Modeling and Calculation of the dynamic Three-Dimensional A^3B^5 Models on the Example of GaAs

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Abstract—The article discusses the dynamic three-dimensional modeling compounds A^3B^5. The initial structure is taken compound GaAs. The resulting model is given for different distances from the central atom. There are the distances from one to six. The result is an uneven growth of the number of atoms grouped along the radius of coverage. For the other elements of the possibility of uniform methods increase the number of atoms, such as Ga. This article briefly describes the algorithms finding the orderly and the semi platonic and Archimedean figures and their complexes for the FCC and BCC structures, which contributes to the increased use of the computer modeling techniques in crystallography and SSP.

Index Terms—Semiconductors; ab initio calculations; crystal structure; Fermi surface.

I. INTRODUCTION

To compound semiconductor type A^3B^5 is GaAs. Its crystal structure is a two face-centered cubic lattice, which are shifted relative to each other by ¼ the space diagonal. In the center of origin of the As atoms there are four nearest neighbors at the vertices of a tetrahedron. Each ion is surrounded by four nearest-neighbor ions, the antithesis of the mark. At a distance, there are four ion with $q_i q_j = -1$, eight ions antithesis sign $q_i q_j = +1$ at a distance. The system nods of the GaAs create the order of the atomic cores of the tetrahedral combinations. The source of difficulty in the calculation of band spectra is a priori is laid in these calculations the translational invariance, which involves the study does not end, real crystals, and the infinite, ideal. Manipulations with infinite objects are allowed in the initial stages of the abstraction of subject area (in our case, solid bodies), but they become simply mathematical trick when trying to obtain information about the physical properties of such complex objects as solid bodies. Solid body, as really existing system, and not a mathematical trick, requires a different approach than adopted for the simple monatomic isolated objects [1].

One of the advantages described technique — applicable to the systems with neighbor order, where Bloch's theorem is not applicable as the initial conditions, since the translational invariance in the real space and in the quasi-momentum space is not the necessary condition for the determination of the crystalline potential, the wave functions of the energy values in the space of wave vectors [1], [2].

Therefore the proposed technique is still the only one well-established technique that is applicable for the analysis

of the band spectrum of finite imperfect crystals.

II. CALCULATION OF THE DYNAMIC THREE-DIMENSIONAL STRUCTURE A^3B^5

Consider the finite crystal with unbroken intervals (except for the crystal boundary violation). For simplicity, we take a large number of cores, when there is a nearly ideal periodicity of the crystal. In this case, the parameters obtained from the mathematical formalism for the analysis of the band spectrum are periodic functions, except for the boundary of the crystal. The crystal potential and wave functions have a period equal to the distance between the cores, depending on the chosen direction. The energies have multiple frequency modulus of the wave vector in the quasi-momentum space [1]-[3].

Now turn to the crystal with a very small number of cores. In such a crystal frequency is not as ideal as in the previous case. The simulation of such a crystal is insurmountable difficulties for traditional methods, but this is the case is taken by us as a basic demonstration version. The object in question is distant from a perfect crystal due to its limited size. And despite this, the technique presented by us showed the periodicity of the above parameters. Thus in our problems are not used the condition of periodicity and Bloch's theorem as the necessary initial conditions. The Fig. 1 shows it on the example of GaAs.
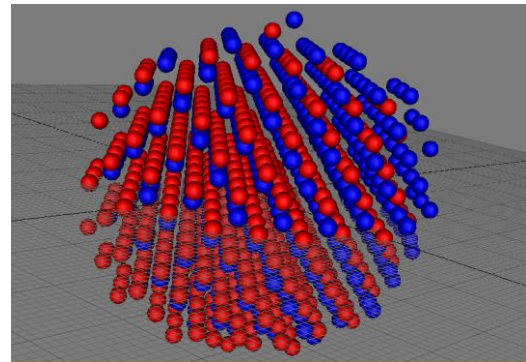

Fig. 1.The As atoms and Ga for the radius of coverage 6. Red marked atoms As, in blue denote atoms Ga. Central atom is As.

In computer modeling of the crystal structure of GaAs, combined with three-and five-valent elements are observed the following regularities (see Table I). When the radius of coverage is two in this range there are 38 cores. As the first atomic core in the center of origin, the four Ga atoms are located at a distance of 3 next 12 As atoms at a distance of 8. Nine Ga atoms at a distance there are 11. Six As atoms at a distance of 16, three Ga at a distance of 19 and three Ga at a distance of 27.

