

“Ab initio” study of helium atoms immobilization in UO_2 crystals

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Abstract. We present density functional theory (DFT) calculation results concerning the uranium dioxide crystals with a helium atom incorporated in the octahedral interstitial position. “Ab initio” calculations were performed using the Wien2k program package. For comparison, a pseudo-potential approach in the generalized gradient approximation was applied using the ABINIT program package. To compute the unit cell parameters 13 atom super-cell was chosen. Parameters of the potential barrier, which the helium atom has to overcome while jumping to the next octahedral interstitial position, were calculated by the help of both the program packages. The results, obtained using two different program packages, are shown in the table and presented graphically. For the so described parameters, the quantum mechanical movement of the helium atom around the equilibrium position is considered. The parameters of Schrödinger’s equation are collected in Table 2, while the results of mean square deviation and thermal occupation of energetic levels are presented in a graph. It is established that the helium atoms are located (with an accuracy of several percent of lattice constant) nearby the equilibrium position and form a local bound state. Applying a two site-model, we evaluated the time for an over-barrier jump. Graphically presented results show that the helium atom over-barrier jump is not possible even for temperatures as high as 1200 K. Influence of potential barrier height on the jump time was also considered.

Key words: uranium • dioxide • DFT+U • LDA • GGA • ABINIT • over-barrier jumps • incorporated helium • harmonic oscillator

Introduction

The first attempt to explain the helium incorporation in a UO_2 crystal was undertaken in the early 1990s [8]. The bond energy of helium atoms in the uranium dioxide crystal equal to -0.1 eV was estimated by using the semi-empirical inter-atomic potentials and the shell model. As the result was negative, so the helium atom could be permanently chemically bond in the uranium dioxide crystal. However, this result arose doubts because it was obtained with not very precise and half-classical methods. The later study, using the density functional theory-generalized gradient approximations (DFT-GGA) [3] framework, did not confirm this result. Conversely, the bond energy was calculated to be positive and according to the authors it was equal to about $+1.3$ eV [7]. The next attempt to determine the energy using the ABINIT [10] program package confirmed the result of the semi-empirical inter-atomic potentials method – the bond energy was evaluated to be about -0.1 eV. After about ten years, counting from the first attempt, the

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calculation were repeated by Gryaznov *et al.* [9] using the “ab initio” method and applying Hubbard’s model (DFT+U). They obtained the value for bond energy equal to +1.3 eV. Several approximations of the exchange-correlation energy functional $E_{xc}[n(\vec{r})]$ both of the local spin density approximations (LSDA) and the generalized gradient approximation (GGA) types were used in the calculations what seems to give reliable results of bond energies lying in the range from +0.77 to 1.83 eV, depending on the applied approximation.

In our previous work [5], considering the noble gases Xe and Kr bonding abilities in the uranium dioxide, we have assumed that the atoms can occupy oxygen vacancies but not the octahedral interstitial positions since the big ionic radii of these atoms practically make it impossible. In the case of helium the situation is different.

In all the above-mentioned models, the helium atom was located in the octahedral interstitial position of the uranium dioxide crystallographic lattice what is obvious as which ever position would be a worse one in terms of total energy consideration. Leaving the results unchallenged [9], the goal of this study is twofold. First, to describe the chances of formation of the stable local helium atom immobilization in the UO_2 . Second, to evaluate the possibility of helium atom to overcome the potential barrier between the neighbouring octahedral interstitial positions.

Method of calculations

“Ab initio” calculations of the electronic structure were performed using the Wien2k program package [2] based on the DFT. The Kohn-Sham (K-S) total-energy functional is used here as follows:

$$(1) \quad E[\Psi_i] = 2 \sum_i \int \Psi_i^* \left(-\frac{\hbar^2}{2m} \right) \nabla^2 \Psi_i d^3 r + \int V_{\text{ion}}(\vec{r}) n(\vec{r}) d^3 r + \frac{e^2}{2} \iint \frac{n(\vec{r})n(\vec{r}')}{|\vec{r}-\vec{r}'|} d^3 r' + E_{xc}[n(\vec{r})] + E_{\text{ion}}(\{\vec{R}_i\})$$

Theoretical studies of uranium compounds are difficult due to the relativistic character of electron motion in the U atom core and the strong electron-electron correlation. Chemical bonds of uranium in compounds is complex and is characterized by a mixed metal-covalent chemical bonding. Taking into consideration the above, in all DFT calculations we use several exchange-correlation energy functional $E_{xc}[n(\vec{r})]$ both within the LSDA and GGA approximations.

