

Xe and Kr bonding abilities in the single crystal oxygen vacancies of the uranium based fuel

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Abstract. The valence electron density distribution of krypton and xenon located in the oxygen vacancy and in its nearest neighbourhood was performed by application of the method “ab initio”. The results are presented on the graphs. The bonding energies of krypton and xenon in the uranium dioxide crystal lattice were calculated. It was found also that krypton and xenon cause a local increase of $\text{UO}_{1.75}\text{Xe}_{0.25}$ and $\text{UO}_{1.75}\text{Kr}_{0.25}$ unit cell and cause its deformation what is presented in tables. The force constants of krypton and xenon were also assigned what gives evidence about the strong bond of krypton and xenon with the $\text{UO}_{1.75}\text{Xe}_{0.25}$ and $\text{UO}_{1.75}\text{Kr}_{0.25}$ single crystal lattice. Obtained results are compared with the analogical studies of He atom incorporation into UO_2 single crystal lattice.

Key words: noble gases • chemical bond • UO_2 single crystal • valence electron density distribution • atomic force constants • bond energy • crystal lattice

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, 26, 27, 30, 37, 38, 41, 46, 48]. Some authors [4, 15, 19, 30, 38, 46, 48] 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 [6, 44] confirmed that bubbles tend to concentrate in the grain boundaries during irradiation. Likewise, some authors [27, 28, 37, 41] 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 UO_2 fuel that is exploited in 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 UO_2 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 relatively low temperature, a large burst release appears at high temperature, about 1800°C [44].

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 $1150\text{--}1450^\circ\text{C}$ [31].

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 [42].

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 [42].

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 induced 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 induced chemical interaction occurs. Significant part of fission gas product is thus expected to be chemically bound in the matrix of UO_2 [42].

From the moment of discovering the rare gases (helium, neon, argon, krypton, xenon and radon) at the end of the XIX century until the beginning of the sixties 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 [7, 23–25, 35, 40].

While many of these can be regarded as meta-stable species, several are actually thermodynamically stable compounds and can be obtained commercially [23].

There is a very interesting report on bonding between noble gas atoms and the actinide metal atom uranium [22].

Experiments with a mixture of noble gases using 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 [22].

The authors believe [22] 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 [42].

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 [39]. Quantity of incorporation energy of helium into the UO_2 lattice was a matter of several studies based on “ab initio” method application [8, 12–14, 21, 33]. The influence of He interstitial on unit cell size and lattice distortion was studied, too. The calculation results for helium we have compared with our calculation results for krypton and xenon.

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 methods widely applied and generally available is the numerical ABINIT program 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. The total-energy functional is expressed using a set of fictitious single-particle orbitals, Ψ_i , as follows:

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

The first term of Eq. (1) describes the kinetic energy of valence electrons, in the second term $V_{\text{ion}}(\vec{r})$ is the electron-ion potential and $n(\vec{r})$ is the electronic density given by:

$$(2) \quad n(\vec{r}) = 2 \sum_i \left| \Psi_i(\vec{r}) \right|^2$$

The third term describes the Coulomb electron-electron interaction, the fourth term $E_{xc}[n(\vec{r})]$ is the exchange-correlation energy functional and the fifth term $E_{ion}(\{\vec{R}_i\})$ is the Coulomb energy associated with interaction among the nuclei at positions $\{\vec{R}_i\}$.

For a given ionic configuration, $\{\vec{R}_i\}$, the minimum value of the Kohn-Sham energy functional is equal to the total energy of the electronic ground state. Therefore, it is necessary to determine the set of wave functions, ψ_i , by minimization of the Kohn-Sham energy functional (1). For this purpose, the plane wave of Bloch's functions are used. The wave function Ψ_i , is demanded as the sum of plane waves. More details are presented in [32]. 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 [36]. 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 [9, 18].

In our calculations we applied the Troullier-Martins pseudo-potential which is adapted for plane wave calculations [43]. The computation results we obtained by counting the interaction of all the valence electrons in the 12 atom super-cells.

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.

