

Bonding xenon on the surface of uranium dioxide single crystal

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Abstract. We present density functional theory (DFT) calculation results of xenon atom interaction with the surface of uranium dioxide single crystal. A pseudo-potential approach in the generalized gradient approximation (GGA) was applied using the ABINIT program package. It has been revealed that close to the surface a potential well is formed for xenon atom due to its interaction with the atoms of oxygen and uranium. Depth and shape of the well is the subject of “ab initio” calculations. The calculations were performed both for the case of oxygenic and metallic surfaces. It has been shown, that the potential well for the oxygenic surface is deeper than for the metallic surface.

Key words: noble gases • uranium dioxide • chemical bond • density functional theory (DFT) • generalized gradient approximation (GGA)

Introduction

It is generally accepted that most of the insoluble inert gas atoms Xe and Kr produced during fissioning are retained in the fuel irradiated at a temperature lower than the threshold [4, 15, 19, 25, 27, 34, 35, 38, 42, 43]. Some authors [4, 15, 19, 27, 35, 42, 43] assume random diffusion of gas atoms to grain boundaries and consider the effect of trapping the atoms at inter-granular bubbles until saturation occurs. To better understand the bulk Xe diffusion mechanism in uranium-based fuel, Anderson *et al.* [1] calculated the relevant activation energies. Others [5, 41] confirmed that bubbles tend to concentrate in the grain boundaries during irradiation. Likewise, some authors [25, 34, 38] further assume that most of the gas atoms are retained in solution in the matrix of grains being there immobilized or are precipitated into small fission gas bubbles.

The experimental data presented in the open literature imply that we can assume that after irradiation exposure in excess of 10^{18} fissions/cm³ the single gas atom diffusion can be disregarded in description of fission gas behaviour. It means that a significant fraction of fission gas products is not available for diffusion. This is a general observation for the whole temperature range of UO₂ fuel that is exploited in the light water reactors (LWR). The above well documented assumption implies that a single gas atom diffusion model cannot be used to estimate the amount of fission gas that will be released from UO₂ during irradiation.

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Out of pile experiments show that during annealing the irradiated UO_2 sample bursts of fission gas release occur. After a small burst release at a relatively low temperature, a large burst release appears at high temperature about 1800°C [41].

The point defects induced by radiation begin to recover at $450\text{--}650^\circ\text{C}$ and are completely almost recovered above 850°C , while defect clusters of dislocations and small intra-granular bubbles require $1150\text{--}1450^\circ\text{C}$ [28].

Thermal recovery of radiation defects and microstructure change in irradiated UO_2 fuels studied by X-ray diffraction and transmission electron microscopy lead to the conclusion that the gas release kinetics from irradiated UO_2 is determined by the kinetics of thermal recovery of the radiation induced defects [39].

If the point defects, defect clusters of dislocations and small intra-granular bubbles are thermally recovered at the temperatures below 1450°C a natural question concerns nature of forces which immobilize the noble gases. Hence, an additional trapping process of inert gas atoms with the uranium dioxide material is suspected to occur [39].

The process of strong binding of the fission gas fragments with the irradiation defects is described as a process of chemical interaction with UO_2 . It is assumed that the vicinity of the fission fragment trajectory is the place of intensive irradiation inducing chemical interaction of the fission gas products with UO_2 [26].

We can further assume that above a limiting value of fission fluency (burn-up) a more intensive process of irradiation inducing chemical interaction occurs. Significant part of fission gas product is thus expected to be chemically bound in the matrix of UO_2 [39].

From the moment of discovering the rare gases (helium, neon, argon, krypton, xenon and radon), at the end of XIX century until to the beginning of the sixties years of the XX century, it was considered that the noble gases are chemically inactive.

The nobility of rare gases started to deteriorate after the first xenon compound was found by Barlett in 1962 [2]. Barlett showed that the noble gases are capable of forming what one could consider as normal chemical compounds, compelling chemists to readjust considerably their thinking regarding these elements.

In a burst of activity in the years that followed after the discovery of the first halogen compound, a number of compounds of noble gases have been reported, especially with xenon. It is observed, that the rare gases make reaction with the most electronegative elements, such as fluorine and oxygen. Later it has been shown that Xe (sometimes Kr) form bonds also with other non-metals, and even with some metals [6, 24, 29, 32, 37].

While many of these can be regarded as meta-stable species, several are actually thermodynamically stable compounds and can be obtained commercially [24].

