"WEIGHT" OF THE OF RECIPROCAL LATTICE NODE IN THE CELL/ SUPER CELL OF THESE LATTICE

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Abstract: *Geometrically, the reciprocal lattice is built on the basis of the lattice of the crystal according to the rule* $\vec{a}_j^* \cdot \vec{a}_k = \delta_{jk}$ *, where the vectors* $\vec{a}_j^*$ *,* $\vec{a}_k$ *are the periods of the crystal and reciprocal lattices corresponding* $\delta_{jk} = 0$ *at* $j \neq k$ *and* $\delta_{jk} = 1$ *at* $j = k$ *(j, k = 1,2,3). The "weight" of the reciprocal lattice node, determined by the structural amplitude of the crystallographic plane corresponding to it, should not be zero, since in this case the reciprocal lattice node will be homologous to any point of the reciprocal space outside the lattice. Crystals with Bravais I, F, C – type cells in the reciprocal lattice are characterized by super cells, periods of which are n – times larger than* $a^* = a^{-1}$ *, where a is the period of the lattice cell. With respect to complex structures, even if they are single-element, the period of the super cell of the reciprocal lattice can exceed* a^* *several times. For a diamond crystal* $a_s^* = 4a^*$ *under the super cell of the reciprocal lattice it is necessary to use the smallest parallelepiped, the "weight" of all vertex nodes of which is not equal to zero.*
KEYWORDS: "WEIGHT" OF THE RECIPROCAL LATTICE NODE , CELL AND SUPER CELL RECIPROCAL LATTICE.

1. Introduction

The crystal lattice assumes regularity in the arrangement of atoms along any direction. This means that when choosing two adjacent identical structural-chemical (homologous) elements with a distance between them - α, on a straight line passing through these two points, there will be homologous or points with a distance $t = n\alpha$, where n is an integer. The value of t is the translation, the transfer of the crystal to which it leads to self-coincidence. Three non-coplanar translations $\vec{a}, \vec{b}, \vec{c}$ selected according to the corresponding requirements, form a parallelepiped called the crystal cell. The cell must meet the following requirements:

1. The point symmetry of the cell is the same as that of the crystal as a whole;
2. The number of right angles in the cell should be maximum;
3. The total cell surface should be the smallest.

The listed requirements allow in most cases to choose one of the many possible options. In the general case, the lattice cell of a crystal is an oblique parallelepiped with three linear (a, b, c) and three angular (α, β, γ) parameters. The cell can be described by the vectors

$\vec{a}, \vec{b}, \vec{c}$ which form the crystallographic coordinate system (kg) (or Bravais rapper). The coordinates of a point within a cell are measured in units of parameters a, b, c.

Tasks to be solved:
1. To show that the assertion that the F-type lattice of the crystal forms a cell I-type in the reciprocal lattice. Statement that the I-cell forms F-type lattice is incorrect, because the cells of the reciprocal lattice can not contain nodes with non-integer parameters.
2. To justify the necessity of introducing the concept of a super reciprocal lattice cell.
3. To show that, along with the coordinate of the reciprocal lattice site, its "weight" determined by the structural amplitude F (h, k, l) must be taken into account.
4. Show that a number of nodes in the indicated reciprocal lattices have zero "weights".

2. The relationship between the cells of the cristal and reciprocal lattices.

An arbitrary plane in the crystal cuts off the coordinates $(x, y, z)_{kg}$ from the crystallographic axes and necessarily has a set of planes homologous to it.
The Interplanar distance between the adjacent planes is equal to d.

Let one of the planes pass through a point with coordinate x_{kg}. The plane homologous to it within the first cell is located at the origin of coordinates. Section $x_{kg} \leq a$. Any crystallographic plane cuts off the segment $x_{kg} = a/h$ from the crystallographic axis, where h is a mandatory integer [1].

In the three-dimensional version, the crystallographic plane passes through points with crystallographic coordinates $(x, y, z)_{kg} = (a/h, b/k, c/l)$. Integers (h, k, l) are called crystallographic indices. It follows from the above that one of the sets of identical planes necessarily passes through two, three, four vertices of the lattice.

The value of the interplanar distance is determined by the method of x-ray electron or neutron diffraction (X-ray, electron and neutron diffraction methods, respectively).