TABLE I: THE COMBINED LATTICE GaAs

№	x	y	z	d^2	Ion	
0	0	0	0	0	As	
1	−1	−1	1	3	Ga	breaking
2	−1	1	−1	3	Ga	
3	1	−1	−1	3	Ga	
4	1	1	1	3	Ga	
5	0	2	−2	8	As	breaking
6	0	2	2	8	As	
7	0	−2	−2	8	As	
8	0	−2	2	8	As	
9	−2	2	0	8	As	
10	−2	−2	0	8	As	
11	2	2	0	8	As	
12	2	−2	0	8	As	
13	−2	0	2	8	As	
14	−2	0	−2	8	As	
15	2	0	2	8	As	
16	2	0	−2	8	As	
17	1	3	−1	11	Ga	breaking
18	1	−1	3	11	Ga	
19	−3	1	1	11	Ga	
20	−1	3	1	11	Ga	
21	3	1	−1	11	Ga	
22	1	−3	1	11	Ga	
23	−1	1	3	11	Ga	
24	3	−1	1	11	Ga	
25	1	1	−3	11	Ga	
26	0	4	0	16	As	breaking
27	−4	0	0	16	As	
28	4	0	0	16	As	
29	0	0	−4	16	As	
30	0	0	4	16	As	
31	0	−4	0	16	As	

TABLE II: CONTINUATION

№	x	y	z	d^2	Ion	
32	3	3	1	19	Ga	breaking
33	1	3	3	19	Ga	
34	3	1	3	19	Ga	
35	1	5	1	27	Ga	breaking
36	5	1	1	27	Ga	
37	1	1	5	27	Ga	

Total number of cores with zero: 38

From this calculation, the differences in distance between the various groups are as (1):

$$\Delta r_1 = r_2 - r_1 = 3$$
$$\Delta r_2 = r_3 - r_2 = 5$$
$$\Delta r_3 = r_4 - r_3 = 3$$
$$\Delta r_4 = r_5 - r_4 = 5 \qquad (1)$$
$$\Delta r_5 = r_6 - r_5 = 3$$
$$\Delta r_6 = r_7 - r_6 = 8$$

We observe quasiperiodic change in the difference. At the border radius of coverage this periodicity is broken. When increasing the radius of coverage this periodicity is restored to the previous radius, but is broken on the new range. Thus, the boundary conditions lead to a violation of the periodicity.

Simulated lattice shown in the following figures. The first figure shows the four first neighbors As in the lattice. Neighbors' ions Ga (blue) form a tetrahedron with the center of As (red).

III. MODELING OF THE DYNAMIC THREE-DIMENSIONAL MODELS OF GaAs

The Fig. 2 shows the grid with a radius of coverage 1. There are 5 atomic cores in it. There is a periodic step structure. The structure of the central ion and its neighbors on the tetrahedron is stored and located in the center of this lattice.
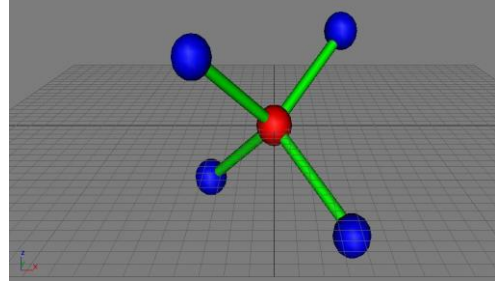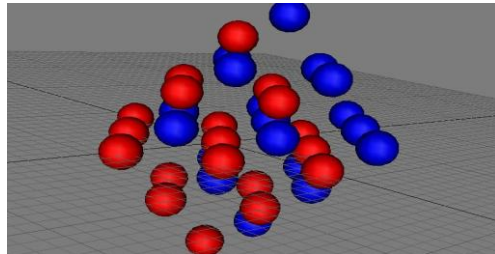

Fig. 2. The grid with a radius of coverage where there are 5 atomic cores.

The Fig. 3 shows the grid with a radius of coverage 2. There are 38 atomic cores in it. There is a periodic step structure. The structure of the central ion and its neighbors on the tetrahedron is stored and located in the center of this lattice.