The above potentials are recommended by the authors of Wien2K program package [2].

All the calculation were performed using the Hubbard model (DFT+U), corrective exchange-correlation energy functional $E_{xc}[n(\vec{r})]$, namely:

- 1) PBE+U
- 2) WC+U
- 3) PBEsol+U
- 4) GGA +U
- 5) LSDA+U
- 6) ABINIT

For comparison, we used also the ABINIT code results as was previously used in the calculations of helium atom bond energy in UO_2 [7]. The ABINIT code utilizes the same functional form (Eq. (1)) as the Wien2k code. The difference consist in the calculation method of the total energy and the electron wave function of atom core. In the Wien2k code the electron wave function of atom core is calculated in a direct way, while in the ABINIT code the participation of the core electrons is considered in the form of pseudo-potential which is separately. Approximation of interactions between core electrons and the valence electrons in the pseudo-potential form are not unambiguous [11]. In our calculations we used the Troullier-Martins pseudo-potential scheme, which is adapted for plane-wave calculations [12]. In both cases the antiferromagnetic electron spin-polarization was taken into account.

Crystal field potential

The fifth term of Eq. (1) describes the dependence of the total energy on the nuclei positions. Therefore, performing calculations at different lattice coordinates of interstitial helium atom, we can numerically determine the potential values of crystal field along the direction of neighbour interstitial octahedral positions. UO_2 is isomorphic, with a face-centered cubic lattice (fcc) of the fluorite type structure, with similar lattice parameters: $a = 5.396 \text{ \AA}$ [1] and space group $\text{Fm-}3m$ (#225). At this structure, the neighbour octahedral interstitial positions have, for instance, the following crystal coordinates $(0, 0, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. Such a potential calculations were performed by the usage of Wien2k program package for the mentioned above all five exchange-correlation energy functional $E_{xc}[n(\vec{r})] + U$ approximations. The value of the correlation energy U was fixed at 4.6 eV, as suggested in Ref. [9]. Additionally, we used also the ABINIT code for comparison. In a view of periodicity of the crystal lattice, the calculations were performed in the range from $(0, 0, \frac{1}{2})$ to $(\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$. The calculation results of the potential appeared, within the error limit, to have the same shape irrespective of the applied method and the inconsiderable differences refer solely to its height. The potential values $V(x)$ of the $\text{UO}_2 + \text{He}$ arrangement were calculated with the usage of PBE+U, LSDA+U potential approximations and using the ABINIT pseudo-potential method for comparison [4]. In the case of uranium dioxide these approximations gave the best results as showed in [4]. All the calculated potentials were normalized to unity and are presented in Fig. 1.

By x it is denoted the He current position $(x, x, \frac{1}{2})$ during displacement between the neighbour octahedral interstitial positions in the range from $x = 0$ to $x = \frac{1}{4}$. The potential value presented in Fig. 1 can be approximated by the Gaussian curve:

$$(2) \quad V = \Delta V \varepsilon_0$$

where $\varepsilon_0 = e^{-\frac{2(x-x_c)^2}{w^2}}$, ΔV – potential barrier height, x – current crystal coordinate of helium atom, $x_c = 0.25$, $w = 0.1468$.

Table 1. Different methods of calculating potential barrier heights for helium, eV, which separates the neighbour octahedral interstitial positions in the crystal lattice of UO₂

E_{XC}	PBE+U	LSDA+U	WC+U	PBEsol+U	W91+U	ABINIT
ΔU_{UO_2+He} (eV)	8.90	8.32	7.83	7.86	7.71	7.97

Table 2. Parameters of the Schrödinger equation for the helium potential well in the octahedral interstitial positions of UO₂

	$\langle \Delta V \rangle$ (eV)	a (eV/Å ²)	ω (s ⁻¹)	x_0 (Å)	E_0 (eV)
U_{UO_2+He}	8.122	1.2498	7.737×10^{15}	0.14273	0.0509

For small x , better approximation is obtained by means of power series:

$$(3) \quad V = \Delta V (8.961x^2 + 433.68518x^4 - 1905.72859x^6), \quad x < 0.08$$

Collected results of potential barrier height ΔV for different E_{XC} potentials are presented in Table 1. The divergence of the results for the E_{XC} potentials is not big. In further calculations we used the average values calculated from the results obtained only by the Wien2k code which are assumed to be equal to 8.122 eV.

