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МОДЕЛИРОВАНИЕ ФИЗИЧЕСКИХ ПРОЦЕССОВ И МЕХАНИЧЕСКИХ СИСТЕМ
MODELING OF PHYSICAL PROCESSES AND MECHANICAL SYSTEMS

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THE MODELING OF CRYSTAL WAVE FUNCTIONS THROUGH POTENTIALS

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Abstract

The aim of this work is to develop exact methods for crystal potentials and wave functions, which would allow to calculate the energy spectra of the electron states in various solids without fitting and use of corrective factors. The article considers the number of structural units of clusters and their physical properties of the GaAs structure. The resulting cluster is investigated and studied based on computer simulation as. We introduced an additional concept of interspherical space, shows certain characteristics that are present in the real space of the crystal lattice in the formation of the structure. Values describing the interspherical space are directly involved in describing the properties of direct and reciprocal space. The values of the variables describe the quasi-bound states of the structural units of the direct and reciprocal spaces. Quasi-bound states determine quantities that are parameters of the characteristics of the corresponding spaces. Computer modeling determines the spatial coordinates relative to the selected number of structural elements of the cluster in direct space. Solving the Poisson equation in reciprocal space, we obtain the electron density and the allowed values of the energy levels. An approach is discussed using the proposed concept of the intersphere space to the structure of GaAs clusters and the results of a computer-analytical study based on this concept, satisfying the solution of the equation of the intersphere oscillator.

Keywords: GaAs, cluster, nanocluster, cores, intercore space, interspherical space, interspherical oscillator, equations of state, electron density, energy levels.

Аңдатпа

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КРИСТАЛДЫҢ ТОЛҚЫНДЫҚ ФУНКЦИЯЛАРЫН ПОЦЕНЦИАЛДАР АРҚЫЛЫ МОДЕЛЬДЕУ

Бұл жұмыстың мақсаты әртүрлі қатты денелердегі электрон күйлерінің энергетикалық спектрлерін түзету факторларын қолданбай және қолданбай есептеуге мүмкіндік беретін кристалдық потенциалдар мен толқындық функциялардың нақты әдістерін жасау болып табылады. Мақалада кластерлердің құрылымдық бірліктерінің саны және олардың GaAs құрылымының физикалық қасиеттері қарастырылады. Алынған кластер компьютерлік модельдеу негізінде зерттеледі және зерттеледі. Біз сфералық кеңістіктің қосымша түсінігін енгіздік, құрылымның қалыптасуында кристалдық тордың нақты кеңістігінде болатын белгілі бір сипаттамаларды көрсетеді. Сфералық кеңістікті сипаттайтын мәндер тікелей және өзара кеңістіктің қасиеттерін сипаттауға тікелей қатысады. Айнымалылардың мәндері тікелей және өзара кеңістіктердің құрылымдық бірліктерінің квази-байланысты күйлерін сипаттайды. Квазишектелген күйлер сәйкес өлшемдердің пропорцияларын анықтайды. Компьютерлік модельдеу тікелей кеңістіктегі кластердің құрылымдық элементтерінің таңдалған санына қатысты кеңістіктік координаттарды анықтайды. Пуассон теңдеуін өзара кеңістікте шеше отырып, біз электронның тығыздығын және энергия деңгейлерінің рұқсат етілген мәндерін аламыз. GaAs кластерлерінің құрылымына ұсынылған сфералық кеңістік тұжырымдамасын қолдану тәсілі және осы тұжырымдамаға негізделген компьютерлік-аналитикалық зерттеу нәтижелері, интерсфералық осциллятор теңдеуінің шешімін қанағаттандыратын әдіс талқыланады.

Түйін сөздер: GaAs, кластер, нанокластер, ядролар, ядроаралық кеңістік, сфера аралық кеңістік, сфералық осциллятор, күй теңдеулері, электрон тығыздығы, энергия деңгейлері.