If the X-ray beam at the slip angle θ (beam 1) falls on the crystallographic plane I (Figure 1), and is reflected from it, and the next plane II (beam 2) interferes with these rays, then the diffraction angle is 2θ. The angular position of the reflex is described by the Wolf-Bragg equation.

$$2d\sin\theta = n\lambda \tag{1}$$

where d is the interplanar distance, λ is the radiation wavelength, n is an integer.
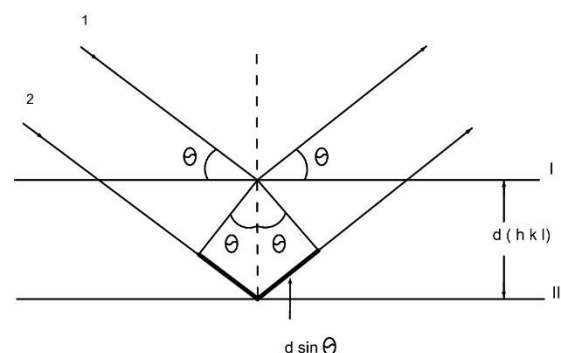

Fig. 1. To the condition of the Wolf-Bragg

The value of d/n is determined experimentally and is considered as $d/n \equiv d$ for the corresponding crystallographic planes. Each of the d (h, $k.l$) planes can be represented as a point of reciprocal space (Figure 2).
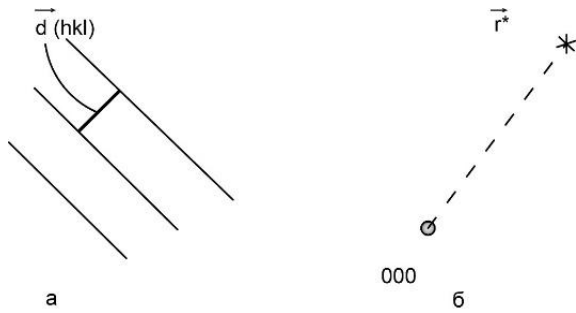
Fig. 2. - (a) - mapping of the d (h, k, l) plane, (b) - in the reciprocal space

The point (*) is a map of the space of a crystal $\vec{d}$ (h, k, l) of the space of a crystal. The radius vector of a point (*) in the reciprocal space is equal to $\vec{r}^* = \vec{d}^{(-1)}$.

Moreover, $\vec{r}^*$ is parallel to $\vec{d}$. It is obvious that the transition from the reciprocal space to the cristal one is also easy to implement. Each node of the reciprocal lattice has integer coordinates (h, k, l) in its crystallographic system, that are linked to the Brave Crystal Rapper.

Nodes (h, k, l) in the reciprocal space form a lattice, but unlike crystal space, this lattice determines only the position of the nodes, but is not a translational symmetry. Each x-ray reflex has its own intensity (I), which characterizes the "weight" of the reciprocal lattice site. The greater I (h, k, l), the greater the "weight" of the node (h, k, l), which we denote F (h, k, l).

In the reciprocal lattice, as in a crystal lattice, an elementary parallelepiped is selected with parameters $a^*, b^*, c^*, \alpha^*, \beta^*, \gamma^*$, moreover, this choice depends on the cell of the crystal lattice, since $(a, b, c, \alpha, \beta, \gamma) = (a_i^0 \, a_i^0)_{i=1,2,3}$ is connected with $(a^*, b^*, c^*, \alpha^*, \beta^*, \gamma^*) = (a_j^* \, a_j^*)_{j=1,2,3}$ with the conditions:

$$a_j^{*(0)} = \frac{a_{j+1}^{0(*)} \, a_{j+2}^{0(*)} \, sin \, \alpha_j^{0(*)}}{V^{0(*)}}, \qquad (2)$$

$$cos\alpha_j^{*(0)} = \frac{cos \, \alpha_{j+1}^{0(*)} cos \, \alpha_{j+2}^{0(*)} - cos \, \alpha_j^{0(*)}}{sin \, \alpha_{j+1}^{0(*)} sin \, \alpha_{j+2}^{0(*)}}, \qquad (3)$$

or

$$sin\alpha_j^{*(0)} = \frac{r^{0(*)}}{sin \, \alpha_{j+1}^{0(*)} sin \, \alpha_{j+2}^{0(*)}}, \qquad (4)$$