Fig. 3.The grid with a radius of coverage 2 where there are 38 atomic cores.

The Fig. 4 shows the grid with a radius of coverage 3. There are 110 atomic cores in it. There is again a periodic step structure. The structure of the previous lattice is preserved. And while the structure of the central ion and its neighbors on the tetrahedron is stored and located in the center of this lattice.
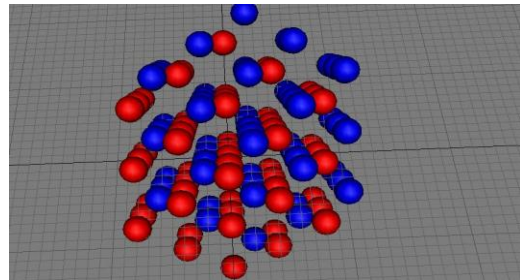

Fig. 4.The grid with a radius of coverage 3. where there are 110 atomic cores.

The Fig. 5 shows the grid with a radius of coverage 4. There are 282 atomic cores in it. Again, there is a periodic step structure. The structure of the previous lattice is

preserved. Again, the structure of the central ion and its neighbors on the tetrahedron is stored and located in the center of this lattice.
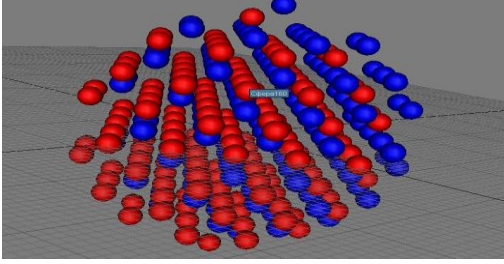

Fig. 5.The grid with a radius of coverage 4. where there are 282 atomic cores.

The Fig. 6 shows the grid with a radius of coverage 5. There are 498 atomic cores in it. There is a periodic step structure. The structure of the previous lattice is preserved. And the structure of the central ion and its neighbors on the tetrahedron is stored and located in the center of this lattice.
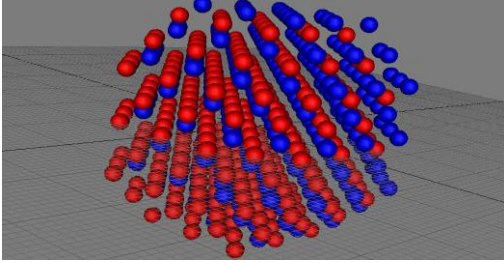

Fig. 6. The grid with a radius of coverage 5. where there are 498 atomic cores.

The Fig. 1 shows the grid with a radius of coverage 6. There are 918 atomic cores in it. There is a periodic step structure. The structure of the previous lattice is preserved. And the structure of the central ion and its neighbors on the tetrahedron is stored and located in the center of this lattice.

IV. DISCUSSION

It can be seen as an increase in the radius of coverage is restored periodicity in the lattice covered by the previous radius and there is a new violation of the periodicity on the boundary spanning lattice. The depth of violation increases with the radius of coverage. This is well observed in the tables you demonstrated for different cores.

On the basis of the direct lattice can construct the reciprocal lattice and define the properties of the Fermi surface. And the radius of coverage can be taken arbitrary (millions of skeletons).

The calculated structure allows to reach a real-time implementation and to take into account of defects and of real devices based on GaAs, because these are high-speed computing now by our proposed method.

On the basis of the direct lattice we can also construct the reciprocal lattice and define the properties of the Fermi surface. And the radius of coverage can be taken arbitrary (millions of skeletons). High-speed computing enables a dynamic computer simulation of the properties of real crystals of the GaAs.

Since the GaAs lattice is identical to the lattice of Si, sphalerite and diamond, we can apply the technology provided by and for these substances.

In calculating of coordination spheres cells of FCC- and BCC-lattices are presented as superlattice structure to fill own nodes by atoms of cells and additional nodes of the simple cubic lattices (SCL) — interstitial atoms [2]. The completing of coordination spheres with atoms is determined on the basis of a small SC-lattice, taking into account octahedral, tetrahedral internodes.

If atoms in the lattice arrange with the dense packing, P-nodes are centers of the inter-body lattices in the methods of presentment of the spatial distribution of atoms and internodes along the coordination spheres in the crystals. Tetrahedral and octahedral internodes in the ion-interionic terminology mean inter-body lattice space surrounded by the atoms in the crystal lattice nodes.