Аннотация
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МОДЕЛИРОВАНИЕ ВОЛНОВЫХ ФУНКЦИЙ КРИСТАЛЛА ЧЕРЕЗ ПОТЕНЦИАЛЫ

Целью работы является разработка точных методов для кристаллических потенциалов и волновых функций, которые позволили бы рассчитывать энергетические спектры электронных состояний в различных твердых телах без подгонки и использования поправочных коэффициентов. В статье рассмотрено количество структурных единиц кластеров и их физические свойства структуры GaAs. Полученный кластер исследуется и изучается на основе компьютерного моделирования. Введено дополнительное понятие межферного пространства, показывающее определенные характеристики, присутствующие в реальном пространстве кристаллической решетки при формировании структуры. Величины, описывающие межферное пространство, принимают непосредственное участие в описании свойств прямого и обратного пространства. Значения переменных описывают квазисвязанные состояния структурных единиц прямого и обратного пространства. Квазиограниченные состояния определяют пропорции соответствующих размерностей. Компьютерное моделирование определяет пространственные координаты относительно выбранного количества структурных элементов кластера в прямом пространстве. Решая уравнение Пуассона в обратном пространстве, получаем плотность электронов и разрешенные значения энергетических уровней. Обсуждается подход с использованием предложенной концепции межферного пространства к структуре кластеров GaAs и результаты основанного на этой концепции компьютерно-аналитического исследования, удовлетворяющего решению уравнения межферного осциллятора.

Ключевые слова: GaAs, кластер, нанокластер, ядра, межъядерное пространство, межферное пространство, межферный осциллятор, уравнения состояния, электронная плотность, энергетические уровни.

Introduction

We consider the crystal as a system of all its constituent elements, the properties of which are determined by the crystal system and there are no outside the crystal in a free state, used a nonlinear superposition of the interactions of these elements are not made outside the assumption of a crystal structure and its size. The known properties of the crystal experiments, for example, the frequency of the elements in the arrangement should be obtained as a consequence of the approach, not postulated in advance.

Methods investigated by computer simulation technology energy bands for metal crystals with structure of face-centered cubic. We used the developed in the works a theoretical approach and experimental data from literature sources [1-3].

We have explored the properties of quantum-well heteronanostructures (QRS) based on A^3V^5 direct-gap semiconductors containing layers of quantum wells (QWs) and quantum dots (QDs) is a determination of their structure and properties of nanosized objects. For instrumental applications, it is necessary to create homogeneous defect-free RS with the necessary geometric values and structural units. to implement their creation, an important component of the study is the analysis of the composition, the functional perfection of the details of the active elements of devices and diagnostics of the optoelectronic properties of quantum-well heterolayers.

Therefore the proposed technique is still the only one well-established technique that is applicable for the band spectrum was analysing of finite imperfect crystals.

In the plane of the quantum well, the motion of electrons remains unbounded. Therefore, electrons in a quantum well are referred to as a two-dimensional electron gas. The energy spectrum of the x- and y-energy components of a 2D gas is quasi-continuous, as in a three-dimensional material [4]. Low concentration electrons and conduction holes are attracted to point defects in semiconductors with deep levels. The concentration of electrons and conduction holes is several orders of magnitude less than the concentration of atoms of the main conductivity of the semiconductor. This proportion of charge carriers in semiconductor materials can have unknown significant effects in the use and manufacture of electronic and optoelectronic devices. Computer modeling of the structures of gallium arsenide shows within the radius of coverage there are discontinuities in the uniform arrangement of structural units. In various technological operations, such dislocations from uniformity affect the electronic properties of quantum-dimensional heteronanostructures. Therefore, it is important to study and develop the theory to improve technology. This, in turn, will lead to improvements in the parameters of devices based on quantum-sized heteronanostructures.

The results of computer simulation of the structure of the A_3B_5 gallium arsenide semiconductor, showing a peculiar defect in the form of a discontinuity located in the atomic crystal lattice with detection of coverage commensurate with the size of several interatomic distances. The crystal lattice of a gallium arsenide semiconductor combines two sublattices of three and five valence atoms, each of which generates its own

defect formation. A small perturbing factor substitutes the action of an atom of the gallium sublattice into the site of the arsenide sublattice. Leading to a violation of the structure of this compound. [5], [6].