where $r^{0(*)} = (1 - cos^2 \, \alpha^{0(*)} - cos^2 \, \beta^{0(*)} - cos^2 \, \gamma^{0(*)} + 2cos \, \alpha^{0(*)} \, cos \, \beta^{0(*)} \, cos \, \gamma^{0(*)})^{1/2}$, $V^{*(0)}$ – the volumes of the reciprocal (cristal) cells of the lattices, determined by the formula:

$$V^{*(0)} = a^{*(0)} \, b^{*(0)} \, c^{*(0)} r^{*(0)}, \qquad (5)$$

The scalar multiplication of the vectors Bravais rapper of the crystal and reciprocal cells are equal $(a_j^* \, a_k^0) = \delta_{jk}$. From conditions (2-5) it follows that the reciprocal lattice of reciprocal lattice is a crystal lattice.

The reciprocal and direct lattices are described by formally symmetric transitions from the parameters of one lattice to the parameters of another, but both of these lattices are characterized by cells as an elementary geometric configuration. These two lattice are significantly different from each other. In the crystal lattice, all cells are absolutely identical with each other. That is, the following is always true:

$$\hat{T}R(x, y, z) = R^{'} (mx, nx, pz), \qquad (6)$$

where $\hat{T}$ – translation operator. Moreover, the points (x, y, z) and (mx, nx, pz) are homologous, that is, they can be swapped, but no properties of the lattice will change. At the nodes of the crystal lattice and, therefore, at the vertices of the cell are homologous

points. It can be a single atom, any point of a molecule, a certain point of a molecular radical, the center of a structural polyhedron, etc. In the cell of the reciprocal lattice the nodes are points with radius vectors.

$$\vec{r}^* = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*, \qquad (7)$$

The vertices of the crystal cell located in the octant of the coordinate system x^*, y^*, z^* are a parallelepiped with coordinates of the vertices 000; 100; 010; 001; 110; 101; 011; 111. In the reciprocal lattice, the cells are identical only geometrically, that is, they are all a parallelepiped with edges a $\vec{a}^*, \vec{b}^*, \vec{c}^*$. Each node of the reciprocal lattice $r^*(hkl)$ defines a plane (hkl) [2]. The structural amplitude of X-ray (electron, neutron) radiation F (h, k, l) determines the "weight" of the reciprocal lattice site. Translation in the reciprocal lattice with F (h, k, l) is absent. The choice of the cell itself is connected with the crystal lattice, that is, the origin of coordinates in the reciprocal lattice and the direction of the axes x^*, y^*, z^* cannot change, since they depend on $\vec{a} \, \vec{b} \, \vec{c}$. Any number of atoms with coordinates (xyz) with values in the range (0 ÷ 1) can be located in a crystal cell. Any point in the space of the crystal has a point homologous to it in the cell, taken as the initial one.

There can not be any nodes of the lattice in the cell of the reciprocal lattice, as their coordinates in the rapper $\vec{a}^*, \vec{b}^*, \vec{c}^*$ are integers. The "weight" of the node of the reciprocal lattice can be zero. In this case, x^*, y^*, z^* to pass non-null node and cell must be constructed so that all its vertices are non-zero "weight". Periods of such super cell as its volume will be multiples (a^*, b^*, c^*, V^*) (2-5).

3. Reciprocal lattice of crystals I, F, C (AB) – types

The "weight" of the reciprocal lattice node is described by the value of the structural amplitude, which is calculated by the formula:

$$F(h, k, l) = \sum_{j=1}^{N} f_j (xyz)_j \, exp2\pi i \, (hx_j + ky_j + lz_j), \quad (8)$$

where f_j – atomic scattering amplitude of the j-th atom (tabular value). N is the number of atoms in the cell, the volume-centered cell of the crystal lattice (type I) [3]. The basis of the I-type cell is the parallelepiped to which the nodes (000) belong; (1⁄2 1⁄2 1⁄2), that is, any point (any atom) with coordinates (xyz) must have a homologous point (atom) with coordinates (x + 1⁄(2), y + 1⁄2, z + 1⁄2). Therefore, the structural amplitude (8) for the I – type of the lattice takes the view:

$$F(h, k, l) = \sum_{j=1}^{N/2} f_j (xyz)_j \{[exp2\pi i \, (hx_j + ky_j + lz_j) + exp2\pi i [h(x_j + {}^1/_2) + k(y_j + {}^1/_2) + l(z_j + {}^1/_2)]\} = 1 + exp2\pi i \, (\tfrac{hkl}{2}) \sum_{j=1}^{N/2} f_j \, exp2\pi i \, (hx_j + ky_j + lz_j), \quad (9)$$