Helium atom in the crystal field potential well of UO₂

According to the above calculation results, the helium atom located in the octahedral interstitial position exists in a deep potential well. This suggests hypothesis that these helium atoms can form bound states in the UO₂ crystal lattices.

The potentials presented in Fig. 1 were computed on the assumption that all the atoms in a crystal lattice, therein the helium atom, are in the set crystal positions and stay all the time there immovably. In the next part of our calculations, in reverse, we consider that the helium atom is movable and is oscillating around local equilibrium positions.

For the above assumptions, movement of the helium atoms can be described with the Schrödinger equation in the form:

$$(4) \quad -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi + V(x)\Psi = E\Psi$$

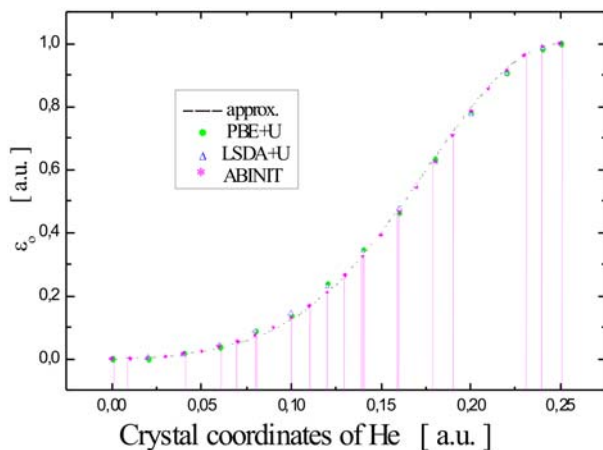


Fig. 1. Crystal field potential $\varepsilon_0 = (E - E_0)/(E_{max} - E_0)$ vs. helium location $(x, x, \frac{1}{2})$ in the UO₂ crystal lattice for the range from $x = 0$ to $x = 0.25$.

where: m – mass of helium atom, ΔV – potential (see, Eq. (3)), E – helium atom energy.

To develop the potential ΔV into power series around the equilibrium position and neglect all terms above the second power, we obtain the well known harmonic oscillator approach. This approach we use to do preliminary calculations and afterwards, using the eigenfunction base of harmonic oscillator we solve Eq. (4) for real potentials ΔV .

Harmonic oscillator approach

The potential energy used in this approach is the following:

$$(5) \quad V(x) \cong 8.961\Delta Vx^2 = ax^2 = \frac{m\omega^2}{2}x^2$$

where ω is the frequency of harmonic oscillator.

The Schrödinger equation takes then the form:

$$(6) \quad -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi + \frac{m\omega^2}{2}x^2\Psi = E\Psi$$

Introducing the characteristic length $x_0 = \sqrt{\hbar/m\omega}$, the eigenfunction Ψ_n can be expressed as:

$$(7) \quad \Psi_n(x) = e^{-\frac{x^2}{2x_0^2}} H_n\left(\frac{x}{x_0}\right)$$

where $H_n(x/x_0)$ is the Hermite polynomial of degree n . In particular,

$$(8) \quad \begin{aligned} H_0(x) &= 1, \\ H_1(x) &= 2x, \\ H_2(x) &= 4x^2 - 2, \\ H_3(x) &= 8x^3 - 12x, \end{aligned}$$

Each next polynomial can be obtained, applying the recursive formula:

$$(9) \quad H_{n+1} = 2xH_n - 2nH_{n-1}.$$

Each of the quoted eigenfunction Ψ_n expressed by Eq. (7), fulfils the Schrödinger Eq. (6).

Solving them, depending on the Ψ_n function form, expressed as:

$$(10) \quad E_n = (n + \frac{1}{2})(n + \frac{1}{2})\hbar\omega \cong (n + \frac{1}{2})E_0 \quad (\text{eV})$$

where $n = 0, 1, 2, \dots, n$ – quantum number.

Numerical values of a, ω, x_0 and E_0 for the considered cases are presented in Table 2.

