
METALS
AND SUPERCONDUCTORS

Structure Stability and Electronic Properties of the Zr–He System: First-Principles Calculations

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Abstract—Ab initio studies are carried out for the atomic and electronic structures of the Zr–He system. It is revealed that zirconium undergoes a phase transition induced by helium. The most preferred position of the impurity in the metal lattice is determined. The energy of dissolution of helium and the excess volume introduced by helium are calculated. It is shown that the presence of helium in the Zr lattice significantly perturbs the valence charge density of the metal and substantially changes its electronic structure.

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1. INTRODUCTION

The behavior of inert gases in metals has been extensively studied over several last decades [1, 2]. Helium has been taking a special interest. Being formed as a result of (n, α) reactions, helium is accumulated in metals and is one of main factors determining the radiative swelling and high-temperature embrittlement of structural materials of nuclear reactors [3, 4]. At low temperatures, helium affects the processes of radiation hardening [5] and fatigue characteristics of a material manifesting itself as an obstacle to dislocation motion [6, 7]. All the factors influence negatively the operating properties of reactor materials.

The understanding of the macroscopic effect occurred because of helium accumulation is mainly hampered by the necessity to consider the problems at many levels beginning from the microscopic (the electronic configuration and the position of helium atoms in a metal crystal lattice and energy characteristics corresponding to them) through the study of diffusion mechanisms, kinetics of nucleation and growth of bubbles to the statement of correlation between evolution of the microstructure and a change in the macroscopic properties of a material [8].

The microscopic consideration of the problem was started in [9–12]. The heat of dissolution and activation energy of helium diffusion in Al, Mg, Ni, Cu, and Pd were calculated. It is shown that a correct description of the helium behavior in a metal lattice requires the inclusion of its quantum nature (zero-point vibrations). However, the noted studies have a semiempirical or model character (jellium model), and their

results were able only qualitatively to solve the problem. As was noted in [11], the difficulties of these methods are due to the fact that helium substantially perturbs the electrons of a host metal and also can distort its lattice. Thus, to obtain quantitatively correct results, the ab initio methods should be used.

The study of metal–helium systems by ab initio methods becomes possible only with the advent of modern power computers. By now, there are a number of reports dealing with calculations of various energy characteristics of helium in various metals [13–18], such as Al, Ni, Fe, Pd, Cu, La, and various alloys and solid solutions based on these metals. However, in the literature, there are no any data on the study of the influence of helium on the structure stability and electronic properties of zirconium which is a metal of high importance for nuclear power engineering. Actually, zirconium is used in fabrication of fuel elements, heat exchangers, and other units of nuclear reactors. As known, during operating water-cooled thermal-neutron reactors, helium atoms with a kinetic energy of ~ 1.8 MeV are created as a result of transmutation; such helium atoms are able to penetrate into materials of intravessel units to a depth of 40 μm [19]. Accumulating, helium atoms create in near-surface region of the metal a solid solution with a high impurity concentration. It can be the reason of concentration polymorphism of zirconium like to that taking place during the dissolution of hydrogen in zirconium [20]. Thus, the problem of stability of zirconium crystal structure in the presence of helium is very topical, since it influences the operation safety of nuclear reactors. To most effectively solve this problem, the extensive theoretical

first-principles study of the physical properties of the Zr–He system is necessary.

The aim of this work is the ab initio study of the phase stability of the Zr–He system, calculation of the energy of dissolution of helium in the Zr lattice, and also the study of influence of helium on the electronic structure and distribution of the valence charge density of zirconium.