The multiplier made for the sum sign is:

$$[1 + e^{\pi i (h+k+l)}] = [1 + e^{i\pi c}], \qquad (10)$$

A constant integer C can take two values C = 2n (even), C = 2n + 1 (odd). Consequently, all nodes of the I – type reciprocal lattice with an odd sum of indices have zero "weight". The reciprocal lattice in this case has the view (Figure 3).
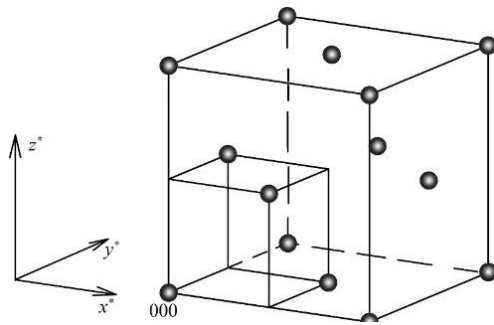
(6)

Fig. 3. - *A super cell of a reciprocal lattice of a crystal with a lattice of type I. ○ - nonzero nodes*

Figure 3 shows the nodes closest to the origin of coordinates the reciprocal lattice with a nonzero "weight". The same figure shows a cell with $a^* b^* c^*$ but it has four nodes with a non-zero "weight" 000, 110, 101, 011. A super cell whose vertices have a non-zero "weight" has periods.

$$\begin{cases} a_s^* = 2a^* = {}^2/_a \\ b_s^* = 2b^* = {}^2/_b \\ c_s^* = 2c^* = {}^2/_c \\ V_s^* = 8V^* \end{cases} \qquad (11)$$

That is, the volume-centered cell in the reciprocal space is described by a face-centered super cell with dimensions (11).

The face-centered crystal lattice is characterized by the Bravais basis 000; 1/2 1/2 0; 1/2 0 1/2; 0 1/2 1/2.

The formula of the structural amplitude for such crystals is

$$F(h, k, l) = \sum_{j=1}^{N/4} f_j (xyz)_j \{ exp2\pi i \left(hx_j + ky_j + lz_j \right) + exp2\pi i [h(x_j + {}^1/_2) + k(y_j + {}^1/_2) + lz_j] + exp2\pi i [h(x_j + {}^1/_2) + ky_j + l(z_j + {}^1/_2)] + exp2\pi i [hx_j + k(y_j + {}^1/_2) + l(z_j + {}^1/_2)] \} = (1 + e^{\pi i(h+k)} + e^{\pi i(h+l)} + e^{\pi i(k+l)}) \sum_{j=1}^{N/4} f_j \, exp2\pi i \, (hx_j + ky_j + lz_j) \qquad (12)$$

The multiplier in front of the sum sign (four-term) is equal to zero if the indices (*hkl*) have different parity: two even ones one odd and vice versa. If (*hkl*) have the same parity, then this four-member is equal to four. Therefore, the reciprocal lattice nodes with indices of mixed parity have zero "weight" (Figure 4).
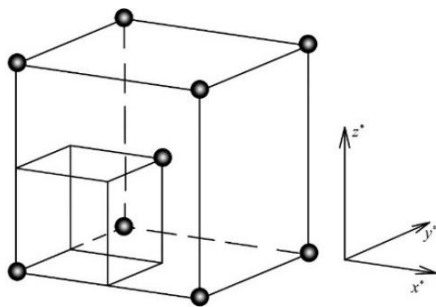

Fig. 4. - *A super cell of a reciprocal lattice of a crystal with an F – type cell*

Figure 4 shows the reciprocal lattice cell, which has only two nodes with a nonzero "weight" (000); (111). The super cell has indices 000, 111, that is, the super cell refers to the volume-centered Bravais cell. The relationships between the supercell parameters of the reciprocal crystal lattice with an *F* – type lattice and the parameters of the reciprocal and crystal cells are the same as in conditions (11).