The Table 1 contains the number of atoms and the distance from the central atom of the diamond-like structure. The distance is given in units of the lattice constant *a*. Let us choose the maximum distance based on these conditions, forming a set of atoms contributions on which the calculation of the potential are taken into account.

In this work we consider the crystal potential for crystals with the diamond structure. The Coulomb potential is the sum of the capacity building of the nucleus and the electrons occupied levels:

$$U_c = U_n + U_0, \tag{2}$$

where $U_n = -2Z/r$. Here, Z — number of the element, r — distance from the atom to the specified point.

Potential U_0 is a solution of the Poisson equation:

$$\nabla^2 U_0 = -8\pi\rho_0(r), \tag{3}$$

where $\rho_0(r)$ — the density of the electrons of the occupied levels at the distance r from the center of the atom. The density is calculated as follows:

$$\rho_0(r) = \sum_{n,l} r^2 R_{nl}^2(r). \tag{4}$$

Function $R_{nl}(r)$ — the radial part of the electron wave function for a hydrogen atom [4], [5]. Using the principle of superposition of the electronic densities and the additivity of the integral equation (3) can solve as follows:

$$U_0(r) = \sum_{i=0}^{I} u(r_i), \tag{5}$$

$$u(r_i) = \sum_{n,l} u_{nl}(r_i), \tag{6}$$

where I — the set of the number of atoms minus one, r_i — the distance from the center of the i-th atom to the specified point

$$\vec{r}_i = \vec{r} - \vec{a}_i. \tag{7}$$

Here a_i — the radius-vector of the i-th atom with respect to the center of origin. Let us obtain the Poisson equation for an electron of i-th atom:

$$\nabla^2 u_{nl}(\vec{r}_i) = -8\pi r_i^2 R_{nl}^2(\vec{r}_i). \tag{8}$$

Solving (8), we obtain

$$u(\vec{r}_i) = -8\pi \sum_{n,l} \iint u_{nl}(\vec{r}_i)d\vec{r}_i^2 \ . \qquad (9)$$

Directly using the functions (5, 6, 7, 8, 9) we find the potential U_0 (r). This approach allows us to calculate effectively and accurately the electronic potential. We rewrite the expression (2) accounted for the entire set of atoms:

$$U_c(\vec{r}) = \sum_i U_n(\vec{r}_i) + U_0(\vec{r}). \qquad (10)$$

Thus, the Coulomb potential is calculated from all the surrounding atoms [1], [6].

This approach allows us to select any line capacity in any direction from the lattice points, and may be any length of line. Moreover, we can specify a curved line capacity.

The cell potential near the nucleus has a singularity, and the distance from the nucleus is close to zero in hyperbole. For a single atom inside the Wigner-Seitz sphere the main contribution comes from the nucleus of an atom [6], [7].

Consider the cell potential obtained at the line potential. In this case, clearly seen the potential frequency, which is created by all the atoms are now set. In passing through the core potential becomes singular. The potential between the atoms is identical and negligible in the magnitude. There is a little effect of the atoms located at the centers of the faces of the two face-centered cubic lattices [8].

The obtained simulation results show the crystal potential, the crystal can be modeled with all its features. In contrast to known methods of calculating of the crystal potential as described in the engineering calculations of the crystal potential is universal. It gives the results without making any correction factors, does not require the use of logarithmic scales, and other non-uniform, allows you to quickly calculate the crystalline potential for all elements of the given crystal structure. There are facilities for the further developments of such technology in the direction of accounting for various disturbances. It will allow a calculating the electronic potential even more precisely. However, even without taking into account the properties of an ideal crystal, this calculation provides sufficiently accurate results. To illustrate the power and versatility of the described technique for the calculating of the potential capabilities it is shown an interaction potential on line drawn along the main diagonals of the two face-centered cubic lattices in Fig. 7.
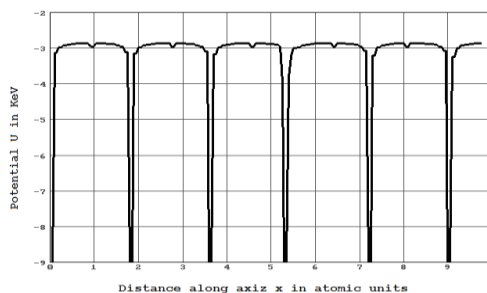

Fig. 7.An interaction potential on line drawn along the main diagonals of the two face-centered cubic lattice.