2. METHOD AND DETAILS OF THE CALCULATION

The self-consistent calculations of the total energy and electronic structure of pure Zr and Zr–He system were performed in terms of the density functional theory using the generalized gradient approximation [21] by the linearized augmented plane wave method [22, 23] implemented in the FLEUR program package [24]. The radii of the muffin-tin spheres of Zr and He atoms were chosen equal to 2.3 and 1.0 au, respectively, which permits to helium atoms to be accommodated in the tetrahedral and octahedral interstitial sites of the hexagonal close-packed (hcp), body-centered cubic (bcc), and face-centered cubic (fcc) lattices of zirconium and also in various interstitial sites of its ω phase. In the expansion of the wave function inside the muffin-tin spheres in spherical harmonics, the terms up to $l = 8$ for Zr and $l = 6$ for He were only taken into account. To reach a required accuracy when calculating the total energy, the cut-off parameter of the plane-wave basis k_{\max} was chosen equal to 4.0 au^{-1} , which corresponds to more than 160 basis functions (augmented plane waves) per atom. During each iteration of the self-consistence, the Hamiltonian eigenvalues were calculated in 140 k points of the irreducible part of the Brillouin zone for the face-centered cubic and hexagonal close-packed structures, in 126 k points for the body-centered cubic structure and in 205 k points for the ω phase. The self-consistence procedure of the electron density was carried out to achieving the convergence of the total energy not worse than 0.02 meV, which corresponds to the convergence of the charge density better than $0.0001 \text{ meV/Bohr}^3$. The density of states $N(E)$ was calculated by a linear tetrahedron method, and its smoothing were performed by Gaussians with the root-mean-square width 0.08 eV.

For convenience of comparison of the total energies, the calculated unit cells were chosen so that the unit cell of pure zirconium contained two zirconium atoms in the hexagonal close-packed, body-centered cubic, and face-centered cubic structures, and the unit cell of the Zr–He system contained two Zr and one He atoms. The total energy of the ω phase in the Zr–He system was compared to the corresponding quantity of the most energetically preferred (it will be shown in what follows) body-centered cubic phase calculated for the unit cell with hexagonal symmetry containing three Zr and one He atoms. The both structures

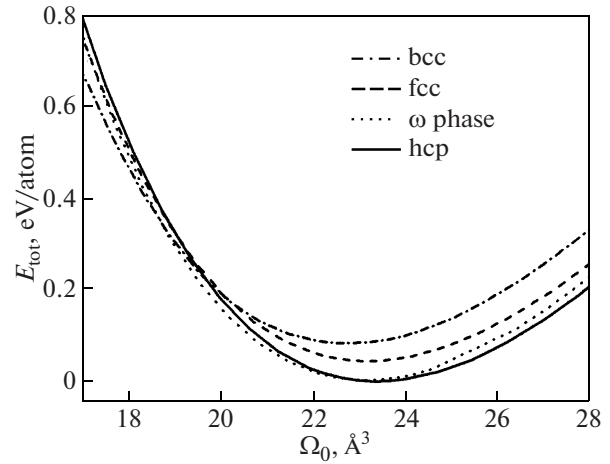


Fig. 1. Dependences of the total energy of pure Zr on the specific volume Ω_0 per atom. The total energy of the hexagonal close-packed structure is taken as the reference point.

(body-centered cubic and ω phases) can be described by the hexagonal lattice with three atoms per unit cell [25] whose positions are determined by coordinates (000), $(1/3, 2/3, 1/3 + z_\omega)$, and $(2/3, 1/3, 2/3 - z_\omega)$, where $z_\omega = 0$ for the body-centered cubic structure and $z_\omega = 1/6$ in ω phase.

For the cubic (face-centered cubic and body-centered cubic) structures, we calculated the dependence of the total energy of the crystal E_{tot} on its unit cell volume Ω . The total energy of the hexagonal (hexagonal close-packed and ω phases) structures was calculated as a function of Ω and the ratio of lattice parameters c/a .

3. RESULTS AND DISCUSSION

3.1. Atomic Structure

Figure 1 presents the calculated dependence of the total energy E_{tot} of the Zr crystal on the specific volume Ω_0 per atom. It is seen that, in the absence of external pressure, the Zr crystal has a hexagonal close-packed structure. Under pressure (decrease in Ω_0), the phase transition occurs from the hexagonal close-packed phase to ω phase which, in turn, transits to the body-centered cubic phase at more higher pressures. This sequence of the pressure-induced phase transitions agrees well with the results of the extensive experimental and theoretical studies [26–28]. The calculated values of the equilibrium volume Ω_0 for the hexagonal close-packed, face-centered cubic, body-centered cubic structures and ω phase are 23.27, 23.06, 22.82, and 23.11 \AA^3 , respectively, and agree well with the experimental [26, 29–31] and theoretical results of other studies [27, 32–34].