To establish the relationship between the forward lattice, as well as to construct an inverse lattice and determine the properties of the Fermi surface and the number of incoming elements, you can use the differentiation rules. When calculating the required accuracy, the radius of coverage can take an arbitrary number of elements. High speed computations make it possible to perform dynamic computer simulation of the properties of real GaAs crystals [2], [7].

The characteristic of the GaAs cell shows that electrons in the conduction band occupy places in the vicinity of the minimum with energies spaced from the minimum by magnitudes much smaller than the width of the band, the magnitude of which is about 1 eV. Similarly, the places of the valence band that are not filled with electrons are located in the vicinity of its ceiling atoms of one substance into another with a constant flow of these atoms in time and a constant gradient of their concentrations.

The crystal potential and calculation the wave functions

Let's consider how the electronic spectrum of the A^3B^5 compounds is arranged near the point of a simple on the number and spatial orientation. Since the energy is a quadratic form of momentum, using the transformation of the coordinate system, depending on the number of nuclei in the cluster and their spatial location, it is possible to diagonalize of the energy changes periodically with different amplitudes. The arrangement of groups of atomic nuclei in different directions of space subjects to certain laws of a series. In various directions of the arrangement of the atomic cores appear parallel intersecting spaces. The real images of these spaces are antisymmetric to the spaces of atomic core. If the law of a number of numerical arrangements of the atomic cores is characterized by integer coordinates, the components of the atomic arrangement of the planes are described by fractional coordinates.

When determining the energy spectra of quantum mechanical problems for periodic structures, translation methods are often used. Using these simple considerations, we can write the following general expressions for a cubic crystal in the case when semiconductors have a periodic structure. The law of electron dispersion in the vicinity of the bottom of the conduction band can be written by the expression:

$$V(\vec{r}) = \left[\sum_{i=0}^N V_n(\vec{r}_i) \right] + U_0(\vec{r}) + V_{\text{exh}}(\vec{r}). \quad (1)$$

where $V_n(r_i)$ – i -th kernel generates a potential at the point r ; the solution of the Poisson equation determines the potential of electrons $U_0(r)$ created at a certain point r by electrons of low levels of atomic orbitals

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

The value $\rho_0(r)$ – denotes the radius-dependent vector r , originating from the atomic center, the electron density of the underlying atomic orbitals; $V_{\text{exh}}(r)$ – the exchange potential radius-dependent vector r is $V_{\text{exh}}(r)$; $r_i = |r - a_i|$ – the distance from the i -th node to the point r ; a_i – the node location; N – relative to the coverage radius, the constituting cluster is selected the number of atomic cores. The method of Hartree-Fock-Slater is used to solve the Schrödinger equation with the potential determined by the composition of the cluster (1).

The following equation is the computed density of a given state:

$$\rho_0(r) = \sum_{n,l} r^2 R_{nl}^2(r). \quad (3)$$

The radial part of the wave function of an electron for a hydrogen atom [1], [4], [5] has the form of a function – $R_{nl}(r)$. For electron densities, we apply the superposition principle, integral equation 3 is characterized by additivity, then its solution looks like this:

$$U_0(r) = \sum_{i=0}^l u(r_i), \quad (4)$$

$$u(r_i) = \sum_{n,l} u_{nl}(r_i), \quad (5)$$

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

$$\vec{r}_i = \vec{r} - \vec{a}_i. \quad (6)$$

the distance from the origin center to the i -th atom is described by the radius vector a_i . The equation of Poisson for the electron of the i -th atom is obtained as follows:

$$\nabla^2 u_{nl}(\vec{r}_i) = -8\pi r_i^2 R_{nl}^2(\vec{r}_i). \quad (7)$$

We have obtained a solution to equation (8), in the following form

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

We find the potential $U_0(r)$ directly using the functions (Eq.4, Eq.5, Eq.6, Eq.7, Eq.8). An efficient and accurately calculated electronic potential is the result of this approach.

In gallium arsenide, the bottom of the conduction band is located at the G-point. The effective mass of an electron in the conduction band is $0.067m_0$. The valence band in GaAs is arranged similar to that in Germany. The band gap at 300 K is 1.424 eV. Gallium arsenide is a straight-band semiconductor. It will be shown later that this fact is the reason for the widespread use of GaAs in light-emitting devices. The value of spin-orbital splitting is 0.3 eV. Absence of an inversion center it leads to a small splitting of energy in the vicinity of the bottom of the conduction band and to its displacement from the G-point in the direction [111].