The Bravais basis of *C* – type cells is 000; 1/2 1/2 0. Therefore, the structural amplitude of such crystals is:

$$F(h, k, l) = \sum_{j=1}^{N/2} f_j (xyz)_j \{ exp2\pi i \left(hx_j + ky_j + lz_j \right) + exp2\pi i [h(x_j + {}^1/_2) + k(y_j + {}^1/_2) + lz_j]\} = (1 + e^{\pi i(h+k)}) \sum_{j=1}^{N/2} f_j \, exp2\pi i \, (hx_j + ky_j + lz_j), \qquad (13)$$

which allows us to state that $F(hkl) \neq 0$ only for an even sum of indices *hk*, the restrictions are not imposed on *l*. The super cell of the reciprocal lattice of such crystals is shown in Figure 5.
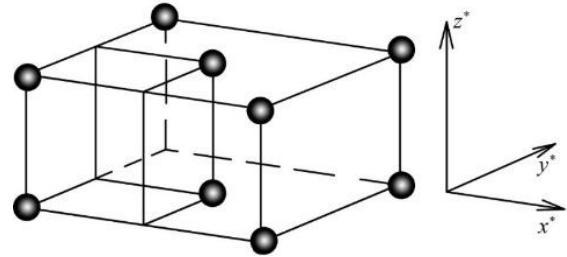

Fig. 5. - *Super cell of a reciprocal lattice of a crystal with a C – type cell*

It can be seen from the figure that the cell of the reciprocal lattice has nodes with zero "weight" in its vertices.

The relations between the parameters of the super cell and the parameters of the cells of the reciprocal and crystal lattices are:

$$\begin{cases} a_s^* = 2a^* = {}^2/_a \\ b_s^* = 2b^* = {}^2/_b \\ c_s^* = c^* = {}^1/_c \\ V_s^* = 4V^* \end{cases} \qquad (14)$$

It is obvious that the *P* – type cells of the crystal lattice in the reciprocal lattice are also characterized by a *P* – type cell, since, when calculating *F* (*hkl*), there are no restrictions on the indices.

For more complex structures, these relations between the cells of a crystal and the super cells of the reciprocal lattice may break. This can be illustrated by the example of diamond.

4. Reciprocal lattice of diamond crystals

Diamond crystals are described by the *Fd3m* space group. Figure 6 (*a*) shows a polyhedral model of the structure of a diamond as a junction of tetrahedra and a cell of its crystal lattice (*b*).

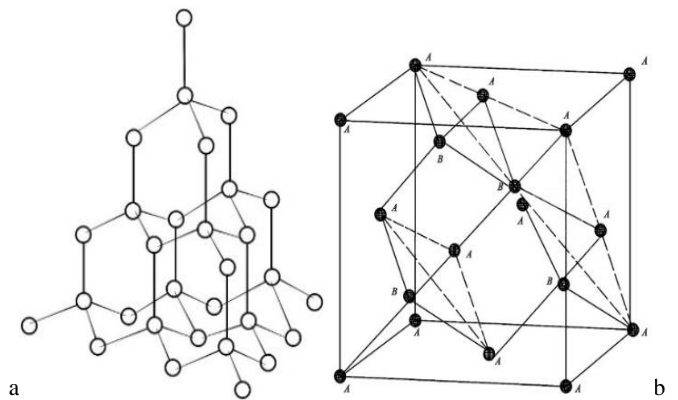a   b

Fig. 6. - *Articulation scheme of carbon tetrahedra (a), a lattice cell of a diamond crystal (b)*

The diamond cell consists of two face-centered cubes that are shifted relative to each other along the main diagonal of the cube for

translation (1⁄4 1⁄4 1⁄4). The coordinates of carbon atoms in the diamond cell are shown in table 1.

Table 1. *- Crystallographic coordinates of atoms in a diamond cell (Figure 6)*

№	1	2	3	4
xyz	000	$\frac{1}{2}\frac{1}{2}0$	$\frac{1}{2}0\frac{1}{2}$	$0\frac{1}{2}\frac{1}{2}$
№	5	6	7	8
xyz	$\frac{1}{4}\frac{1}{4}\frac{1}{4}$	$\frac{3}{4}\frac{3}{4}\frac{1}{4}$	$\frac{3}{4}\frac{1}{4}\frac{3}{4}$	$\frac{1}{4}\frac{3}{4}\frac{3}{4}$

The period of crystal lattice of diamond and minimum atomic distance have values: $a = 3,57$Å, $(r_{c-c}) = 1,54$Å.

