EFFECT OF IRRADIATION AND DEUTERIUM BEHAVIOR IN Li-BASED TRITIUM BREEDING CERAMICS

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The behavior of implanted deuterium in advanced lithium orthosilicate (Li_4SiO_4) pellets with addition of lithium metatitanate (Li_2TiO_3), and in reference Li_4SiO_4 pellets, has been investigated. Thermal desorption (TD) spectroscopy was used to study the deuterium interaction with radiation defects in materials. Computational evaluation of deuterium desorption within the framework of the diffusion-trapping model allowed to associate characteristics of experimental TD spectra with specific trapping sites in the material. It was found that deuterium desorption is limited mainly by intragranular diffusion of deuterium and its trapping by radiation defects associated with Li-vacancy traps. Deuterium gas release from both ceramics demonstrated similar trend indicating weak dependence of deuterium trapping behavior on phase composition. The change of the morphology and elemental composition of the pellets surface has been analyzed. SEM examination indicated that ion irradiation and subsequent thermal desorption annealing of two-phase ceramics leads to an increase in surface destruction processes.

INTRODUCTION

Fusion reactors, which will operate with a closed tritium-deuterium fuel cycle, have a potential to be used for future commercial purposes. However, there are several crucial scientific and technological challenges, which need to be resolved. One of the most important technological challenges for DEMO (Demonstration fusion power plant) or any commercial fusion power plant is to ensure the tritium self-sufficiency.

In nature, tritium (^3H) is generated by cosmic rays in the upper atmosphere layers of Earth by $^{14}N(n,^3H)^{12}C$ nuclear transmutation reactions. However, due to the relatively short half-life of the generated tritium nucleus (12.32 years, beta decay), its natural abundance is too low to be economically exploited. Therefore, in ITER (International Thermonuclear Experimental Reactor), which is currently under construction at Cadarache, France, several designs of DEMO relevant Test Blanket Modules (TBMs) will be tested in order to verify and compare the proposed solid and liquid form tritium breeding concepts under real operational conditions of fusion reactor [1].

In the proposed TBMs, tritium will be generated by the nuclear transmutation reactions of lithium with neutrons. Naturally occurring lithium is composed of two stable isotopes, lithium-6 (7.5%) and lithium-7 (92.5%). The cross-section of $^6Li(n,\alpha)^3H$ nuclear transmutation reactions is significantly higher in comparison to the cross-section of $^7Li(n,n',\alpha)^3H$ reactions. Therefore, the tritium breeder material will be enriched with the lithium-6 isotope in order to increase the tritium production [2].

Li_4SiO_4 and Li_2TiO_3 in the form of ceramic spheres (further in the text referred as "pebbles") were internationally accepted as two leading candidate materials for the tritium breeding in the solid breeder TBM concepts [3].

The top priority for tritium breeder materials is the tritium release performance [4]. Understanding of the release behavior of bred tritium from solid breeder materials is necessary to design tritium recovery system from blanket of a fusion reactor because permeation loss of bred tritium in the piping system or type of tritium recovery system depends on the tritium release behavior [5].

Induced radioactivity and high chemical activity of tritium leads to complex and rigid safety procedures. Therefore, in order to investigate the generated tritium diffusion and release behavior, nuclear reactor irradiation tests are traditionally simulated by implantation of other non-radioactive hydrogen isotope ions (protium and deuterium), which are easier to handle and study.

The purpose of this study is to clarify the desorption behavior of the implanted deuterium in the Li_4SiO_4 pellets with addition of Li_2TiO_3 and to evaluate the deuterium trapping and release characteristics from the irradiated ceramic breeder materials. The brittle crush and changes in the elemental composition of the pellets after irradiation are also investigated.

1. EXPERIMENTAL PROCEDURE

The advanced Li_4SiO_4 pellets with 10% of Li_2TiO_3 as a secondary phase were investigated together with the reference Li_4SiO_4 pellets. The reference Li_4SiO_4 pebbles (0 mol.% Li_2TiO_3) consisted of two crystalline phases, Li_4SiO_4 as the primary phase and Li_2SiO_3 as a secondary phase due to 2.5 wt.% excess of SiO_2 (Table 1).

Table 1

Phase composition of the advanced ceramic

Item No	Phase composition, mol.%
1	90% Li_4SiO_4 + 10% Li_2TiO_3
2	90% Li_4SiO_4 + 10% Li_2SiO_3

The advanced pebbles were produced by an enhanced melt-based process at the Karlsruhe Institute of Technology (Germany), while the reference pebbles were fabricated by a melt-spraying process at the Schott AG (Mainz, Germany). To achieve an operation relevant microstructure and phase composition, the fabricated Li_4SiO_4 pebbles with content of Li_2TiO_3 were thermally treated up to 1220 K for 3 weeks in air atmosphere.