Chemical bonding of xenon and krypton in uranium dioxide single crystal

By exploitation the numerical "ab initio" the code ABINIT [17], was applied to make computer simulation of xenon and krypton chemical bonding in uranium dioxide single crystal. Computations were performed for the particular chemical compositions $\text{UO}_{1.75}\text{Xe}_{0.25}$ and $\text{UO}_{1.75}\text{Kr}_{0.25}$. The simulation goal was to explain the possibility of incorporation the xenon and krypton atoms into the oxygen lattice positions of the UO_2 single crystal. Calculations have shown that the minimal internal energy demands enlargement of unit cell dimensions from 5.472 to 6.207 Å in the case of xenon and to 6.000 Å in the case of krypton. The unit cell itself undergoes deformation. It concerns mainly the position of uranium atoms what is exemplified in Tables 1 and 2 below.

The calculated results, presented in Tables 1 and 2 were obtained by successive computations of Xe and Kr binding energy for different geometric positions of the gas atoms and uranium atoms optimizing their

Table 1. Reduced coordinates of uranium in the presence of xenon

Original position	Final position
0.0, 0.0, 0.0	-0.022, -0.022, 0.022
0.0, 0.5, 0.5	-0.022, 0.522, 0.478
0.5, 0.0, 0.5	0.522, -0.022, 0.478
0.5, 0.5, 0.0	0.522, 0.522, 0.0220

Table 2. Reduced coordinates of uranium in the presence of krypton

Original position	Final position
0.0, 0.0, 0.0	-0.020, -0.020, 0.020
0.0, 0.5, 0.5	-0.016, 0.515, 0.480
0.5, 0.0, 0.5	0.520, -0.020, 0.480
0.5, 0.5, 0.0	0.5125, 0.513, 0.0150

position in order to obtain the maximal binding energy of the noble gases.

The bond energy of the two considered atoms was computed too. In the case of xenon the energy is equal to -1.23 eV, and -3.42 eV in the case of krypton. Since both energies are negative, so such a chemical bond can exist as a stable one. This is confirmed additionally by atomic force constants calculated for Xe and Kr equal to $C_{Xe} = 5.5$ eV/Å² and $C_{Kr} = 7.9$ eV/Å², respectively. These are large values what confirms that detachment of Xe and Kr atoms from the UO_2 crystallographic lattice is not easy.

Also, the electron density distribution for the two solid solutions were calculated. Computation results for $\text{UO}_{1.75}\text{Xe}_{0.25}$ chemical compound are presented in Fig. 1.

Similar results are for $\text{UO}_{1.75}\text{Kr}_{0.25}$ what is presented in Fig. 2. Figures 1 and 2 give evidence of Xe and Kr chemical binding with the single crystal uranium dioxide.

Discussion

Several authors [8, 12–14, 21, 33] studying the He atom incorporation into the octahedral interstitial position of the UO_2 lattice revealed a series of approaches: the incorporation energy is positive and lies within the range $0.77 \div 1.38$ eV depending on the method applied and

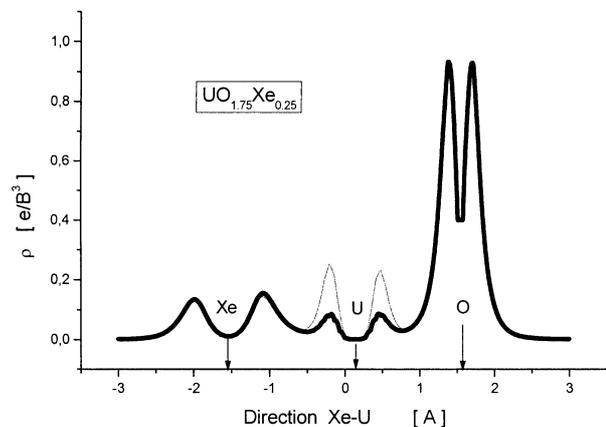


Fig. 1. Electron density of xenon and oxygen electrons round- about uranium. Dashed line – before occupation of the oxygen vacancy; full line – after occupation of the vacancy.

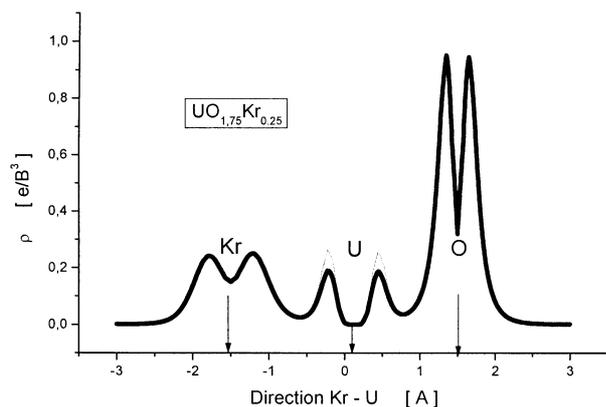


Fig. 2. Electron density of krypton and oxygen electrons roundabout uranium. Dashed line – before occupation of the oxygen vacancy; full line – after occupation of the vacancy.