Figure 2 shows the calculated $E_{\text{tot}}(\Omega)$ dependence for the Zr–He system when the zirconium atoms form

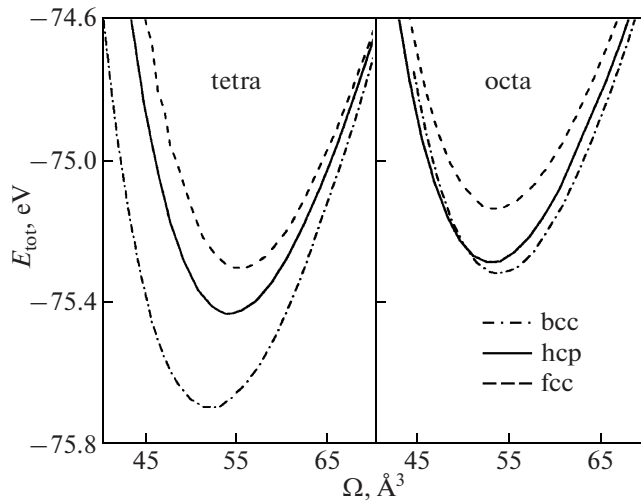


Fig. 2. Dependences of the total energy of the Zr–He system on the unit cell volume Ω of the hexagonal close-packed, face-centered cubic, and body-centered cubic lattices of Zr for the tetrahedral and octahedral coordinations of the helium atom. The reference point is the total energy of the hexagonal close-packed structure of pure Zr.

the hexagonal close-packed, body-centered cubic, and face-centered cubic lattices and helium atoms occupy the tetrahedral and octahedral interstitial sites. Here, Ω is the unit cell volume containing two Zr and one He atoms. As follows from Fig. 2, the body-centered cubic structure of Zr is the most energetically preferred at both the tetrahedral and octahedral arrangement of the helium atoms, and the tetrahedral interstitial site is more preferred than the octahedral that for all three the structures considered.

When an impurity is implanted to a crystal, it changes the crystal volume. This change is determined as the difference between the volume of the crystal containing an impurity and the pure-crystal volume and is called the excess volume. Table 1 lists the excess volumes which helium atoms contribute to the Zr lattices. It is seen that helium atom arranged in a tetrahedral interstitial site of the body-centered cubic lattice contributes a lower excess volume than helium atoms

Table 1. Excess volume introduced by the He atom into the Zr lattice

Lattice type	Excess volume, \AA^3	
	tetrahedral interstitial site	octahedral interstitial site
bcc	6.51	7.90
hcp	7.25	6.57
fcc	8.86	7.31

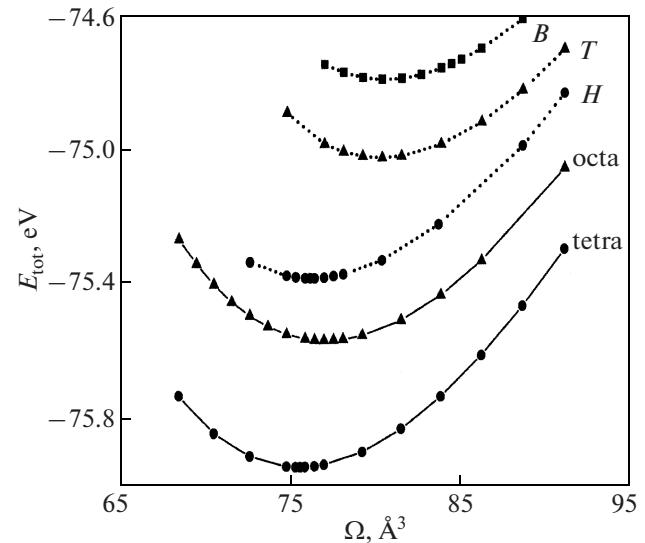


Fig. 3. Dependences $E_{\text{tot}}(\Omega)$ for the Zr–He system, where the zirconium atoms are in the body-centered cubic (solid lines) and ω phases (dotted lines). The letters *B*, *H*, and *T* correspond to the helium atom sites with the coordinates $(0, 0, 1/2)$, $(1/2, 1/2, 0)$, and $(1/2, 1/2, 1/4)$ in the lattice of the Zr ω phase, respectively. As in Fig. 2, the energy is given with respect to the minimum of the total energy of the hexagonal close-packed structure of Zr, which is normalized to the number of atoms in the unit cell.

occupying octahedral interstitial sites. The opposite situation is observed in the hexagonal close-packed and face-centered cubic lattices. It can be understood based on the fact that the coordination polyhedrons in the face-centered cubic and hexagonal close-packed structures are regular polygons; in this case, the tetrahedrons are half in volume as the octahedrons. It follows that, when the impurity atom is placed in the tetrahedral interstitial site, the Zr unit cell increases (the shape being unchanged) to a greater degree than in the case of the octahedral coordination.