For the irradiation and implantation experiments, the pebbles were powdered using an agate mortar and were pressed into 10 mm pellets (height: ~ 2 mm) using a

manual hydraulic press (Fig. 1). The pellets instead of pebbles were used in order to eliminate the effect of surface curvature, thereby providing normal ion beam incidence to the entire target surface.
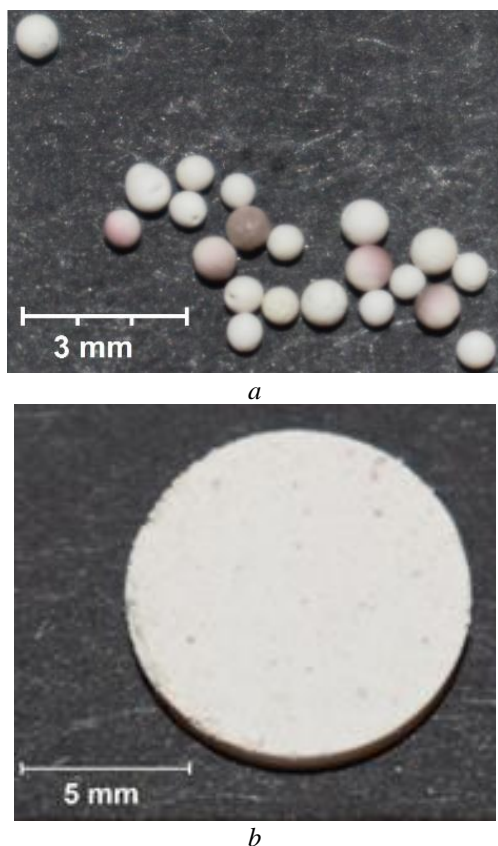

a

b

Fig. 1. The advanced pebbles (a),
and a pressed pellet (b)

The pellets were irradiated in the target chamber of ESU-2 installation [6] with a 25 keV D_2^+ ion beam separated by an 85-degree magnetic mass analyzer and incident on the target approximately along the normal with a current density of 6 $\mu A/cm^2$ at a temperature of 290 K. The central section of the sample surface with a diameter of d ~ 7 mm was subjected to irradiation. To calibrate the beam current, a Faraday cup was used, which was introduced along the path of the beam in front of the sample. Uniformity of irradiation within the beam trace on the target was ensured by defocusing.

The distribution profiles of the radiation damages and the implanted deuterium ions in the irradiated pellets were calculated using SRIM code [7] (Fig. 2).
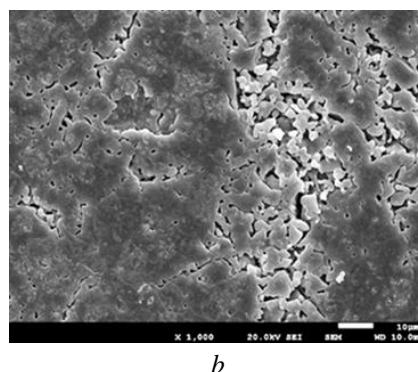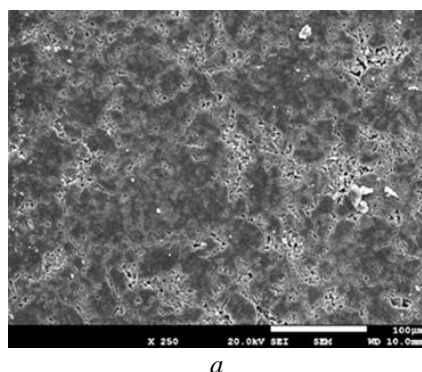
The implanted deuterium release was investigated by the thermal desorption technique in the temperature range from 290 to 1200 K at a rate of 6 $K \cdot s^{-1}$. The gas release was registered by a monopole mass-spectrometer. Irradiations and measurements of TDS were performed in one chamber, to exclude contact of the specimens with air that prevented the formation of artifact trap sites associated with the surface oxide. The residual gas pressure in the experimental chamber was measured to be ~ $5 \cdot 10^{-5}$ Pa.
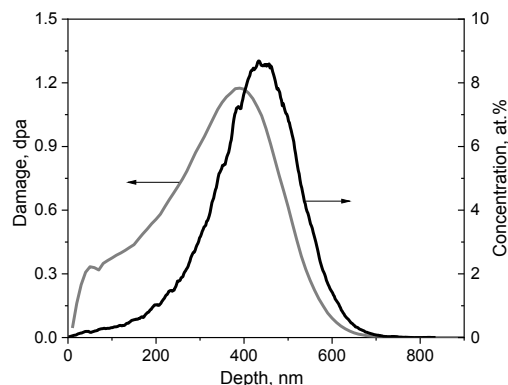

Fig. 2. Depth distribution profiles of damage and
concentration for 25 keV deuterium ions in Li_4SiO_4
ceramic calculated by SRIM for a dose
of $1 \cdot 10^{17}$ D^+/cm^2

The sample holder made of Ta plate was used to fix pellets, and the sample was heated by indirect resistive heating during the annealing. The surface temperature of the pellet and the temperature of the sample holder were measured up to 1200 K, by using a thermocouple. The temperature difference between the surface of the pellets and the sample holder was approximately 300…400 K at each irradiation temperature.