In determining the energy spectra of quantum-mechanical problems for periodic structures, it often uses methods of the broadcast. In particular, semiconductors have a periodic structure. The crystal potential, having the grating period, usually modeled by the expression [1], [9]:

$$V(\vec{r}) = \left[\sum_{i=0}^{N} V_n(\vec{r}_i)\right] + U_0(\vec{r}) + V_{exh}(\vec{r}). \qquad (11)$$

where V_n (r_i) — the potential created by the i-th nucleus at the point $\mathbf{r}$; U_0 (r) — the electronic potential, formed by the electrons of the core at some point $\mathbf{r}$ and is determined from the Poisson equation

$$\nabla^2 U_0(\vec{r}) = -8\pi\rho_0(\vec{r}). \qquad (12)$$

Here $\rho_0(\mathbf{r})$ — the electronic density of the occupied levels at a distance r from the center of the atom; $V_{exh}(\mathbf{r})$ —the exchange potential at point $\mathbf{r}$; $\mathbf{r}_i = |\mathbf{r}\text{-}\mathbf{a}_i|$ — the distance from the i-th node to the point $\mathbf{r}$; $\mathbf{a}_i$ — the node location; N — the number of neighbors taken into account relatively to the cores. The solution of Schrödinger equation based on the potential (11) is carried out by the Hartree-Fock-Slater [10].

The specificity of a solid compared to other bodies, is the decisive role of spatial-structural properties: a lattice type, a location and an interaction of the defects, a structure of core lattices and inter-ionic space. The period of the inter-ionic lattice coincides with the period of the core lattice. Spatially periodic structure of two weakly coupled and oppositely charged objects is the cause of the stability of rigid body — in this case the semiconductor GaAs — because between these objects appear spatially periodic Coulomb forces. In the geometric structure of each inter-ionic space surrounded on six sides by positive ion cores, and the ionic core in turn — intervals.

For a uniform distribution of electrons in the space of interaction between them becomes energetically unfavorable. There is the possibility of an orderly arrangement of electrons in space, the emergence of the so-called Wigner or "electron crystal".

The geometrical structure of the crystal consists not only of the atomic cores, but inter-ionic space intervals. The valence electrons in inter-ionic space intervals are also elements of the crystal, along with the atomic cores. The inter-ionic space is gap, i.e. the most probable location of the valence electrons. In addition, inter-ionic space intervals are also still a kind of "elements" of the crystal. But then the conclusion is that in the crystal lattice there are two — the well-known lattice consisting of the atomic cores, and another, equally important for the existence of the crystal lattice of the valence electrons are concentrated between the cores. The lattice periodicity of the atomic cores immediately implies the lattice periodicity of the inter-ionic space.

Even more natural in such a conclusion, if you do not forget that the atomic cores of the crystal lattice — not a point in space, but the figures, which occupy a significant part of the whole space of the crystal, and inter-ionic space also has a periodic structure, as well as skeletons. The period of this lattice coincides with the usual of the core of the lattice. Fig. 8 shows a two-dimensional lattice with the lattice constant a_0. The coordinate origin of the system *Oxy* is at the center of one of the cores, and the origin of the coordinate system *O'x'y'* is located in the center of one of the inter-ionic cells. The

coordinate system $O'x'y'$ is formed by the translation of the coordinate system Oxy in $a_0n/2$, where $n = \{0, 1, 2, ...\}$. We assume inter-ionic intervals are the inter-ionic elements of the lattice, which is shifted with respect to a core of the lattice by half a lattice constant in all coordinate axes.
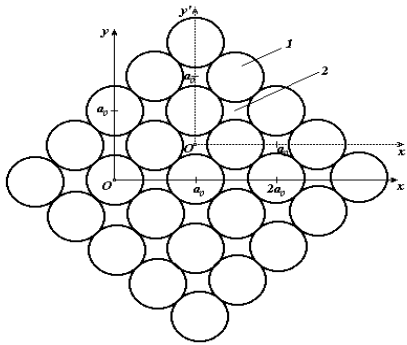

Fig. 8.A two-dimensional lattice with the lattice constant a0.