The volumes of the octahedral interstitial sites in the body-centered cubic lattice are twice as large as those of the tetrahedral ones. However, the coordination polyhedrons in the body-centered cubic structure are not regular: the tetrahedron edges differ in length (one edge is a and five edges are $a\sqrt{3}/2$) and the octahedrons are strongly flattened in a direction, although their edges have the same length. These specific features of the coordination polyhedrons of the body-centered cubic lattice lead to the fact that larger non-metallic atoms can implant to the tetrahedral interstitial sites than atoms implanted to the octahedrons [35]. In our case, this circumstance is manifested in the fact that the helium atom located in the octahedral interstitial site increases the Zr unit cell volume to a greater degree than the helium atom located in the tetrahedral interstitial site.

Figure 3 shows the calculated $E_{\text{tot}}(\Omega)$ dependence for the Zr–He system, where the zirconium atoms are in the body-centered cubic and ω phases. In these systems, the He concentration in the Zr lattice is lower (for three Zr atoms there is one He atom) than in aforementioned case (for two Zr atoms there is one He atom). Comparing Figs. 2 and 3, one can see that, as the helium concentration in the body-centered cubic lattice of zirconium decreases, the tetrahedral position of the impurity remains energetically more preferred than the octahedral that. Moreover, it follows from Fig. 3 that the body-centered cubic structure of zirconium with the tetrahedral and even octahedral arrangement of helium is energetically more preferred than the ω phase of Zr with all possible interstitial sites of the impurity under consideration.

Table 2 lists the energies of dissolution of helium atoms in the Zr lattice calculated by the formula

$$\Delta E = E_{\text{tot}}(\text{Zr}_n\text{He}) - [nE_{\text{tot}}(\text{Zr}) + E_{\text{tot}}(\text{He})],$$

where $E_{\text{tot}}(\text{Zr}_n\text{He})$, $E_{\text{tot}}(\text{Zr})$, and $E_{\text{tot}}(\text{He})$ are the total energies of the Zr_nHe system, pure Zr, and an isolated helium atom. For the latter quantity, we obtain value -78.5044 eV from the self-consistent calculation of helium atom in vacuum at zero temperature. The calculated energies of dissolution are positive for all the cases considered. This circumstance shows that helium is not dissolved in zirconium at the normal conditions and it can penetrate into zirconium bulk only under specific conditions, e.g., as a result of implantation (irradiation with α particles) or nuclear reactions occurring in the material. As follows from Table 2, for all the considered structures, helium has the minimum energy of dissolution in the tetrahedral interstitial site, and its energy of dissolution in the both interstitial sites of the body-centered cubic lattice is lower than the corresponding values for other considered structures.

Unfortunately, we failed to find in the literature any data on the energy of dissolution of helium in Zr, because of this, we compared our results with the data for Al, Mg [9], and α -Fe [16]. The pseudopotential calculations [9] performed in terms of the theory of nonlinear screening give the following energies of dissolution of helium: in Al, $\Delta E_{\text{octa}} = 4.06$ eV and $\Delta E_{\text{tetra}} = 5.77$ eV; in Mg, $\Delta E_{\text{octa}} = 2.71$ eV and $\Delta E_{\text{tetra}} = 3.28$ eV. Hence, it was concluded in [9] that the octahedral interstitial site of the Al and Mg lattice is more preferred for the placement of helium than the tetrahedral interstitial site is. This conclusion is contradictory to our conclusion that helium exhibits the tetrahedral coordination in the face-centered cubic and hexagonal close-packed lattices of Zr. Likely, this circumstance can be due to the fact that Al and Mg are simple metals, while Zr is a transition metal. Really, Zr $4d$ electrons are stronger localized in space than the valence s – p electrons of Al and Mg are, because of this

Table 2. Energies of dissolution of helium in zirconium

Lattice type	Energy of dissolution, eV	
	tetrahedral interstitial site	octahedral interstitial site
bcc	2.63	3.02
hcp	3.08	3.19
fcc	3.09	3.28

they undergo a stronger repulsion from the strongly coupled core $1s$ electrons of implanted helium.