The state becomes energetically unfavorable with a uniform distribution of electrons in space, the interaction between them. The appearance of the so-called Wigner or "electronic crystal" is possible with an ordered organization of electrons in space [5], [8].

If in GaAs one of the atoms of the sublattices is replaced by an atom with a higher valence, an atom with a valence of 5 will take the place of the "native" atom. It is obvious that in the valence band, which is all filled, there is no places, and therefore the states with the lowest energy are in the conduction band. Once in the conduction band, an additional valence electron spreads throughout the crystal. The impurity atom thus becomes a positively charged ion, since the valence electrons "compensate" only a charge equal to the number of valence electrons of the "native" atom. Thus, there is an electric field of attraction of an electron trapped in the conduction band to an impurity atom. The crystal is in a stable state due to the ordered arrangement of opposite charges.

Results of Computational Crystalline Potential Modeling of the diamond structure of GaAs are shown gaps of the potential at the distance 1.4 a.u. where the atom of main diagonal is located. In figure 1 is shown the GaAs potential along Ox axis through three Ga atoms. In figure 2 is shown the GaAs potential along the main diagonal of the crystal lattice.

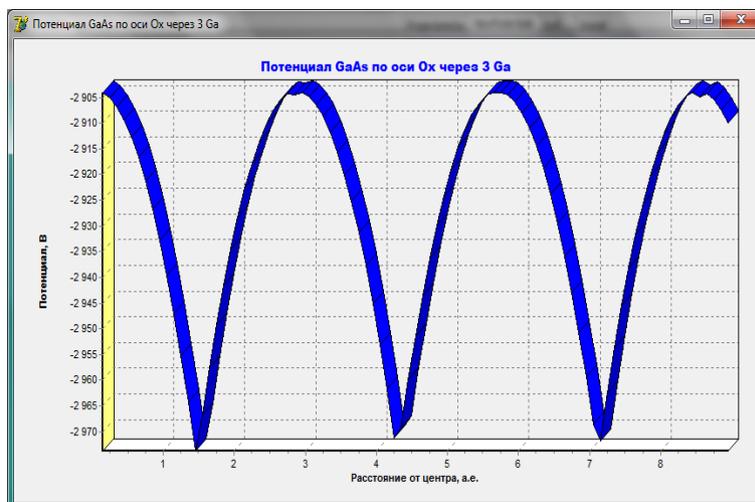


Figure 1. The GaAs potential along Ox axis through three Ga atoms

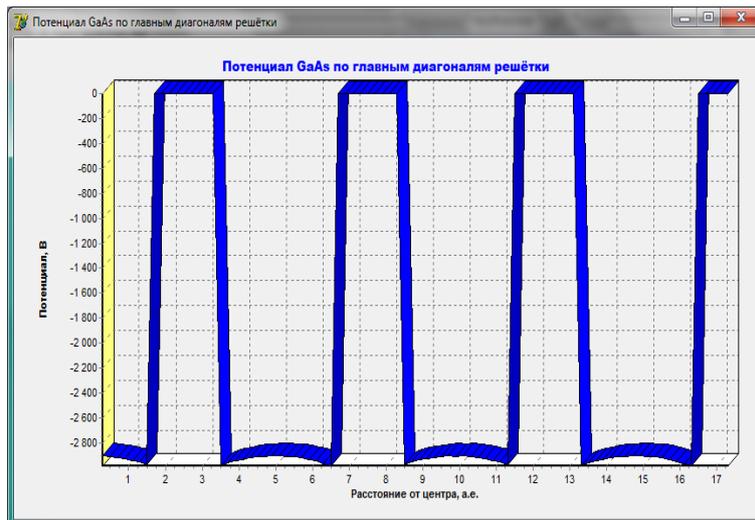


Figure 2. The GaAs potential along the main diagonal of the crystal lattice

Our results of modeling the crystal potential show that a crystal can be modeled taking into account all its features. It is clear from the definition that the potential of the central cell is markedly different from zero only near the impurity atom at distances of the order of the lattice constant. If the size of the electron orbit is much larger than the lattice constant, then the contribution from the potential of the central cell can be considered as a perturbation. The correction to the energy of the impurity state due to the potential of the central cell is commonly called a chemical shift, since this correction depends on the chemical nature of this impurity center, whereas the Coulomb interaction and the impurity spectrum caused by it depend only on the magnitude of the impurity charge.