Taking into account the coordinates of atoms (table 1), the structural amplitude (8) will take the following from after the transformation:

$$F(hkl) = f_c[1 + exp\pi i(h+k) + exp\pi i(h+l) + exp\pi i(k+l)1 + exp\pi i(h+k+l)2, \qquad (15)$$

The first bracket in this expression is not equal to zero for indices with the same parity. If the indices are even, but their sum equals $4n + 2$, then $F(hkl) = 0$. Therefore, the first nonzero nodes lying on the coordinate axes of the reciprocal lattice for the Super Diamond Cell are as follows: 400; 040; 004. Indices (hkl) in the coordinate system $\vec{a}$ $\vec{b}$ $\vec{c}$ all odd, then $F(hkl) \neq 0$. If the indices are even, then their sum should be divisible by 4 without any balance.

Super cell cube reciprocal lattice diamond has a period $a_s^* = 4a^* = \frac{4}{a}$. All faces centered: 220; 202; 022.

Reciprocal lattice nodes with all odd indices are inside the super cell and have indices: 111; 311; 131; 331; 113; 313; 133; 333

Nodes with odd indices form a cube with the edge $(a')^{(*)} = 2a^* = \frac{2}{a}$, which is inside the super cell of the reciprocal lattice of the diamond.

If a trio of nodes of the reciprocal lattice $(x^*y^*z^*)_1$ are chosen as a structural element and the translation $x_t^* = x_1^* + 4$ is taken into account, then we get the distribution of nodes in table 2.

Table 2 *– Bringing the super cell of the reciprocal lattice of the diamond to the super cell F – type*

$(x^*y^*z^*)_1$	000 111 $\overline{1}\overline{1}\overline{1}$	220 331 $\overline{3}\overline{3}\overline{1}$	202 313 $\overline{3}\overline{1}\overline{3}$	022 133 $\overline{1}\overline{3}\overline{3}$
$(x^*y^*z^*)_t$	000 111 333	220 331 113	202 313 131	022 133 311

Each vertex node is located in the center of the tetrahedron from the nodes of the reciprocal lattice. Node 000 lies in the tetrahedron of the nodes 111 $\overline{1}\overline{1}\overline{1} \equiv 333$, $1\overline{1}\overline{1} \equiv 133$, $\overline{1}\overline{1}\overline{1} \equiv 313$. The other nodes of the first super cell are coordinated by nodes with odd indices on the similar scheme.

Nodes with odd indices are also found in tetrahedrins, the vertices of which are nodes in the vertices of the super cell and the three nodes of the coordinating face.

A tetrahedron that coordinates nodes with even indices can be considered as "some super knot" of the reciprocal lattice. In this case, it is obvious that the Super diamond Cell refers to the *F*-type.

5. Conclusion

When studying the diffraction of *X*-rays it is assumed that when the node of the reciprocal lattice is on the sphere of the Ewald, there will be a reflected beam (reflex) on the radius-vector of the node of this sphere. The intensity of the reflex determines the "weight" of the node, which is equal to the structural amplitude. Depending on the type of cell of the Bravais lattice of the crystal, some reciprocal lattice units have a zero weight. In the vertices of the reciprocal lattice cell must be nodes with $F(hkl) \neq 0$. This condition is only for *P*-type lattice.

Cell of the reciprocal lattice is based on the rapper $a^* = r^*(100)$, $b^* = r^*(010)$, $c^* = r^*(001)$. Such a cell can not include the nodes of the lattice , as their indices would have fractional values. It is shown that the assertion that the cell *F*–type lattice of a crystal is characterized by the cell *I* –type in the reciprocal lattice wrong. These types in the reciprocal lattice belong to super cell with parameters to an integer the number a_j^*.

For the analysis of crystals with non primitive cells, the concept of super cells must be used.

For example, the diamond crystal shows that the lattice of *F*–type in the reciprocal space of the super cell is also related to the *F*–type.

Super cell of the reciprocal lattice of the crystals with Bravais cells of crystals with a lattice of *C*–type have a volume $V_s^* = 4V^*$ for *F*– and *I*–type $V_s^* = 8V^*$, for diamond $V_s^* = 64V^*$, where V^*– cell volume of the reciprocal lattice with parameters $a^*b^*c^*$.

6. References

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