According to the more recent ab initio calculations [16], the energies of dissolution of helium in α -Fe are $\Delta E_{\text{octa}} = 4.58$ eV and $\Delta E_{\text{tetra}} = 4.40$ eV. This means that the tetrahedral interstitial site of the α -Fe lattice is more preferred than the octahedral that for the placement of helium. This conclusion agrees well with the results of our calculations for body-centered cubic lattice of zirconium. As for the energies of dissolution, they are larger by a factor of more than 1.5 than the corresponding values which we obtained for zirconium. It is most likely due to the fact that the number of the valence d electrons in iron is larger than that in zirconium by a factor of three.

3.2. Electronic Structure

3.2.1. Density of states. Since the body-centered cubic structure of Zr with the helium tetrahedral coordination is energetically most preferred, we consider, in what follows, only this structure. Figure 4 shows the calculated densities of electronic states of pure Zr and the Zr–He system. Our results for pure zirconium agree well with the data from [36, 37]. As seen from Fig. 4, the presence of helium in the zirconium lattice markedly changes its electronic structure.

(1) Below the conduction band bottom of Zr, a narrow (~ 0.7 eV) band of helium s states arises; it is separated from the valence states of zirconium by a gap of ~ 13 eV.

(2) The conduction band width of Zr decreases from 5.25 to 4.15 eV, i.e., by 1.1 eV.

(3) The peak in the density of states peak at the energy 0.28 eV vanishes.

(4) The high peak of $N(E)$ at 4.4 eV is shifted to the Fermi level by 1.3 eV and its height decreases by 2.5 states/eV.

Moreover, the Zr conduction band narrowing occurs owing to the fact that helium atom replaces the zirconium s – p states in the muffin-tin spheres and their tails in the interatomic region of the crystal from the energy range from -5.25 to -4.18 eV.

Helium atom has two electrons in the s state. At the chosen muffin-tin sphere radii, 62% of the electronic charge density of helium atom is in its muffin-tin

