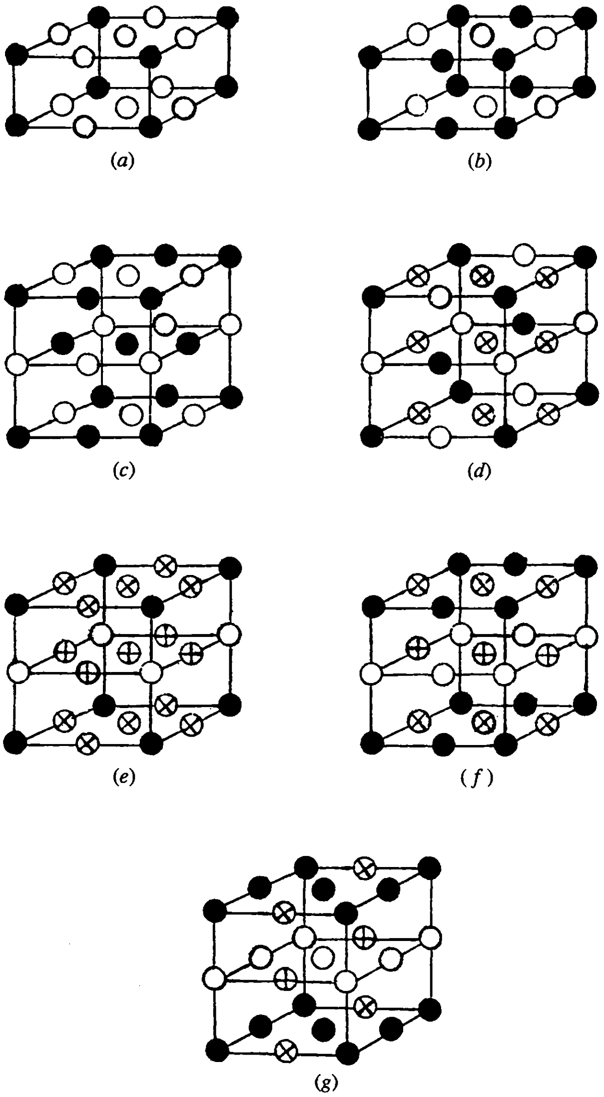
(*a*) (*b*) (*c*) (*d*) (*e*) (*f*) (*g*)

Fig. 3. Superstructures determined in Table 2.

This work was partially supported by the State Committee on Science and Technologies of the Ukraine (grant no. 2.2/205).

References

Bugaev, V. N. (1978). *Ukr. Fiz. Zh.* **23**, 1073–1080.

Bugaev, V. N. & Chepulskii, R. V. (1995). *Phys. Status Solidi B*, **192**, 9–16.

Bugaev, V. N. & Tatarenko, V. A. (1989). *Interaction and Arrangement of Atoms in Interstitial Solid Solutions Based on Close-Packed Metals.* Kiev: Naukova Dumka. (In Russian.)

Dmitriev, V. P., Rochal, S. B., Gufan, Yu. M. & Toledano, P. (1989). *Phys. Rev. Lett.* **62**, 2495–2498.

Fontaine, D. de (1979). *Configurational Thermodynamics of Solid Solution. Solid State Physics*, Vol. 34, edited by H. Ehrenreich, F. Seitz & D. Turnbull, pp. 73–274. New York: Academic Press.

Fromm, E. & Gebhardt, E. (1976). *Gase und Kohlenstoff in Metallen.* Berlin: Springer-Verlag.

Gufan, Yu. M. (1982). *Structural Phase Transitions.* Moscow: Izd. Nauka. (In Russian.)

Gufan, Yu. M. & Dmitriev, V. P. (1982). *Fiz. Met. Metalloved.* **53**, 852–861.

Khachaturyan, A. G. (1973). *Phys. Status Solidi B*, **60**, 9–37.

Khachaturyan, A. G. (1978). *Ordering in Substitutional and Interstitial Solid Solutions. J. Prog. Mater. Sci.* **22**, 1–150.

Khachaturyan, A. G. (1983). *Theory of Structural Transformations in Solids.* New York: John Wiley.

Khachaturyan, A. G. & Shatalov, G. A. (1975). *Acta Metal.* **23**, 1089–1102.

Kovalev, O. V. (1965). *Irreducible Representations of the Space Groups.* New York: Gordon and Breach.

Krivoglaz, M. A. (1969). *The Theory of X-ray and Thermal Neutron Scattering from Real Crystals.* New York: Plenum Press.

Krivoglaz, M. A. & Smirnov, A. A. (1964). *The Theory of Order–Disorder in Alloys.* London: Macdonald.

Landau, L. D. (1937). *Phys. Z. Sowjet Union*, **11**, 26.

Landau, L. D. & Lifshitz, E. M. (1980). *Course of Theoretical Physics*, Vol. 5: *Statistical Physics*, Part 1. Oxford: Pergamon Press.

Lifshitz, E. M. (1942). *J. Phys. (Moscow)*, **6**, 61, 251.

Sanchez, J. M., Gratias, D. & de Fontaine, D. (1982). *Acta Cryst.* A**38**, 214–221.

Solov'eva, M. I. & Shtern, D. M. (1990). *Izv. Vuzov. Fiz.* No. 6, pp. 90–94.

Zhorovkov, M. F. (1993). *Izv. Vuzov. Fiz.* No. 8, pp. 13–25.

Zhorovkov, M. F., Fuks, D. L. & Panin, V. E. (1975). *Phys. Status Solidi B*, **68**, 379–385.

---

* In general, the assemblage of the interstices forms the complex (with the basis) crystal lattice. However, the case of interstitial-atom distribution predominantly within one of the interstitial sublattices only is widely observed in experiment. Such a situation can be caused by both the energy non-equivalence of the (symmetry different) interstitial sublattices and the strong repulsion between the interstitial atoms that occupy the neighboring (even energetically equivalent) sublattices (see *e.g.* Khachaturyan & Shatalov, 1975; Khachaturyan, 1983).