Investigations of surface microstructure were performed using scanning electron microscope JEOL JSM-7001F. Chemical composition of the samples was determined by energy dispersive X-ray spectroscopy – EDS.

2. RESULTS AND DISCUSSION

Effect of irradiation on morphology of the pellets surface. The visual inspection of the samples after irradiation at the room temperature revealed a color change − the darkening in the surface of pellets. This could be an effect of oxygen vacancies provoked by the ionizing radiation [8].

a

b

Fig. 3. Surface morphology of the 90% Li_4SiO_4 + 10% Li_2SiO_3 ceramics in the as-received state (a),
surface area at higher magnification (b)

The SEM micrographs of the 90% Li_4SiO_4 + 10% Li_2SiO_3 ceramics in the as-received state and after irradiation and annealing up to 700 K are shown in Figs. 3 and 4, respectively.

For all samples, along with the undamaged zones, numerous damaged areas on the surface of pellets can be identified. Although these destructions could be partly caused by forceful removal from the irradiation capsules, it was found that the irradiation and annealing processes contribute to an increase in destruction: the observed crush and the formation of cracks and porosity are intensified (see Fig. 4,a).

On the surface of the ceramics the formation of small cavities and nearby fragments of the same shape of extruded material with a diameter of about 1 μm are observed (see Fig. 4,b, marked with circles). Such changes in the surface relief were observed only in samples subjected to deuterium exposure and annealing, and are probably the result of their joint influence.
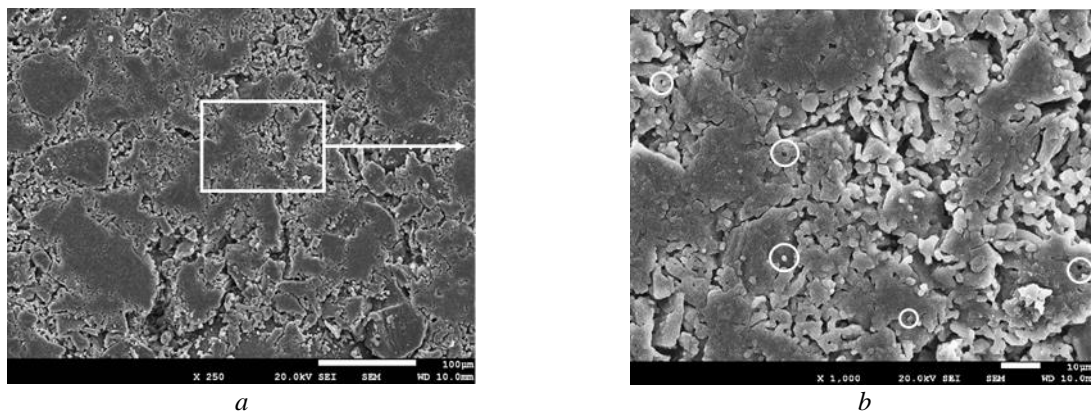

Fig. 4. Morphology of the pellets surface after irradiation and annealing (a),
surface area at higher magnification (b)

Effect of irradiation on elemental composition of the pellets surface. Elemental analysis of undamaged and damaged areas of samples after irradiation and annealing up to 700 K was performed. Areas of the surface from which EDS X-ray spectra were taken, and an example of EDS spectrum are shown in Fig. 5. The focus was mainly on the silicon and oxygen content. Lithium was not analyzed because the window on the detector was made of beryllium. Traces of platinum were fixed because of creation of a conductive layer on the ceramic surface.

Careful analysis of the ceramic surface revealed some areas containing traces of carbon. The origin of these carbon traces is not entirely clear and could be the result of pollution that arose during the experiment. However, the presence of carbon has attracted interest from the viewpoint of its effect on the redistribution of the elemental composition on the ceramic surface. Fig. 6 shows different areas of the surface polluted with carbon, and an example of EDS spectrum.
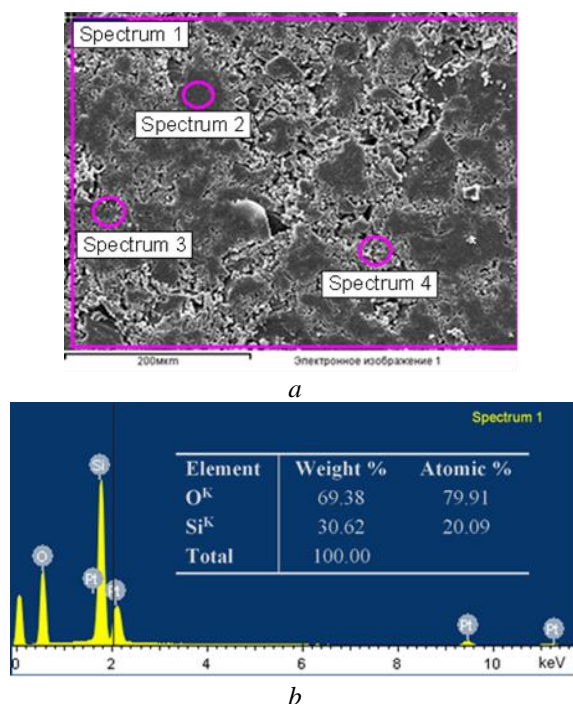