Hamiltonian matrix (6), $H_{mn} = \langle \Psi_m | H | \Psi_n \rangle$, for any of the functions Ψ_m for which Ψ_n is its eigenfunction

(7), is obviously a diagonal one. As these are stationary solutions, this means that if any helium atom is found at any particular level \mathbf{n} – then it may be there for a freely long time. In reality this does not happen because of crystal phonons interaction with the helium atom. At the temperature equal to absolute zero, only the zero level ($\mathbf{n} = 0$) is occupied and the remaining levels are empty. As the temperature increases, according to the Boltzmann distribution law, the higher levels become occupied. These probabilities for ^4He atoms which are bosons are equal to:

$$(11) \quad P_n = \frac{A}{\exp(E_n / k_B T) - 1}$$

where $A^{-1} = \sum_n [\exp(E_n / k_B T) - 1]^{-1}$

When the temperature is not equal to absolute zero, the helium atom can occupy each energy level, but the probability of such an event decreases according to Eq. (11). The thermodynamic equilibrium wave function of helium atoms is not already a pure eigenfunction described by Eq. (7), but superposition of these functions. In order to accomplish the condition (11) the thermodynamic equilibrium wave function of helium atom should get the form:

$$(12) \quad \bar{\Psi}_{\text{equilibrium}} = p_n \bar{\Psi}_n$$

where $p_n = \sqrt{P_n}$, because then the condition $\langle |\Psi_{\text{equilibrium}}|^2 \rangle = 1$ is accomplished at any temperature.

Occupation of quantized energy levels of helium in UO_2 at different temperatures is presented in Fig. 2. We can see that even at the temperature equal to 1200 K the zero energy level is occupied prevalently (over 65%), and occupation of the next energy levels strongly decreases with quantum number \mathbf{n} .

The solution of Eq. (4) for the real potential V

The form of the real crystal field potential V is presented in Fig. 1 and its approximations are expressed by the formulas (2), and (3). Solving of Eq. (4) by using the Hermite polynomials, leads to the Hamiltonian matrix $H_{mn} = \langle \Psi_m | H | \Psi_n \rangle$, which is no longer diagonal

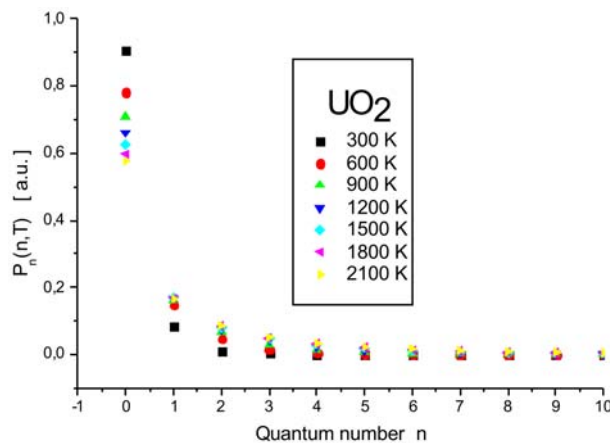


Fig. 2. Energy level occupation probability of helium in UO_2 vs. quantum number n at different temperatures.

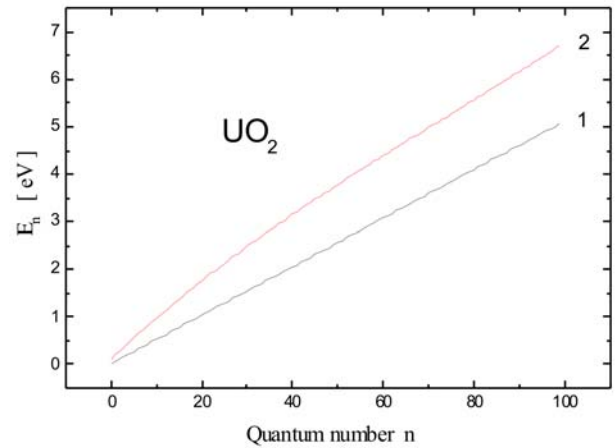


Fig. 3. Energy levels of helium atom in UO_2 vs. quantum number. 1 – Calculated according to Eq. (10); 2 – obtained in the result of diagonalization.