There is a very interesting report on bonding between noble gas atoms and the actinide metal atom uranium [23].

Experiments with a mixture of noble gases using the infrared spectroscopy (IR), coupled with theoretical calculations provide strong evidence for direct bonds between Ar, Kr, or Xe atoms and the U atom of the CUO molecule [23].

The authors believe [23] that the experimental and the theoretical data presented in their report make a strong case for the interactions between the U atom of CUO and the noble gas (Ng) atoms. The U-Ng bond distances are short, and the U-Ng interaction is strong enough to change the spin state of the CUO molecules. Because of the positive charge, the UO_2^{2+} ion, which is isoelectronic with CUO, should form even stronger bonds with noble gas atoms, which could lead to growing number of complexes, that contain direct noble gas-to-actinide bonds.

The examples of rare gas compounds show that noble gas chemistry is much richer than it would be expected. New chemical bonds between strange bedfellows, like noble metals, actinides and noble gases, can still be found [39].

At the very end, we will mention about the analogical problem of helium atoms, which, in particular, are produced mainly as a result of α -decay. The concentration of He can be as high as 1%, which, depending on the temperature and fluency, can contribute to gas bubble formation [36]. Quantity of incorporation energy of helium into the UO_2 lattice was a matter of several studies based on "ab initio" method application [7, 12–14, 21, 31]. The influence of He interstitial on unit cell size and lattice distortion was studied there, too.

In Ref. [8] another approach of the issue was presented. Instead of chemical bond – the helium atom immobilization in a deep potential well inside the crystallographic lattice was proposed. The methods estimate the energy barrier between interstitial sites in perfect lattice UO_2+He on about 8 eV. We have shown there that in these circumstances the helium atom creates local bond state and performs oscillation of small amplitude, so the probability of over barrier jump to neighbour interstitial site, and hence the diffusion coefficient are close to zero.

In our work [9] in contrast to [8] in the calculations we took into account changes in local deformation during He wandering between vacancies and its impact on the barrier height, what appeared to be significant. We have shown that over barrier jump of helium to neighbour interstitial site is associated with a high potential barrier about 4 eV to be overcome. According to our calculations, diffusion value for the potential barrier 4.15 eV at 300 K should be in the case of a perfect crystal without defects about $10^{-48}\text{ cm}^2\cdot\text{s}^{-1}$. Such a small value of diffusion coefficient effectively prevent from any helium movement in the crystals even at very high temperatures.

However, in the case of xenon the situation is different. In Ref. [23] the authors show that argon forms with uranium and oxygen a weak chemical bond. They also suggest that this should include the krypton and xenon. Xenon is heavier and has a lower ionization potential. In our opinion it should, therefore, has a greater ability to produce chemical bonds than argon.

It is proved also that irradiating the UO_2 pellets in the presence of natural xenon, part of the gas atoms is imbedded into the pellet. The xenon is found to be firmly attached to the UO_2 surface such that only 1% of the attached gas can be removed after annealing samples for over 12 h at 1400°C [22].

Nuclear fuels are characterized by a total surface area depending on its density. The aim of this study is to test the ability of UO_2 surface to bond the gas Xe.

Method of calculations

Many problems of low energy physics, chemistry and biology can be explained by the quantum mechanics of electrons and ions using the contemporary numerical methods of advanced quantum theory. One of the method is widely applied and generally available namely the numerical ABINIT program package [17] which is based on the density functional theory, DFT, developed by Hohenberg and Kohn [16] and Kohn and Sham [20]. The DFT provided some hope of a simple method for describing the effects of exchange and correlation in an electron gas.

The Kohn-Sham total energy functional for a set of doubly occupied electronic states contains beside the Coulomb energy of electron-electron and their kinetic energy, also the Coulomb energy associated with interactions among the nuclei (or ions), the static total electron-ion potential and the exchange-correlation functional.

For this purpose, the plane wave of the Bloch's functions are used. The wave function ψ_i , is demanded as the sum of plane waves. More details are presented in [30]. To obtain computation process advance the pseudo-potential method is applied.

It consists in replacing the chemical inert electrons in the core by the effective potential. This idea goes back to the early work of Fermi [11] and afterwards developed in the works of Philips and Kleinman [33]. This assumption is justified by the fact that the change of valence electron wave function during chemical reaction practically does not influence the wave function of the core electrons which are strongly bound. In other words, the core electron wave function and the valence electron wave function are perpendicular to each other.