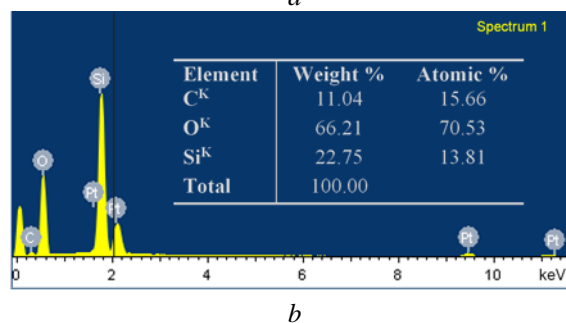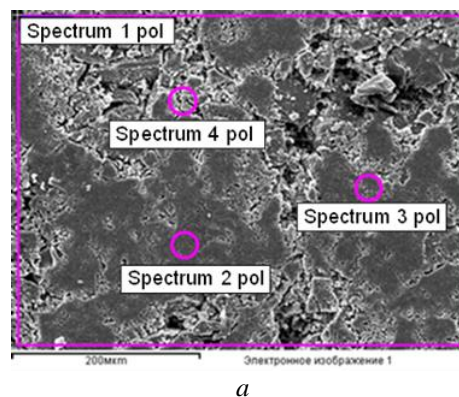*Fig. 6. The location of EDS-spectra on the surfaces of ceramic polluted with carbon (a) and spectrum 1 (b)*

Fig. 5. The location of EDS-spectra on the surfaces of ceramic (a) and spectrum 1 (b)

Fig. 7 summarizes the elemental concentrations of silicon, oxygen and carbon for both clean and carbon-polluted surfaces of ceramic after irradiation and annealing up to 700 K. In the Spectrum 1 taken from the clean area of surface (see Fig. 5), the ratio of oxygen to silicon is fixed as 4:1, which corresponds to the chemical formula. In the Spectrum 2 taken from the undamaged area of the same sample, the ratio of oxygen to silicon is fixed as 3.4:1, that is, a slight decrease in the amount of oxygen is recorded. In the spectra taken from the damaged areas of the sample (see Spectra 3 and 4 in Fig. 5), the ratio of oxygen to silicon is fixed as 1.5:1 and 1.1:1, indicating a considerable decrease in the amount of oxygen and a simultaneous increase in silicon content.
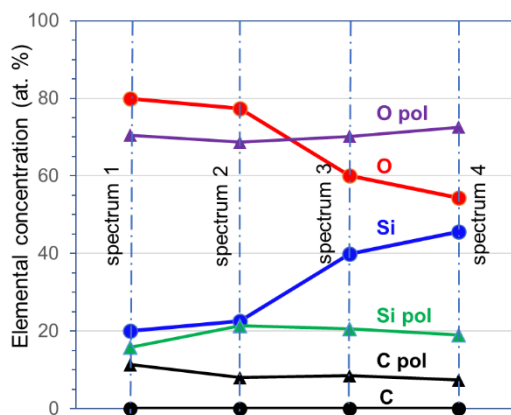

Fig. 7. Elemental concentrations of silicon, oxygen and carbon for both clean and carbon- polluted surfaces of ceramic samples

Similar change in the content of oxygen and silicon on the surface of ceramic was previously reported in [1]. The SEM-EDX spectrometry data on the depth distribution of the atomic composition of lithium titanate before and after irradiation with deuterium ions indicate that the trace impurities of oxygen, silicon, titanium were found on the surface of heat-treated improved Li_4SiO_4 pebbles. Changes in the content of oxygen and silicon and in alteration microstructure after irradiation and annealing were associated with the release of molecular O_2 and the formation of cracks and micropores.

An unexpected result was obtained on carbon-polluted areas of the sample. As can be seen from Fig. 10, the ratio of oxygen to silicon in undamaged and damaged parts of surface is fixed as 4.3:1, 3.0:1, 3.6:1 and 3.5:1 for Spectra 1–4 (see Fig. 6,a), respectively. This observation implies that the presence of carbon can contribute to the stabilization of the elemental composition of the ceramic surface under irradiation.

As was recently shown in [9], the crush load of Li_4SiO_4 pebbles declined sharply after deuterium gas exposure. This study didn't give a detailed analysis for the major factors responsible for the changes of mechanical strength and phase composition of ceramic breeder pebbles.