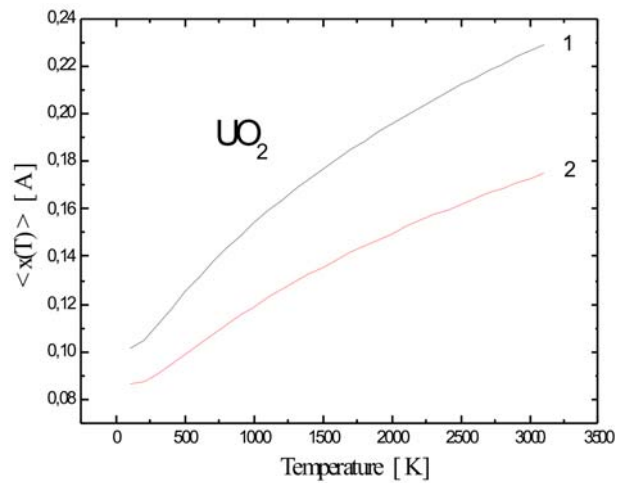


Fig. 4. The mean square deviation of helium atom vs. temperature for UO_2 . 1 – Calculated according to harmonic oscillator approach; 2 – obtained in the result of diagonalization.

and the formerly found states are not stationary. Using the numeric diagonalization methods and using the same Hermite polynomials as basic functions, we can find stationary values and eigenvectors of this system. In our case we applied the Jacobi numerical methods. The calculated values of energy levels for UO_2 in comparison with the values obtained according to Eq. (10), are presented in Fig. 3.

Helium atoms during thermal oscillation deviate from their equilibrium positions. The higher is the temperature the bigger is the deviation. The mean square deviation of helium atom vs. temperature for UO_2 is presented in Fig. 4.

As it is seen, the deviations are small and, even at very high temperatures, for instance at about 1200 K, they are below 4% of the lattice constant a_0 .

At the end of this section, it should be mentioned, that the harmonic oscillator approach with the parameters obtained as a result of neglecting all the higher terms above the second power of the potential V is not the best one from the standpoint of the diagonalization. The result can be more quickly obtained by applying the potential in the parabola form what is presented in Fig. 5. Application of such a potential enables to obtain significantly smaller not diagonal

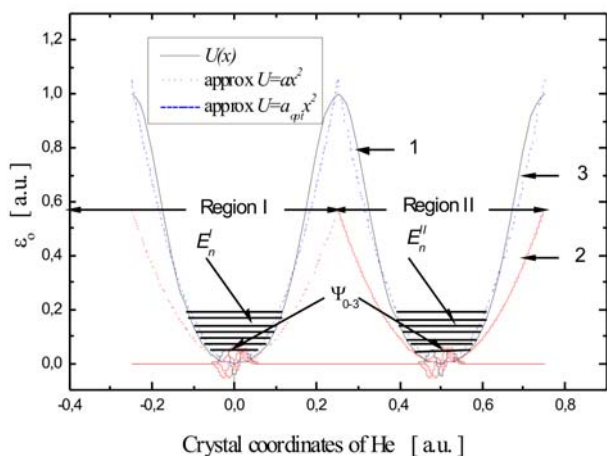


Fig. 5. Two-site model schema. E_n^I, E_n^{II} – energy levels in the regions I and II, respectively; Ψ_{0-3} first four graphs of wave functions $\Psi_n(x)$, localized in the I and II positions; 1, 2, 3 – parabola approximations and optimal parabola approximations of potential $U(x)$, respectively.

terms $H_{mn} = \langle \Psi_m | H | \Psi_n \rangle$, what, in turn, reduces the number of iterations and in the consequence the time, during diagonalization process. Obviously, the choice of potential, and so the choice of basis functions, does not affect in the slightest way the final result, calculated for the real potentials $V(x)$.

Over-barrier jump of helium atoms by crystal field potential barrier of UO₂

The wave functions of helium atom $\Psi_{\text{equilibrium}}(x)$, described by Eq. (12), also after diagonalization contain the exponential factor and rapidly decline with distance. Nevertheless, although to some small extent, the waves penetrate beyond the potential barrier and this means that the helium atom can be found on the other side of the barrier.

Let us consider the two-site model, consisting simultaneously of occupied (region I) and not occupied adjacent octahedral interstitial positions (region II). We believe therefore, that the helium atom has available energy levels of the two octahedral interstitial positions, but it occupies one of them. The potentials of the two positions, their parabola approximations and the first four graphs of wave functions $\Psi_n(x)$, localized in the two positions are illustrated symbolically in Fig. 5. There are also symbolically marked energy levels in both the regions. We see, as already confirmed earlier, the mean square deviations that the shown wave functions are concentrated on small distances from the positions of equilibrium. Below, we assess the time required for over-barrier jump in function of temperature.