on the assumed model. In our case the bond energies for Xe and Kr are negative both for oxygen vacancy occupation. This result is understandable comparing the chemical activity of helium, which practically does not react with other elements, with the chemical activity of Xe and Kr and chlorine group or oxygen. It is difficult to evaluate a priori accuracy of our computation, however in order to compute the incorporation energy it is necessary to compute cohesive energy, which in our case is computed to be 22.88 eV/ UO_2 . Computation accuracy of it co-decide of the final accuracy of the computed incorporation energy. Our computed value of the cohesive energy can be compared with the experimentally measured equal to 22.31 eV [45]. Our computation is closer to the experimental data than the result presented in [34] (18.3 eV), in [10] (22.23) and in [47] (20.26). However our values of the bond energies one should treat as estimated ones.

Our computations refer also to the atomic force constants describing the values of force which bind the considered atoms with the basis or matrix of UO_2 . The obtained values are large for the oxygen vacancy occupation equal to 5–8 eV/Å². It is the second parameter independently computed characterizing stability of atom joint. The so big values of atomic force constants may suggest the occurrence of just this situation.

Summarizing, the evaluated values of atomic force constants suggest that the Kr and Xe atoms can be in a stable way placed in the oxygen vacancies.

The second approach – is the change of lattice constants. In the case of He the lattice constant is increased by ~ 0.04 Å [14] for the 13 atom super-cell. In our case the increase of the lattice constant due to Xe and Kr replacing the oxygen is by about 0.5–0.6 Å. The larger lattice constant increase is for Xe and Kr than for He because of very different ionic radiuses.

The third approach – is the deformation of crystal lattice in nearby of the strange atom (He, Kr or Xe). In the case of He atom the uranium atoms stay in their original positions of the unit cell, and dislocate only the oxygen atoms. In the case of Kr or Xe inversely, move the uranium atoms but oxygen atoms remain in their positions. It is connected, in the obvious way, with the lattice positions settled by He and Kr or Xe. He atoms settle at vacant octahedral site, while Kr or Xe replace the oxygen atoms. The values of deformation in our case is far bigger than for the helium atom.

Remarks and conclusions

Since the examples of rare gas compounds are formed by applying the classical chemical methods, the more the noble gas species in the conditions of neutron and fission fragments irradiation of the UO_2 fuel type can be expected [42].

This assumption is suggested by the fact that the ClXeCl has been found to form after irradiation with 501.7 nm laser light of Cl_2 -doped xenon matrices. It appears that after excitation of the Cl_2 there is little or no barrier for the rearrangement to ClXeCl [5].

The fission fragments are striped of about 20 electrons along most of their paths in the medium in which the fission takes place and are still 10 near the end of their paths [29].

Fission fragments are at the same time very energetic and highly charged particles; they interact strongly with electrons of the material losing their energy mainly by ionisation but also by elastic collisions with atoms as a whole.

As the UO_2 fuel is highly defected, ionised with very energetic and highly charged fission fragments, it appears that during irradiation there is little or no barrier for the formation of rare gas atom compounds with the UO_2 molecule and fission products. There would be a strong interaction between the U atom of UO_2 , fission products and the noble gas (Ng) atoms. This further implies that a significant part of the fission fragments after dissipating all their energy and stopping in the material being still highly ionised at the end of their paths react chemically with the fuel [42].

Keeping in mind that the gas release kinetics from irradiated UO_2 is determined by the kinetics of thermal recovery of the radiation induced defects and associating it with the idea of the noble gas atoms trapped in clathrates (where no chemical bonds between gas atoms and the surrounding occur), we can postulate that in point defects, dislocation loops and gas bubbles the rare gas atoms with the closed-shell electronic structure can be immobilised. In this sense, there exists no true diffusion for the fission gas in the UO_2 fuel [42].

Calculation results show that a chemical bond of noble gas with the uranium dioxide fuel can exist as a stable one. Large values of their bonding confirm that the detachment of Xe and Kr atoms from the UO_2 crystallographic lattice is not easy. Moreover, the bond is so big that Kr and Xe atoms placed in the oxygen vacancies of uranium dioxide single crystal do not undergo destruction due to lattice vibrations.