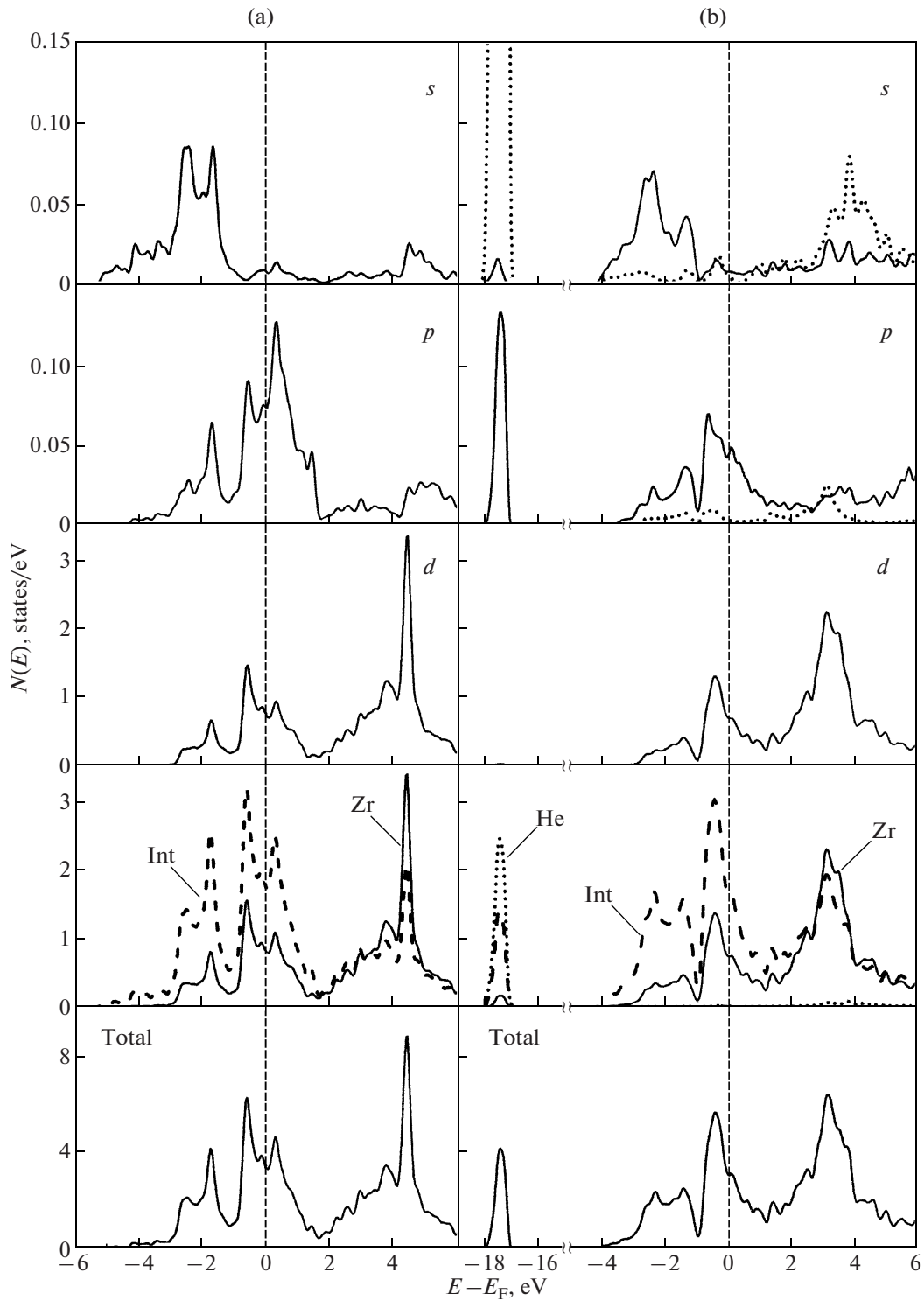


Fig. 4. Density of states $N(E)$ for the body-centered cubic structure of (a) pure Zr and (b) the Zr–He system with the tetrahedral coordination of the He atom. The bottom panel presents the total density of states (Total); the panel second from the bottom shows the local density of states in the interatomic region (Int) and in the muffin-tin spheres of zirconium and helium atoms; and the three upper panels show the partial densities of states of the s , p , and d types.

sphere, 34% fall on the crystal interatomic region, and 4% fall on the muffin-tin sphere of zirconium. The peak in the density of states peak of the p type in the

muffin-tin sphere of zirconium is exactly due to the penetration of the helium atom s state tails to the muffin-tin sphere of zirconium.

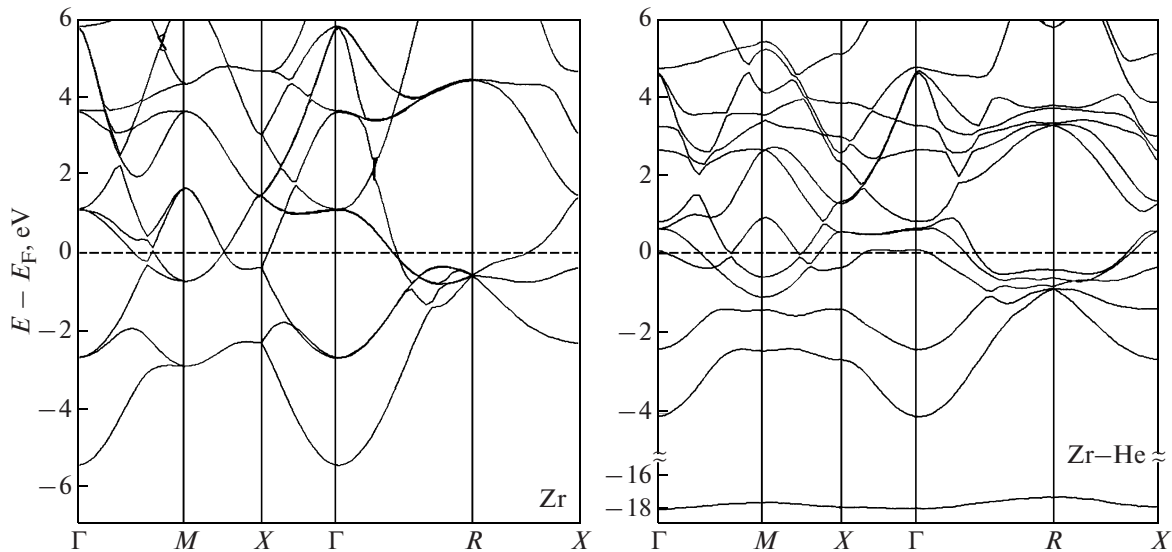


Fig. 5. Dispersion curves $E(k)$ for Zr and Zr-He in the body-centered cubic structure with helium in a tetrahedral interstitial site.