If the helium atom occupies a certain energy level in the octahedral interstitial position I (see Fig. 5), then its state describes the wave function $\Psi^I_{\text{equilibrium}}(x)$. If, on the contrary, the octahedral interstitial position II is occupied, and the position I is empty – we have an analogous situation; the arrangement is in the quantum state $\Psi^{II}_{\text{equilibrium}}(x)$. The wave functions of such an arrangement are analogous, but located in the second position, what is symbolized by the index II. However, the

matrix elements, containing the functions $\Psi_{\text{equilibrium}}(x)$ from different regions are different from zero:

$$(13) \quad H^{I-II}_{\text{equilibrium}} = \langle \Psi^{II}_{\text{equilibrium}} | H | \Psi^I_{\text{equilibrium}} \rangle = H_{12} \neq 0$$

The matrix elements, containing the functions $\Psi_{\text{equilibrium}}(x)$ from the same regions are:

$$(14) \quad H_{11} = H^{I-I}_{\text{equilibrium}} = \langle \Psi^I_{\text{equilibrium}} | H | \Psi^I_{\text{equilibrium}} \rangle = H_{22}$$

According to the general principals of quantum mechanics, the amplitude of C_i states, which previously were constants, begin to depend on time. This is described by the linear system of differential equations [6]:

$$(15) \quad \begin{aligned} i\hbar \frac{dC_1}{dt} &= H_{11}C_1 + H_{12}C_2 \\ i\hbar \frac{dC_2}{dt} &= H_{21}C_1 + H_{22}C_2 \end{aligned}$$

where C_1, C_2 are the state amplitudes $\Psi^I_{\text{equilibrium}}(x)$ and $\Psi^{II}_{\text{equilibrium}}(x)$, respectively.

Once summing up and once subtracting the sides of the above differential equations we get two separated, easy to solve differential equations. Omitting the technical details, we obtain finally:

$$(16) \quad \begin{aligned} C_1(t) &= \exp\left(-\frac{iH_{11}t}{\hbar}\right) \cos\left(\frac{H_{12}t}{\hbar}\right) \\ C_2(t) &= \exp\left(-\frac{iH_{11}t}{\hbar}\right) \sin\left(\frac{H_{12}t}{\hbar}\right) \end{aligned}$$

The amplitude C_1 decreases with time as a cosine function and reaches the value of zero after $t = \pi\hbar / 2H_{12}$, while C_2 increases as a sine function and reaches the value of 1 for the same time t . In other words the helium atom moved from the region I to region II after time t . Results of numerical calculations are presented in Fig. 6.

The results of calculations presented in Fig. 6 show that the diffusion of helium in UO₂ is impossible even at high temperatures as high as 1200 K. The time that must elapse for the helium atom to over-barrier jump from one to the neighbouring octahedral interstitial position, distant only about 3.9 Å, at a temperature of 1200 K is about 10²⁸. They are unimaginably long times,

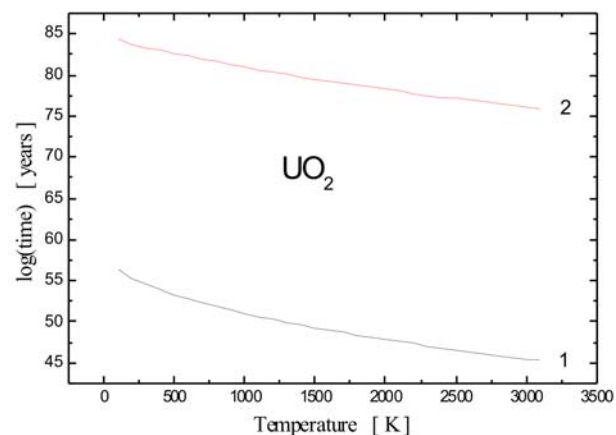


Fig. 6. Over-barrier jump time of helium atom in UO₂ in function of temperature. 1 – Parabola approximations of potential ΔV ; 2 – real potential ΔV .