Regardless of whether the field exists in the space surrounded by the shell or not in the empty space surrounded by the shell, the electric field is zero. For GaAs, the radius of the ground state of the donor is approximately 100 Å. The ionization energy of the donor in GaAs is about 5.8 MeV and is almost the same for germanium and silicon atoms taking the place of gallium atoms. Impurities whose localized states are located near the edges of the zones are called fine. If the impurity levels are located deep in the zone, then such impurities are called deep. To describe the state of deep impurities, it is necessary to take into account both the contribution to the wave function of several energy zones and the potential of the central cell. In these cases, the transition of an electron through electron shells occurs due to quantum mechanical effects.

The modeling of the structure GaAs

During the formation of a gallium arsenide crystal, the electronic configuration of the 4s4p states changes. Therefore, it is possible to extend the integration to infinite limits, and for the dependence of the electron energy on momentum, use this dependence near the bottom of the conduction zone. Electrons in the conduction band and holes in the valence band can be considered as an ideal Fermi gas. This is an approximation, since the electrons in the conduction band interact with each other as well as with charged impurities. However, in semiconductors at not very low temperatures, the kinetic energy of the electrons is greater than the Coulomb energy, so the electrons can be considered as free. [2], [9]. Then, to determine the band spectrum, you can use the wave function obtained with respect to these potentials. In figure 3 is shown the wave function of a crystal of copper for the $n = 4$.

It can be seen from this figure that the fluctuations of the wave functions coincide with breaks of potentials in simple structures such as Cu, and in complex structures as GaAs.

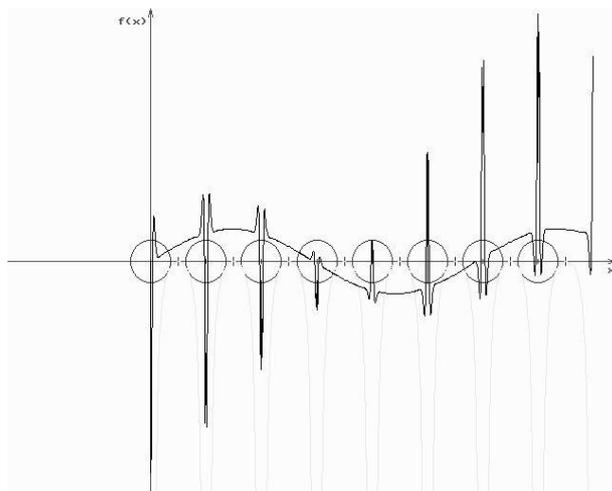


Figure 3. The wave function of a crystal of copper for the $n = 4$

Conclusion

When considering the movement of electrons in a crystal in weak fields, it was shown that in a constant weak electric field, the movement of electrons is finite. Therefore, this consideration cannot explain the flow of current in conductive crystals. The reason for this is that we considered the motion of an electron in an ideal crystal. In this approximation, we were able to establish the law of electron dispersion and develop methods to describe it. However, we have neglected the imperfection of the crystal (or lattice defects), which is essential for the description of the crystal. This "imperfection" of the crystal can be described within the framework of perturbation theory, since the potential that it creates is small compared to the self-consistent Hartree-Fock potential [8], [10]. The atoms inside the unit cell oscillate synchronously in acoustic vibrations. For optical oscillations, the displacement vector refers to the change in the distance between the atoms inside the unit cell, since in this type of oscillation, the center of mass of the unit cell remains stationary. It is obvious that with any translation of the crystal as a whole, the energy of the electron does not change. But when the phonon wave vector tends to zero, acoustic vibrations describe the vibrations of the crystal as a whole.

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