It is generally assumed that the binding energy over 6 Ry (~ 81.6 eV) is of the core characteristic.

A review of pseudo-potential method can be found in the articles [10, 18].

In our calculations we applied the Troullier-Martins pseudo-potential which is adapted for plane wave calculations [40]. An energy cut-off of 120 Ry was chosen.

While computing we look for the optimal atom location that ensure a minimum value of internal energy. Each time the forces acting on the atoms (ions) are also computed. The calculations take into account the impact of eight $5s^25p^6$ electrons of xenon, six $5f^36d^17s^2$ electrons of uranium and six $2s^22p^4$ electrons of oxygen. The remaining electrons were included into shell of cores and took into account as appropriate Troullier-Martins pseudo-potentials. The electron spin-polarization was taken into account.

Xe-O and Xe-U interaction

Using the above-described ABINIT software package, we received the potential dependencies of two-particles interactions for Xe-O and Xe-U, which are shown in Fig. 1. As can be seen from the calculations, the largest bonding energy for Xe-O is 0.730 eV, and realized at an optimum distance of 1.86 Å, and for Xe-U respectively -0.309 eV at a distance of 3.06 Å. For comparison, in the same way we calculated potentials Ar-O and Ar-U,

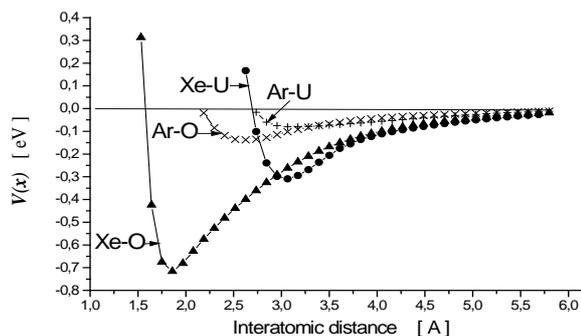


Fig. 1. Inter-atomic potential for Xe-O, Xe-O, Ar-O and Ar-U vs. mutual distance of atoms.

which turned out to be equal to 0.138 eV and 0.081 eV (3.18 and 1.87 kcal/mol). The calculation results are also shown in Fig. 1. These latter results were also studied in detail in the context of multi-particles interactions of complex CUO-Ar. The energy of the interaction was about 3.7 kcal/mol (0.16 eV) [23] which corresponds to the values obtained by us for two-particles potentials. However, the interaction of xenon, in comparison with argon are much stronger, in particular with oxygen (over 5-fold). This situation should favour bonding of xenon atoms to the surface of UO_2 .

UO_2 surface

Compound UO_2 is isomorphic, with a face-centred cubic lattice (fcc) of the calcium fluorite type structure, with similar lattice parameters $a = 5.396$ Å [3] and space group $Fm-3m$ (#225).

If the plane yz is accepted as the surface, then going from the surface down, we are faced with alternating atoms of uranium, oxygen, uranium, oxygen, etc. There are, therefore, two possibilities – either the surface is determined by the oxygen atoms of S_o (oxygenic) or uranium S_u (metallic). Both of these cases were the subject of our calculations. In each of these cases, there are two extreme positions in the xenon atoms to oxygen atoms, and uranium, namely (a) such as Xe atoms are located exactly opposite to the oxygen atom, and (b) when they are in front of the uranium atom.

Both of these situations are shown in Figs. 2a and 2b and refer to the configuration S_o . Further, these configurations will be briefly designated as $S_{o,a}$ and $S_{o,b}$, respectively.

An analogical situation exists when the surface is determined by the uranium atoms. Here, too, we have two analogous situations, which we denote as $S_{u,a}$ (xenon atoms are located exactly opposite to the oxygen atoms) and $S_{u,b}$ (xenon atoms are in front of the uranium atom), respectively. That can be easily imagined, if in Figs. 2a and 2b xenon atoms are located on the left side of shown super-cells.