3.2.2. Dispersion curves. As was noted above, in the calculation of the electronic structure of the body-centered cubic phase of pure zirconium and the Zr-He system, we used the unit cell containing two Zr atoms. Thus, the $E(k)$ dispersion curves (Fig. 5) were calculated along the symmetric direction of the irreducible part of the simple cubic lattice.

It follows from Fig. 5 that the calculated results for pure Zr agree well with similar data available in the reference book [36]. It is seen from this figure that the presence of helium splits abundant electron states along all the symmetric directions of the Brillouin zone. The Fermi surface topology changes noticeably. The character of dispersion of many bands lying both above and below the Fermi level is modified. Some energy bands exhibit portions with very weak dependence on the wave vector. Near the Fermi level, there are parallel bands with different Fermi wave vectors. All above results change the spectrum of both single-particle and collective excitations of the electron subsystem of the crystal and influence its optical properties.

3.2.3. Valence charge density. Figure 6 shows the calculated spatial distributions of the valence charge density of pure Zr and the Zr-He system in the (001) plane containing both zirconium and helium atoms. Being implanted to the zirconium lattice, helium strongly changes the distribution of the valence charge density of zirconium. It is most clearly seen from Fig. 6c which presents the difference between the charge densities of the Zr-He system, on the one hand, and pure zirconium with a helium atom, on the other hand. The heavy curve shows the isoline corresponding to zero difference of the densities. The brighter areas correspond to the negative differences and the darker areas correspond to the positive differ-

ences. It is seen that helium replaces the electron charge density of Zr from the tetrahedral interstitial site and even from the muffin-tin sphere of zirconium. In a larger part of the interatomic region of the crystal, the charge density increases. Moreover, the charge density significantly increases in some regions of the muffin-tin sphere of zirconium. An analysis of the orbital distribution of the charge of the system under study shows that helium decreases the charge of the valence s and d electrons in the muffin-tin sphere of zirconium by $0.025e$ and $0.017e$, respectively, and increases the charge of the valence p electrons by $0.028e$. Here, e is the electron charge. As a whole, the muffin-tin sphere of zirconium loses the charge of $0.011e$.

Thus, helium implanted to zirconium causes very strong and a fairly complex redistribution of the valence charge density of both the interatomic region of zirconium and its muffin-tin sphere.

4. CONCLUSIONS

We have carried out the ab initio calculations of the electronic structures of pure Zr and the Zr-He system for the hexagonal close-packed, face-centered cubic, body-centered cubic structures and ω phase. The studies of the stability of the Zr-He system show that, at normal conditions, the hexagonal close-packed structure of pure Zr is energetically more preferred, and the presence of helium stabilizes the body-centered cubic lattice of zirconium. The tetrahedral position of helium in the zirconium lattice is the most preferred for all the structures studied.

The calculated energy of dissolution is positive for all the cases considered. This circumstance testifies that helium is not capable to be dissolved in zirconium