In the current study, low-energy deuterium ion irradiation and subsequent annealing of two-phase

ceramics leads to noticeable increase in surface destruction processes. The evolution of the surface morphology is accompanied by local enrichment in silicon at the sites of surface destruction. Thus, the redistribution of components in the presence of deuterium may be a possible reason for the change in mechanical properties. However, further investigations are needed to understand the mechanism of these phenomena.

Examination of deuterium thermal desorption from Li-based ceramics. Fig. 8 shows the TD spectra of deuterium from 90% Li_4SiO_4 + 10% Li_2SiO_3 and 90% Li_4SiO_4 + 10% Li_2TiO_3 samples. Deuterium evolution is observed in the temperature range of 290…650 K and is probably characterized by the superposition of at least two close TD peaks at around 400 and 500 K.
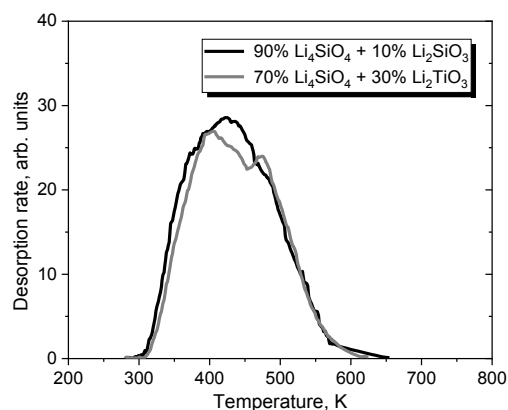

Fig. 8. Deuterium TD spectra from 90% Li_4SiO_4 + 10% Li_2SiO_3 and 90% Li_4SiO_4 + 10% Li_2TiO_3 ceramics irradiated with 25 keV deuterium ions to a dose of $1 \cdot 10^{21}$ D/m² at room temperature

A similar gas release stage with a maximum temperature of 410…430 K was registered in the TD spectra of deuterium from Li_2TiO_3 [10] and Li_4SiO_4 [11] as a low-temperature desorption stage in the structure of a more complex spectrum. The complication of the spectra in studies [10, 11] could be attributed to an order of magnitude higher irradiation dose. The TD spectra in Fig. 8 are very similar, so it is expected that the mechanism of thermal desorption in studied ceramics is associated with the same processes.

Computational evaluation of hydrogen isotopes desorption within the framework of the diffusion-trapping model [12] provides the ability to assess activation energies of de-trapping processes and to associate characteristics of experimental TD spectra with specific trapping sites in the material.

This was accomplished by numerically solving the equations for diffusion in a field of traps. According to McNabb and Foster formalism [13], upon irradiation, the concentration of hydrogen at point x at time t in a crystal containing defects, under the assumption that no more than one hydrogen atom is trapped by one defect, is described as:

$$\frac{\partial C(x,t)}{\partial t} = D(T)\frac{\partial^2 C(x,t)}{\partial x^2} - \sum_k \frac{\partial G_k(x,t)}{\partial t} + \varphi(x), \qquad (1)$$

$$\frac{\partial G_k(x,t)}{\partial t} = 4\pi R_k D(T) \left\{ C(x,t)[W_k(x,t) - G_k(x,t)] - G_k(x,t)zN_V \exp\left(-\frac{Q_k}{k_Б T}\right) \right\}, \qquad (2)$$

where C is the concentration of hydrogen in the solution; G_k is the concentration of hydrogen in traps of k-type; R_k is the radius of defect trap; m_k is the number of hydrogen atoms per trap; z is the number of solution sites per host atom; N_V is the atomic density of the host; W_k is trap concentration; $\varphi(x)$ is the distribution of the hydrogen introduction rate through the depth; Q_k is the binding energy of hydrogen atom with the trap; k_B is Boltzmann's constant; and $D(T) = D_0 \cdot \exp(E_m/k_B T)$ is the deuterium diffusivity.

Such parameters as the concentration of traps and the binding energy of the hydrogen atom with the trap are varied during calculations for the best agreement between the experimental and calculated curves.

Equations (1), (2) have been used previously [12, 14] to determine the trapping characteristics of ion-implanted hydrogen isotopes in metals and alloys. Nevertheless, although the potential relief for hydrogen transport in ceramic materials appears to be more complicated [15] compared to a metal matrix, the proposed approach can be used to estimate the deuterium diffusion and trapping parameters in the present case as well.

According to previous studies, the release rate of tritium is limited by the diffusion stage in many Li-based ceramics, such as Li_2O, $LiAlO_2$ and Li_2ZrO_3 [16]. Meanwhile, the tritium diffusion constants varied by more than six orders of magnitude [15]. In particular, the experimentally determined values of tritium activation energy for diffusion for Li_2TiO_3 vary from 0.63 to 1.5 eV [17–19] with a considerable uncertainty under different temperatures and in various samples.