Potential well

For numerical calculations, we have chosen 25 atomic super-cell of dimensions $4a \times a \times a$ ($21.88 \times 5.47 \times 5.47$ Å) which we filled half of it with 8 uranium atoms and 16 oxygen atoms. The second half of the super-cell is

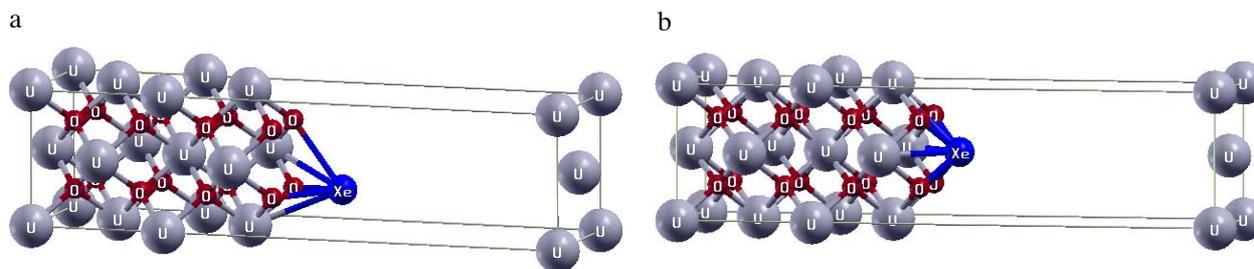


Fig. 2. Bonding of xenon on the surface of uranium dioxide in the position over (a) an oxygen atom, (b) an uranium atom. $S_{O,a}$ configuration.

a space free from oxygen and the uranium atoms. In this space we placed the xenon atom in positions $S_{O,a}$; $S_{O,b}$; $S_{U,a}$ and $S_{U,b}$. Because the xenon atom is separated from the nearest oxygen atoms or uranium atoms by a distance of nearly two lattice constants (Figs. 2a and 2b), we assume that Xe interacts really only with U and O atoms, located on the left side, it means with the atoms of the surface and subsurface layers. It does not interact with the atoms located on the right side, and belonging to the next, periodically repeated super-cell. Binding energy depending on the distance between Xe- UO_2 surface, and thus the shape and depth of the potential well, in which the xenon atom is close to the surface, for the configuration of $S_{O,a}$, $S_{O,b}$ are shown in Fig. 3a, and for the configuration of $S_{U,a}$ and $S_{U,b}$ in Fig. 3b.

For comparison, in Figs. 3a and 3b also is shown the same relationship for the super-cells with identical geometrical dimensions with the difference that only $1/4$ of it is filled with 4 uranium atoms, 8 oxygen atoms and xenon. The numerical calculations show that the oxygenic surface, irrespective of the size of super-cells, bonds more strongly the xenon atoms than the surface of uranium metal, what is shown in Table 1. It is also apparent from the curves according to Figs. 3a and 3b. Given the fact that the oxygen-xenon bonding is more than two times higher than uranium-xenon bonding, and that are realized on the shorter distances – energetically more favourable configuration of S_{O} does not

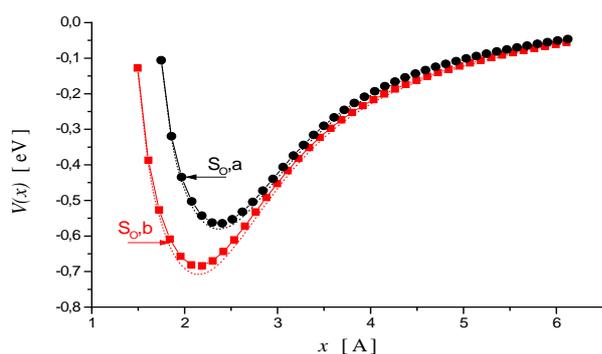


Fig. 3a. The bonding energy depending on x in the following configurations: ● – $S_{O,a}$, and 25 atoms super-cell, ■ – $S_{O,b}$ – 25 atoms super-cell, dotted curves – $S_{O,a}$ – 13 atoms and $S_{O,b}$ – 13 atoms super-cell, respectively x – Xe distance from the surface of UO_2 .

seem to be a surprise. This is in full correlation with the values of the inter-atom potentials Xe-O and Xe-U as presented in Fig. 1.

Summary of the bonding energy of all configurations and the optimum distance from the surface are shown in Table 1. In this table is also shown, for comparison, the same data, but for the typical 13-atom super-cells.

As can be seen from Figs. 3a and 3b and the data, shown in Table 1 doubling of the number of atoms in super-cell leads to small, only just several percent changes of the potential of the well. Given the fact that the interaction potentials presented above (Figs. 1, 3a and 3b) decreases exponentially with distance, assumption that 25 atom super-cell is large enough to represent an infinitely large crystal is confirmed. In other words, the interaction of xenon atoms to the surface of the crystal at a depth of more than two lattice constants can be neglected.