Further, the calculations presented above show that during chemical bonding of Kr and Xe the enlargement of unit cell dimensions are expected. This expectation is supported by the measurement of the lattice parameter of irradiated UO_2 fuel which is progressively expanded in the burn-up range 0–70 GWd/tM [3].

References

1. Anderson DA, Uberuaga BP, Nericar PV (2011) U and Xe transport in UO_{2+x} : Density functional theory calculations. *Phys Rev B* 84:054105–17

- Barlett N, Sladky FO (1968) The relative fluoride ion donor abilities of XeF_2 , XeF_4 and XeF_6 , and a chemical purification of XeF_4 . *J Am Chem Soc* 90;19:5316–5317
- Baron D, Spino J, Papaioannou D, Ray I (2002) Rim formation gas behaviour: some structure remarks. In: Proc on Fission Gas Behaviour in Water Reactor Fuels, 26–29 September 2000, Cadarache, France. Published by OECD, pp 247–268
- Bellamy RG, Rich JB (1969) Grain boundary gas release and swelling in high burn-up uranium dioxide. *J Nucl Mater* 33;1:64–76
- Bieler R, Spence KE, Janda KC (1992) The dynamics of noble gas-halogen molecules and clusters. *J Phys Chem* 95:5058–5064
- Burbach J, Zimmermann H (1985) Spaltgasverhalten in bestrahltem UO_2 bei out-of-pile-Gluehungen von 1400 bis 2000°C. *KfK 3997*:1–39
- Cotton FA, Wilkinson G, Murillo CA, Bochmann M (1999) *Advanced inorganic chemistry*. John Wiley & Sons, New York
- Crocombette JPJ (2002) *Ab initio* energetics of some fission products (Kr, I, Cs, Sr and He) in uranium dioxide. *Nucl Mater* 305:29–36
- Denteneer P, Haering W (1985) The pseudopotential-density-functional method in momentum space: details and test casus. *J Phys C* 18:4127–4134
- Dudarev L, Nguyen Manh D, Sutton AP (1997) Effect of Mott-Hubbard correlations on the electronic structure and structural stability of uranium dioxide. *Philos Mag B* 75:613–621
- Fermi E (1934) Sullo spostamento per pressione dei termini elevati delle serie spettrali. (On the pressure displacement of higher terms in spectral series). *Nuovo Cimento* 11:157–166
- Frazer BC, Shirane G, Cox DE, Olsen CE (1965) Neutron-diffraction study of antiferromagnetism in UO_2 . *Phys Rev A* 140:1448–1452
- Freyss M, Vergnet N, Petit T (2006) *Ab initio* modeling of the behavior of helium and xenon in actinide dioxide nuclear fuels. *J Nucl Mater* 352:144–150
- Gryaznov D, Heifets E, Kotomin E (2009) *Ab initio* DFT+U study of He atom incorporation into UO_2 crystals. *Phys Chem Chem Phys* 11:7241–7247
- Hargreaves R, Collins DM (1976) A quantitative model for fission gas release and swelling in irradiated uranium dioxide. *J Br Nucl Energy Soc* 15:311–318
- Hohenberg H, Kohn W (1964) Inhomogeneous electron gas. *Phys Rev B* 136:864–871
- <http://www.abinit.org>
- Ihm J, Zunger A, Cohen ML (1979) Momentum-space formalism for the total energy of solids. *J Phys C* 12:4409–4415
- Ito K, Iwasaki R, Iwano Y (1985) Finite element model of fission gas release from UO_2 fuel. *J Nucl Sci Technol* 22;2:129–138
- Kohn W, Sham IJ (1965) Self-consistent equations including exchange and correlation effects. *Phys Rev A* 140:1133–1138
- Kudin KN, Scuseria GE, Martin RL (2002) Hybrid density – functional theory and the insulating gap of UO_2 . *Phys Rev Lett* 89:266402–4
- Li J, Liang BE, Andrews L (2002) Noble gas-actinide compounds: complexation of the CuO molecule by Ar, Kr and Xe atoms in noble gas matrices. *Science* 295:2242–2245
- Lorenz M, Rasanen M, Bondybey VE (2000) Neutral xenon hydrides in solid neon and their intrinsic stability. *J Phys Chem A* 104;16:3770–3774