The theoretically calculated constants also demonstrate a wide range of values which could be attributed to the strong anisotropy of the tritium diffusivity. For instance, the calculations of charged tritium diffusion over interstices in Li_2TiO_3 [20] using the density functional theory (DFT) indicate that the activation energy for diffusion in the xy plane is 0.33 eV, while for diffusion in the z direction the barrier is much higher and estimated as 1.00 eV.
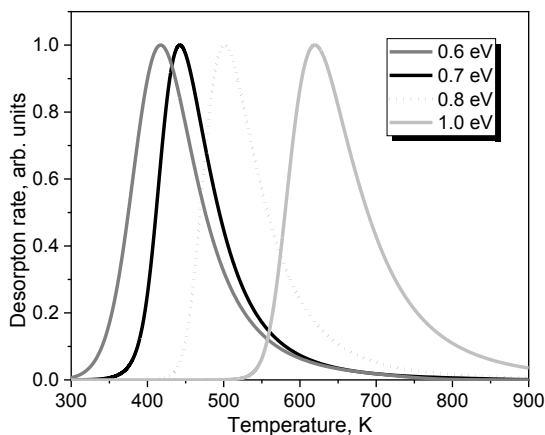
Fig. 9 shows the simulated deuterium TD spectra calculated under the assumption of its diffusion with different values of the diffusion activation energy.

It is seen from Fig. 9 that at activation energies for diffusion above 0.7 eV, the temperature range of deuterium release (controlled exclusively by the diffusion process) is characterized by higher temperatures than those observed in the experiment (see Fig. 8). Moreover, according to our calculations, at diffusion activation energies above 0.7 eV, the deuterium diffusivity in the bulk of the material is very limited at room temperature, that contradicts the experimental data [21] obtained by nuclear reactions analysis on the study of the spatial distribution of ion-implanted deuterium in lithium ceramics. The results [21] showed strong difference between the measured concentration profile and that calculated using SRIM, suggesting a high deuterium diffusivity even at room temperature.

Despite the fact that the diffusion of tritium in crystal grains is an important step in the process of tritium release, it is also affected by various radiation-induced defects (lithium vacancy, oxygen vacancy, and broken bond). The formation of oxygen vacancies caused by ionizing radiation [8] was mentioned in the previous section as a possible reason of darkening in the surface of pellets after irradiation. Meanwhile, the lithium vacancy is considered to be the initial defect caused by irradiation in lithium-based materials, since lithium atoms are constantly knocked out from their positions or consumed to form tritium under irradiation [22].

As shown above, the structure of the experimental TD spectra, consists of at least two closely spaced peaks. Therefore, we speculated that, in addition to the diffusion stage, the spectrum contains a peak associated with deuterium de-trapping from radiation-induced traps. The simulation result is shown in Fig. 10, where the experimental TD spectrum for 90% Li_4SiO_4 + 10% Li_2SiO_3 is shown for comparison.
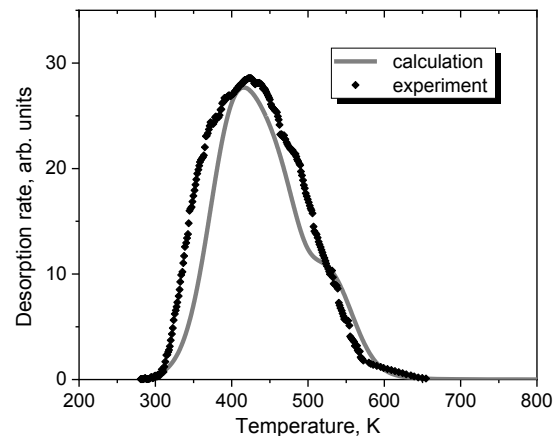
Fig. 9. Simulated (normalized per unit) deuterium TD spectra depending on the value of activation energy for diffusion

Fig. 10. Experimental points and calculated curve of deuterium thermal desorption from 90% Li₄SiO₄ + 10% Li₂SiO₃ ceramic after irradiation with deuterium ions

The simulated spectrum in Fig. 10 was obtained using the following parameters: the activation energy for

diffusion $E_m = 0.59$ eV, the deuterium binding energy with traps $Q = 0.40$ eV.

The de-trapping energy of deuterium bound to radiation induced trap represents the sum of the diffusion activation energy and the binding energy, $E_m + Q$, and reaches almost 1 eV. The results of recent DFT study [15] showed that tritium can diffuse through the interstices of a ceramic lattice with a barrier of 0.52 eV. When the tritium ion becomes bound to a defect of the lithium vacancy type, the energy required for the release of tritium from the vacancy increases to 1.06 eV.

Thus, the values obtained in the current study are in reasonable agreement with those predicted by the DFT calculations. Overall, the obtained results indicate that the desorption of deuterium is limited by the intragranular diffusion of deuterium and its trapping by radiation defects associated with Li-vacancy traps.

