About the energy levels of GaAs

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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.

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 A^3B^5 of semiconductor compounds it is used compound GaAs.

The case of uniform distribution of electrons in the space of interaction between them becomes energetically unfavorable. There is a possibility of an orderly configurations of the electrons in space. One more subtlety of crystal structure in calculating properties of the crystal related to the fact that the radii of the spheres accrue uniformly covering to a certain radius (for example, GaAs structure up to 498), then this is a violation of uniformity. Next violation of uniformity arises after a group of 918 atoms. Figures 1 and 2 are a group of atoms and their arrangement.

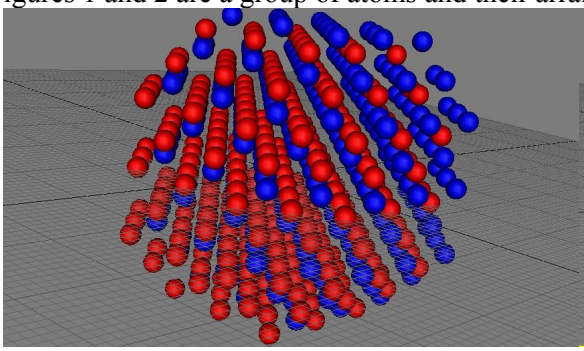

Fig. 1. The grid with a radius of coverage 5. where there are 498 atomic cores.

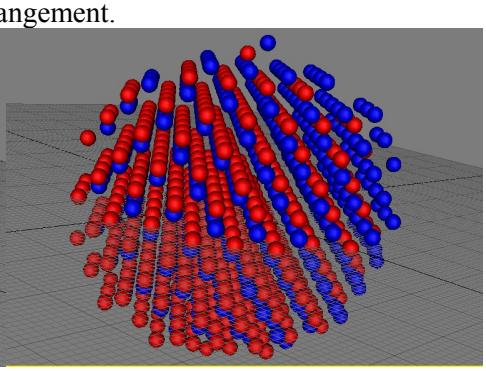

Fig. 2. The As atoms and Ga for the radius of coverage 6. Red marked atoms As, in blue denote atoms Ga. Central atom is As.

But in fact, such a violation of uniformity means that it is impossible to carry out "and self-evident and obvious" extrapolation of the results and methods of calculation for the "normal covered by the scope" on large radii, which is doing traditionally.

Links between the structural units play a dominant role. Coulomb attraction between electrons and nuclei combined into a solid unit. But again arise the question of the relationship of the spatial arrangement of the free electron gas with atomic nuclei in the crystal lattice. Contact in turn, arise from the nature of the electron distribution in space. In the existing models are impermeable ions crystal spherical. According to to the Pauli principle [1] and the theory of closed shells follows that atom is characterized by a stable electronic configuration. When crystal formation by being socialization electron leaving atomic orbital forms a defect in an electronic configuration resulting in an increase width of the unfilled valence [2-4]. In the crystal, when approaching to each other ions because of their impenetrability is broken quantum-mechanical effects. The main contribution to the total energy contributes strongly repulsive inter-ion Coulomb interaction. Much of the energy amounts electron-electron interaction in the calculation, which by existing methods there are big difficulties. The motion of the ions is inextricably linked with the movement of valence electrons [4, 5]. The total energy of the crystal depends on the location not only of ions and the electrons.

Therefore, in the calculation of the energy spectrum, it is necessary to consider the interaction of the electron and the probe with the cores and intercores. Oscillations are tightened to the centers of the cores and increase their amplitude with increasing levels of energy. This is explained the combined effects of strong impact of all cores and intercores on the test electron in the higher energy states. In the even states (2nd and 4th) are clearly visible the envelopes of the plane wave. In these states, the geometry of the crystal increases the total contribution of all the cores and the intercores in the amplitude of the envelope wave (the core and intercore lattice acts as a amplitude resonator). The energy

levels obtained in the space of wave vectors are periodic functions:

$$E_j(k_x+g) = E_j(k_x),$$

where g is a reciprocal lattice vector. The periodic dependence of the energy $E_j(x, k_x)$ from the one-dimensional wave vector k_x with a period $2k_x/a_0$ (where a_0 is the lattice period) throughout the entire crystal is obtained without regard the periodicity conditions.

Figures 3 and 4 shows the plots of the energy $E_j(x, k_x)$ of the coordinates of x and the wave vector k_x for a group of 498 atoms with an energy of 3.12 eV and 913 –2.93 eV.

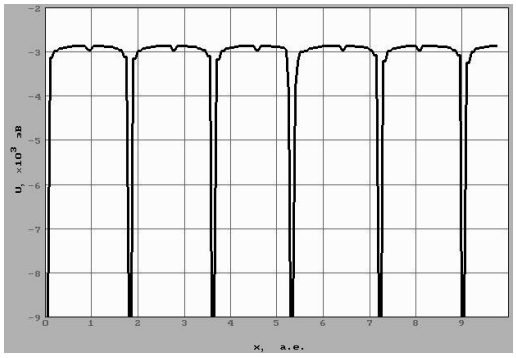

Fig. 3. The grid with a radius of coverage 5, where there are 498 atomic cores with an energy of 3.12 eV.

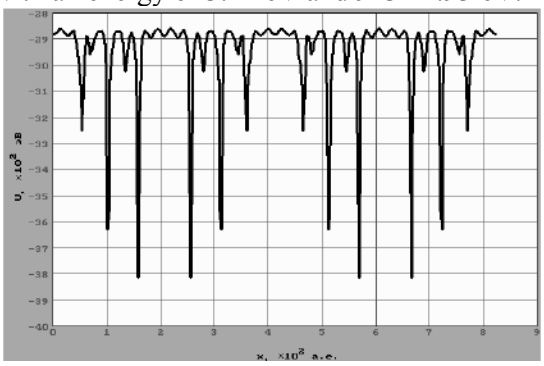

Fig. 4. The As atoms and Ga for the radius of coverage 6, where there are 913 atomic cores with an energy of 2.93 eV.

References

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