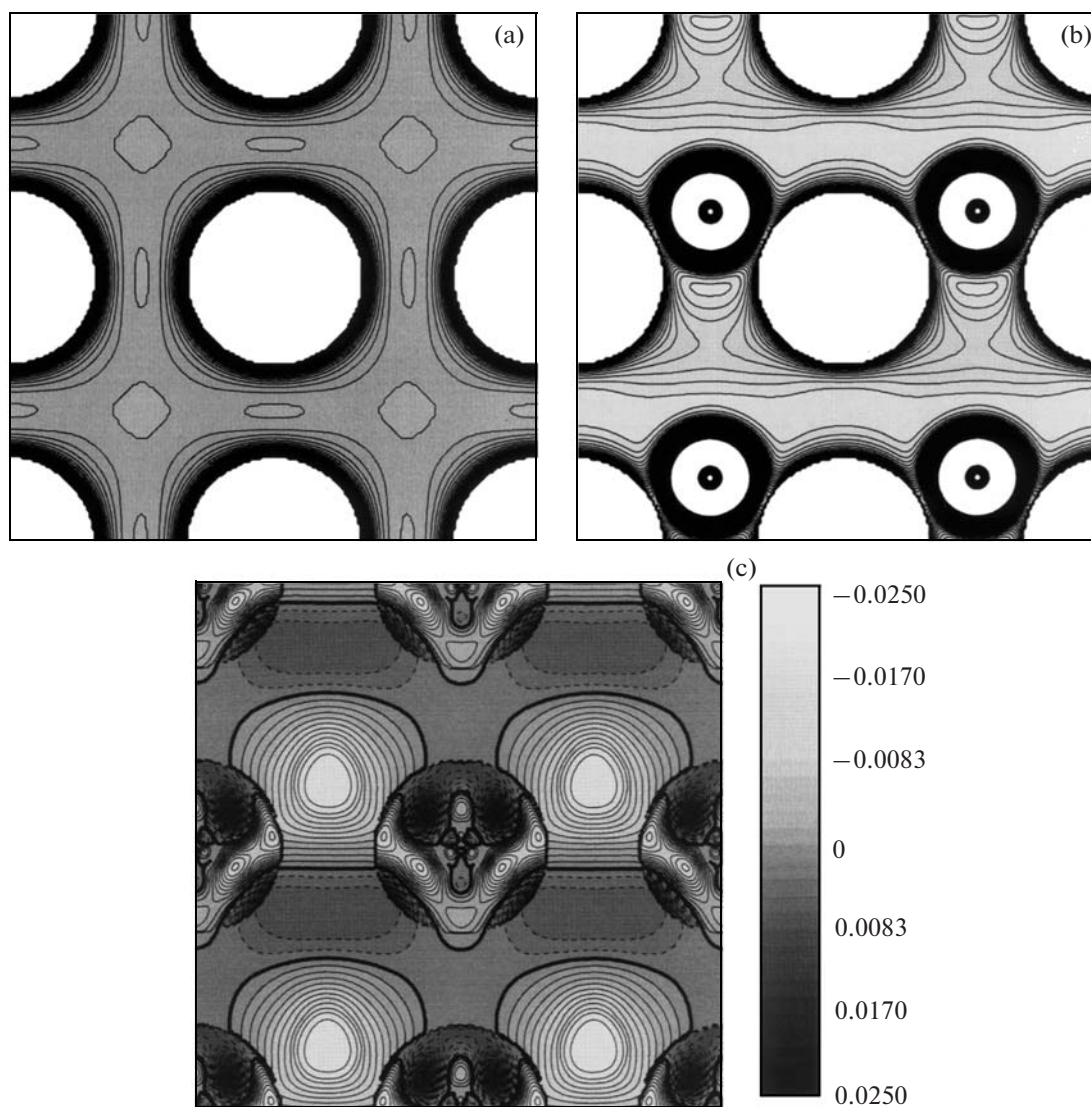


Fig. 6. Distribution of the charge density $\rho(r)$ in the body-centered cubic structure of (a) pure Zr ($\rho_{\text{Zr}}(r)$) and (b) Zr–He system ($\rho_{\text{Zr-He}}(r)$). (c) Difference between the valence densities $\rho(r) = \rho_{\text{Zr-He}}(r) - (\rho_{\text{Zr}}(r) + \rho_{\text{He}}(r))$.

and can penetrate to zirconium bulk only under specific conditions, e.g., during implantation (irradiation with α particles). Helium contributes a fairly large excess volume to the zirconium lattice (from 6.51 to 8.86 \AA^3 per He atom), which can be a reason of occurrence of internal stresses in the Zr–He system.

The presence of helium in the zirconium lattice significantly changes the electronic energy spectrum of zirconium, namely, splits some bands, leads to appearance of flatten portion in them. This can substantially change the spectrum of single-electron and collective excitations of the zirconium. Moreover, helium causes a significant redistribution of the valence charge density inside zirconium which can influence the bond type between its atoms.

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