CONCLUSION

In the present study, deuterium interaction with Li_4SiO_4 ceramics with and without Li_2TiO_3 addition has been investigated by means of ion irradiation combined with thermal desorption spectroscopy. Scanning electron microscopy was used for surface structure characterization. The samples were treated with 12.5 keV/D^+ ions to a fluence of $1 \cdot 10^{21}$ m^{-2} at 290 K. Characteristics of experimental TD spectra were associated with specific trapping sites in the material on the base of computational evaluation of deuterium desorption within the framework of the diffusion-trapping model. The main results are summarized as follows.

Ion-implanted deuterium is rather easily desorbed in the temperature range of 290…650 K. Deuterium gas release from studied ceramics demonstrates similar trend indicating weak dependence of deuterium trapping behavior on phase composition.

The desorption of deuterium is limited predominantly by intragranular diffusion of deuterium and its trapping by radiation defects. The binding energy of deuterium with Li-vacancy associated traps was estimated as 0.4 eV.

Ion irradiation and subsequent thermal desorption annealing of two-phase ceramics leads to an increase in surface destruction processes: the crush and formation of cracks and porosity. The evolution of the surface morphology is accompanied by local enrichment in silicon at the sites of surface destruction.

REFERENCES

1. Artūrs Zariņš. *Formation, accumulation and annihilation of Radiation-induced defects and radiolysis products in advanced two-phase ceramic tritium breeder pebbles*: Doctoral thesis, 2018, 118 p.

2. Y. Poitevin et al. Tritium breeder blankets design and technologies in Europe: Development status of ITER Test Blanket Modules, test & qualification strategy and roadmap towards DEMO // *Fusion Engineering and Design*. 2010, v. 85, p. 2340-2347.

3. R. Knitter, P. Chaudhuri, Y.J. Feng, T. Hoshino, and I.-K. Yu. Recent developments of solid breeder fabrication // *Journal of Nuclear Materials*. 2013, v. 442, s420-s424.

4. L.M. Giancarli et al. Overview of the ITER TBM Program // *Fusion Engineering and Design*. 2012, v. 87, p. 395-402.

5. A. Vītiņš, G. Ķizāne, J. Tīliks, J. Tīliks, and E. Kolodinska. Tritium release from breeding blanket materials in high magnetic field // *Fusion Engineering and Design*. 2007, v. 82, p. 2341-2346.

6. G. Tolstolutskaya, V. Ruzhitskij, I. Kopanets, V. Voyevodin, A. Nikitin, S. Karpov, A. Makienko, T. Slyusarenko, Accelerating complex for study of helium and hydrogen behaviour in conditions of radiation defects generation // PAST. 2010, N 1, p. 135-140.

7. http://www.srim.org/

8. M.H.H. Kolb, J.M. Heuser, R. Rolli, H.-C. Schneider, R. Knitter, M. Zmitko. The HICU PIE results of EU ceramic breeder pebbles: General characterization // *Journal of Nuclear Materials*. 2020, v. 531, p. 152023.

9. Shouxi Gu, Qiang Qi, Yingchun Zhang, Baolong Ji, Haishan Zhou, Guang-Nan Luo. Mechanical strength stability of tritium breeding materials under high temperature deuterium conditions // *Ceramics International*. 2020, v. 46, issue 1, p. 1195-1202.

10. M. Oyaidzu, Y. Nishikawa, T. Suda, A. Yoshikawa, Y. Oya & K. Okuno. Study on Chemical Behavior of Energetic Deuterium Implanted into Li_2TiO_3 // *Fus. Sci. Tech.* 2007, v. 52, p. 1002-1006; http://dx.doi.org/10.13182/FST07-A1625

11. T. Luo. XPS analysis on chemical states of Li4SiO4 irradiated by 3 keV D2+ // *J. Nucl. Mater*. 2011, v. 408, p. 7-11; https://dx.doi.org/10.1016/j.jnucmat.2010.10.019

12. S. Karpov, V. Ruzhits'ky, I. Neklyudov, V. Bendikov, G. Tolstoluts'ka, Parameters of trapping and the thermoactivated output of the deuterium ion-implanted into the Cr18Ni10Ti steel // *Metallofizika i Noveishie Tekhnologii*. 2004, v. 26(12), p. 1661-1670 (in Russian)

13. F. Besenbacher, J. Bottiger, and S. M. Myers. Defect trapping of ion implanted deuterium in nickel // *Journal of Applied Physics*. 1982, v. 53, p. 3536-3541; doi:10.1063/1.331132

14. G. Tolstolutskaya, V. Ruzhytskyi, V. Voyevodin, I. Kopanets, S. Karpov, A. Nikitin. The role of radiation damage on retention and temperature intervals of helium and hydrogen detrapping in structural materials // *Journal of Nuclear Materials*. 2013, v. 442, S710-S714; doi:10.1016/j.jnucmat.2013.02.053.