- Lundell J, Chaban GM, Gerber RB (2000) Anharmonic vibrational spectroscopy calculations for novel rare-gas-containing compounds: HXeH , HXeCl , HXeBr , and HXeOH . *J Phys Chem A* 104;34:7944–7949
- Lyczko K (2002) Chemistry of the noble gases. *Wiadomości Chemiczne* 56:771–792
- McInnes DA, Winter PW (1988) The effect of the chemically inert fission products on the chemistry of irradiated UO_2 . *J Phys Chem Solids* 49;2:143–150
- Mac Iwan JR, Stevens WH (1964) Xenon diffusion in UO_2 . *J Nucl Mater* 11;1:77–93
- Matthews JR, Small GJ (1988) Towards a mechanistic understanding of transient fission gas release. In: Proc of a Technical Committee Meeting, 18–22 September 1988, Preston, England. IAEA-TC-659/4.1. IAEA, Vienna, pp 195–202
- Moak CD, Lutz HO, Bridwell LB, Nothcliffe LC, Datz S (1968) Equilibrium charge states of Br and I ions in solids and gases in the energy range 10–180 MeV. *Phys Rev* 176;2:427–437
- Nakajima T, Saito H (1987) A comparison between fission gas release data and FEMAXI-IV. *Nucl Eng Des I* 101;3:267–279
- Nogita Y, Une K (1993) Thermal recovery of radiation defects and microstructural change in irradiated UO_2 fuels. *J Nucl Sci Technol* 30;9:900–910
- Payne MC, Teter MP, Allan DC, Arias TA, Joannopoulos JD (1992) Iterative minimization techniques for *ab initio* total – energy calculations: molecular dynamics and conjugate gradients. *Rev Mod Phys* 64;4:1045–1097
- Petit T, Lemaingn C, Jollet F, Bigot BF, Pasturel A (1998) Point defects in uranium dioxide. *Philos Mag B* 77;3:779–786
- Petit T, Morel B, Lemaingn C (1996) Cohesive properties of UO_2 . *Philos Mag B* 73;6:893–904
- Pettersson M, Lundell J, Rasanen M (1999) New rare-gas-containing neutral molecules. *Eur J Inorg Chem* 4:729–737
- Philips C, Kleinman L (1959) New method for calculating wave functions in crystals and molecules. *Phys Rev* 116:287–294
- Ray ILF, Thiele H, Matzke H (1992) Transmission electron microscopy study of fission product behaviour in high burnup UO_2 . *J Nucl Mater* 188:90–95
- Rest J, Cronenberg WA (1987) Modeling the behavior of Xe, I, Cs, Te, Ba and Sr in solid and liquefied fuel during severe accidents. *J Nucl Mater* 150;2:203–225
- Sattonay G, Vincent L, Garrido F, Thome L (2006) Xenon versus helium behavior in UO_2 single crystals: A TEM investigation. *J Nucl Mater* 355;1/3:131–135
- Stein L (1983) The chemistry of radon. *Radiochim Acta* 32:163–171
- Szuta M (1994) The diffusion coefficient of fission-product rare gases in single crystal uranium dioxide during irradiation. *J Nucl Mater* 210:178–186
- Szuta M (2006) Chemical activity of noble gases Kr and Xe and its impact on fission gas accumulation in the irradiated UO_2 fuel. In: Proc of the 6th Int Conf on WWER Fuel Performance, Modelling and Experimental Support, 19–23 September 2005, Albena. Institute of Nuclear Energy of the Bulgarian Academy of Sciences, Sofia, pp 345–354
- Troullier N, Martins JL (1991) Efficient pseudopotentials for plane – wave calculations. *Phys Rev B* 43;3:1993–2006
- Une K, Kashibe S (1990) Fission gas release during post irradiation annealing of BWR fuels. *J Nucl Sci Technol* 27:1002–1016
- Veal BW, Lam DJ (1974) The band structure of UO_2 : an angle resolved and resonant photoemission study. *Phys Rev B* 10:4902–4911
- White RJ, Tucker MO (1983) A new fission-gas release model. *J Nucl Mater* 118:1–38

-
47. Yun Y, Kim H, Kim H, Park K (2005) *Ab initio* calculations of strongly correlated electrons: antiferromagnetic ground state of UO_2 . Nucl Eng Technol 37;3:293–298
 48. Zimmermann H (1978) Investigations on swelling and fission gas behaviour in uranium dioxide. J Nucl Mater 75:154–161