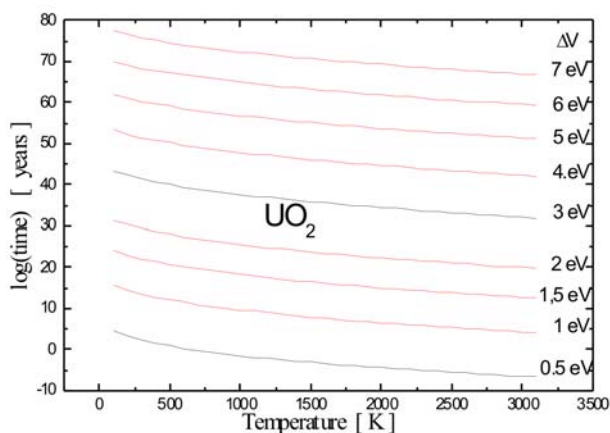


Fig. 7. Over-barrier jump time of helium atom in UO_2 vs. temperature for different barrier heights.

and virtually exclude the possibility of helium diffusion in these compounds.

Penetration of helium atoms by the crystal field potential barrier of UO_2 depending on the height of the barrier

The results of our previous calculations show that even small changes of the potential in UO_2 lead to large changes in the probability of over-barrier jump. Therefore, we decided to check if any, unavoidable errors when calculating the potential parameters using the “ab initio” cannot traverse the results obtained above. We analyzed this problem and the calculation results are presented in Fig. 7. During the calculations, we kept the same as before the width of the barrier. If it is assumed as a criterion, the time of over-barrier jump to neighbour interstitial position, distance of about 3.9 Å, as one year, (dotted line in Fig. 7), the diffusion time in the crystal at a distance of the order of centimeters will require about 10^8 years.

The criterion is fulfilled even at a temperature of 1200 K for UO_2 at ΔV larger than 3.4 eV. At 300 K, this limit shifts to 1.3. Therefore, it does not seem likely that our estimated values of barrier heights at 8 eV is below this criterion.

Discussion

The hitherto existing research described in the open literature, on bonding the helium atoms in UO_2 crystals by the “ab initio” method relied on the incorporation energy calculations. This of course makes a crucial sense for bonding the helium atoms which are solely very close to the crystal surface. Whereas in the case when the helium atom occupies already the octahedral interstitial position, in order to get out of the crystal the atom has to make many over-barrier jumps what practically is impossible, as show our evaluations. Merely, the value and sign of the incorporation energy for the helium atom, being inside the crystal, virtually does not apply to explain the problem of He immobilization in the crystal. Helium atoms resulting from the radioactive decay as α -particles have the energy thousands of times greater than the 8 electronvolt barrier and can easily

move in the crystal occupying free octahedral interstitial positions. The old mineral materials containing fissile isotopes hold fairly a lot of noble gases.

The accuracy of numerical calculations remains to be discussed. Incorporation energy calculations presented in paper [9] which were done with methods similar to ours, show a divergence of +1.83 to +0.77 eV, that is about ± 0.5 eV, and the divergence of the most utmost results, obtained in papers [3, 7, 8] do not exceed ± 1 eV. Since the potential barrier values obtained by us are equal to about 8 eV, therefore even two times of overestimation of the barrier does not change the main conclusion that the diffusion process of helium cannot be observed even at very high temperatures of 1200 K what is an analogical conclusion presented in Ref. [8]. However, authors [8] evaluated the barrier height at about 3.8 eV and they also considered that the barrier significantly reduces the helium atom diffusion in the not defected UO_2 single crystal.

Conclusions

Helium atom located in the octahedral interstitial position of crystal lattice fcc UO_2 is submitted to strong repulsive forces from the surrounding metal and oxygen atoms, which means that it is in a deep potential well of a depth equal to 8 eV, preventing it from any movement in the crystals even at very high temperatures reaching even thousands of K. Thus, the octahedral interstitial positions in uranium dioxide are effective traps for helium atoms. The helium trapped there is immobilized and may stay in the crystal for an arbitrarily long time. This is supported by some old minerals, where alpha decay occurs, such as uraninite which holds fairly a lot of helium during hundreds of millions of years and which could exist in a certain geological period where the temperature was very high.

The α -particles occurring during radioactive decay have a large enough energy to penetrate the crystal and to occupy the octahedral interstitial positions – incorporation process into the crystals.

Shape of the potential barrier is close to the Gaussian curve and its height is equal to 8.122 eV for UO_2 with its width about 1.120 Å.

Quantum-mechanical analysis showed that helium atoms in a crystal form local, stable in time and bound states performing small oscillations around the equilibrium position.

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