15. K. Goswami and S. Murphy, Influence of Lithium Vacancy Defects on Tritium Diffusion in β-Li_2TiO_3 // *J. Phys. Chem. C*. 2020, v. 124, N 23, p. 12286-12294; https://dx.doi.org/10.1021/acs.jpcc.0c02551

16. C.E. Johnson. Tritium behavior in lithium ceramics // *J. Nucl. Mater.* 1999, v. 270, p. 212-220; https://dx.doi.org/10.1016/s0022-3115(98)00905-2

17. T. Kinjyo, M. Nishikawa, M. Enoeda, S. Fukada. Tritium diffusivity in crystal grain of Li_2TiO_3 and tritium release behavior under several purge gas conditions // *Fusion Eng. Des.* 2008, v. 83, p. 580-587; https://dx.doi.org//10.1016/j.fusengdes.2007.11.011

18. T. Tanifuji, D. Yamaki, S. Nasu, K. Noda. Tritium release behavior from neutron-irradiated Li_2TiO_3 single crystal // *J. Nucl. Mater.* 1998, v. 258−263, p. 543−548; https://dx.doi.org/10.1016/s0022-3115(98)00103-2

19. D. Zhu, T. Oda, Y. Shono, S. Tanaka. Release behavior of hydrogen isotopes thermally sorbed in Li_2TiO_3 single crystal // *J. Nucl. Mater.* 2013, v. 442, S437-S441; https://dx.doi.org/10.1016/j.jnucmat.2013.02.062

20. Y. Shi, J. Qi, Y. Han, T. Lu. Anisotropic diffusion of a charged tritium interstitial in Li_2TiO_3 from first-principles calculations // *Phys. Rev. Appl.* 2018, v. 10, p. 024021; https://dx.doi.org/10.1103/physrevapplied.10.024021

21. E. Carella et al. // *Journal of Nuclear Materials.* 2013, v. 438, p. 193-198.

22. Kun Li, Wen Yang, Wei-Hua Wang, and Yong-Tang Li. First Principles Study of Tritium Diffusion in Li_2TiO_3 Crystal with Lithium Vacancy // *Materials.* 2018, v. 11, p. 2383; doi:10.3390/ma11122383

ВПЛИВ ОПРОМІНЕННЯ ТА ПОВЕДІНКА ДЕЙТЕРІЯ У КЕРАМІЦІ НА ОСНОВІ ТРИТІЮ

Сергій Карпов, Валерій Ружицький, Галина Толстолуцька, Ганна Ростова

Досліджено поведінку імплантованого дейтерію у вдосконалених таблетках ортосилікату літію (Li_4SiO_4) з добавками метатитанату літію (Li_2TiO_3), а також у еталонних таблетках Li_4SiO_4 без добавок. Методом термодесорбційної (ТД) спектроскопії вивчено взаємодію дейтерію з радіаційними дефектами у матеріалах. Розрахункова оцінка десорбції дейтерію в межах моделі дифузійного захоплення дозволила пов'язати характеристики експериментальних ТД-спектрів з конкретними місцями захоплення в матеріалі. Встановлено, що десорбція дейтерію лімітується переважно внутрішньозеренною дифузією дейтерію та його захопленням радіаційними дефектами, пов'язаними з пастками типу вакансій Li. Виділення газоподібного дейтерію з обох керамік показує схожу тенденцію, що свідчить про слабку залежність захоплення дейтерію від фазового складу. Проаналізовано зміну морфології та елементного складу поверхні таблеток. SEM-дослідження показали, що іонне опромінення та подальший ТД-відпал двофазної кераміки призводить до посилення процесів руйнування поверхні.

ВЛИЯНИЕ ОБЛУЧЕНИЯ И ПОВЕДЕНИЕ ДЕЙТЕРИЯ В КЕРАМИКЕ НА ОСНОВЕ ТРИТИЯ

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Исследовано поведение имплантированного дейтерия в усовершенствованных таблетках ортосиликата лития (Li_4SiO_4) с добавками метатитаната лития (Li_2TiO_3), а также в эталонных таблетках Li_4SiO_4 без добавок. Методом термодесорбционной (ТД) спектроскопии изучено взаимодействие дейтерия с радиационными дефектами в материалах. Расчетная оценка десорбции дейтерия в рамках модели диффузионного захвата позволила связать характеристики экспериментальных ТД-спектров с конкретными местами захвата в материале. Установлено, что десорбция дейтерия лимитируется в основном внутризеренной диффузией дейтерия и его захватом радиационными дефектами, связанными с ловушками типа вакансий Li. Выделение газообразного дейтерия из обеих керамик демонстрирует схожую тенденцию, что указывает на слабую зависимость захвата дейтерия от фазового состава. Проанализировано изменение морфологии и элементного состава поверхности таблеток. SEM-исследования показали, что ионное облучение и последующий ТД-отжиг двухфазной керамики приводит к усилению процессов разрушения поверхности.