Cores and inter-ionic space two-dimensional lattice include 1) frame, 2) inter-ionic space.

The determining the location of the centers of the inter-ionic intervals can be easily receive from the definition of the basis vector for the nodes of the crystal (the core) of the lattice with any structure. But it should be noted that by increasing the radius of inter-ionic volumes (not just their centers) there is a change the number under the consideration inter-ionic space compared to the amount covered by the cores. Since you want to cover all inter-ionic space surrounding covered the skeletons, the radius of coverage inter-ionic space few more skeletons examined.

Crystal is in a stable condition thanks to the orderly arrangement of opposite charges. Most of the properties of crystals (eg, electrical conductivity, magnetic susceptibility), are caused not only property of the host lattice, but also the existence of inter-ionic lattice.

This inter-ion lattice in addition to the core determines the physical properties of the crystal.

Specificity of a solid compared to other bodies is that in them play crucial role spatial structural properties: the lattice type, location and interaction of defects, the structure of the nucleus and inter-ion lattice. The period of the inter-ion lattice coincides with the period of the core lattice. Spatially periodic structure of two weakly coupled and oppositely charged objects is the cause of the stability of rigid body — in this case the GaAs — because between these objects appear spatially periodic Coulomb forces. In the geometric structure of each inter-ionic cell surrounded on six sides by positive ion cores, and the ionic core in turn — the inter-ionic gaps.

Computer simulation of the properties of the crystal lattice gives to use up to $10^{10} \div 10^{12}$ atoms. Using the described technique can be obtained from any of these atomic systems, as well as changes in the radii of coordination spheres at various distances. Simultaneously, you can get a number of nearby neighbors, the location of atoms on the coordination sphere.

Thus, algorithms are developed for the FCC, BCC and diamond-like structures for determining the orderly and semiregular Archimedean and Platonic figures, as well as their complexes.

V. CONCLUSION

We can develop an algorithm for constructing the structure of compound semiconductor-type A^3B^5, based on this principle. For example, to the type of A3B5 of semiconductor compounds it is used compound GaAs. It is crystal lattice of two face-centered cubic lattices shifted relative to each other at j spatial diagonal. Each Ga atom has four nearest neighbors located at the tops of a tetrahedron. Each ion is surrounded by four nearest neighboring ions of opposite sign. There are four ions with $q_i q_j = -1$ at a distance $a_0 2^{1/2}/2$, eight ions of opposite sign of $q_i q_j = +1$ at the 2 distance $a_0 2^{1/2}$. The system of links of the GaAs structure establishes the order of the atomic body along tetrahedral combinations [2], [3]. For such compounds of the tetrahedral group of atoms is one-eighth of the basic lattice, so it is convenient to consider as a superstructure. The cell of the GaAs lattice consists of four tetrahedral sublattices.

One of the advantages of the described technique is its application to systems with short-range order, which does not use Bloch's theorem as the initial conditions. This was possible due to the fact that translational invariance follows as a consequence of the calculations, and not postulated initially. Thus, translational invariance in real space and in the quasi-momentum space is not a prerequisite for the determination of the crystal potential, wave functions and energies in wave vector space.

This, in turn, allows you to define these parameters not only for infinite crystals, but also for the real limits on the size of the crystals. Therefore, it is possible to determine the properties of crystals with impaired structure of a single scheme, with no additional idealizations. Individual interest is a violation of the periodicity on the boundary of the crystal. In fact, it is inherent in all real crystals violation of the ideal (i.e. infinite) crystal structure.

The violation of a perfect crystal at the border no doubt affects the theoretical study of the band spectrum. Boundary effects appear in the form of decay phase portraits of the main parameters (the crystal potential, the wave functions and energies in wave vector space) in all directions of the crystal boundaries (in our case spherical).

In the study of solid-state we considered two sites within the crystal, virtually connected to each other. A theoretical study of solid-state is easily accomplished with the use of these facilities both qualitative and quantitative methods. But the most effective way of investigating solids is to use a direct computer simulation, and that we have done for simple structures.

Thus, the use of techniques discussed in the article allows the calculation of real properties of GaAs crystals with defects and other constraints.

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