As can be seen from Table 1 from the four configurations of the 25 atomic super-cells, two of them, namely $S_{O,b}$, from the oxygenic surface and $S_{U,a}$, from the metallic side, have the lowest energy and they will be referred in the process of bonding. Only these two configurations, as preferred, will be dealt with in later work. These configurations, in which the xenon atom from its nearest neighbours has 4 oxygen atoms ($S_{O,b}$ configuration), or 4 atoms of uranium ($S_{U,a}$ configuration). Rejected configurations are those where the nearest neighbour is either a single oxygen, or a single uranium.

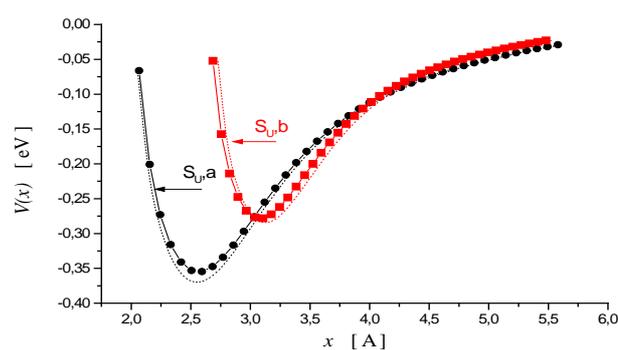


Fig. 3b. The bonding energy, depending on x in the following configurations: ● – $S_{U,a}$, and – 25 atoms super-cell, ■ – $S_{U,b}$ – 25 atoms super-cell, dotted curves – $S_{U,a}$ – 13 atoms, and $S_{U,b}$ – 13 atoms super-cell, respectively x – Xe distance from the surface of UO_2 .

Table 1. Summary results of the well depth U_0 and the optimal distance from the X_{opt} surface for various configurations and sizes of the two super-cells

Configuration	$S_{O,a}$ 13at	$S_{O,b}$ 13at	$S_{U,a}$ 13at	$S_{U,b}$ 13at	$S_{O,a}$ 25at	$S_{O,b}$ 25at	$S_{U,a}$ 25at	$S_{U,b}$ 25at
X_{opt} (Å)	2.3702	2.1487	2.5536	3.1241	2.3668	2.1472	2.56401	3.0813
U_0 (eV)	0.5801	0.70769	0.36957	0.2843	0.5652	0.6843	0.35497	0.2783

Discussion

Noble gases, such as e.g., xenon, form a bonding with the most electronegative elements, such as fluorine and oxygen. The heavier the element, the stronger chemical bonding creates. In particular, xenon with oxygen, forms a trioxide of xenon, which is the bonding energy of about 4.16 eV (402 kJ/mol) [6]. The oxide is also obtained (by interaction of XeF₆ with HOPOF₂ [6]) but there is lack of literature data on the bonding energy of Xe-O in this compound. Bearing in mind that the bonding energy of XeO₃, per one bond is about 1.39 eV, – received by us, using the “ab initio” method, value of 0.730 eV is not surprising. It is known that xenon also enters into chemical reactions with metals such as tungsten and gold, but with much less bonding energy of oxygen and fluorine. Xe-W energy measurements give a value of 0.364 eV (35 kJ/mol), and the gold is estimated at about 0.901 eV (87 kJ/mol) [6]. Our calculation of the pair interaction potential of xenon with uranium gives value of 0.309 eV, what is close to the value of tungsten. As it turned out, xenon also reacts with the surface of the UO₂ crystal. The calculated bonding energy of the xenon atom to the surface of UO₂ (or differently, shape and depth of the well potential) was found to be close to the bonding energy of Xe-O (from the oxygenic surface), or Xe-U (from the metallic surface).

Conclusion

Xenon atom interacts with the surface of uranium dioxide similarly as in the case of Xe-O and Xe-U particles. As a result, the potential well of large depth is formed.

This potential well traps xenon atoms with sufficient degree to create a condition for a bond state. It is, in addition to previously known, as trapping in the bubbles and trapping due to irradiation induced chemical bonding in the bulk of the fuel, an additional process for trapping fission gases by uranium dioxide fuel.

Conducive circumstances to such a phenomena is a significant interaction energy of Xe-U and Xe-O compounds.

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