Л.Н. Гумилев атындағы Еуразия ұлттық университетінің ХАБАРШЫСЫ.
ISSN: 2616-6836. eISSN: 2663-1296

ФИЗИКА. АСТРОНОМИЯ СЕРИЯСЫ/ PHYSICS. ASTRONOMY SERIES / СЕРИЯ ФИЗИКА. АСТРОНОМИЯ

IRSTI 29.15.53
Scientific article

https://doi.org/10.32523/2616-6836-2025-150-1-162-185

Investigation of tin-lithium alloy behavior in high-temperature hydrogen isotope environments: sorption and desorption analysis

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Abstract. Nuclear fusion's effectiveness relies heavily on managing the intense power loads that strike the first wall, especially the divertor in plasma-physical devices. Due to their self-regulating liquid surfaces, liquid metals, such as lithium and tin, present a promising alternative to solid plasma-facing materials. A promising candidate is a tin-lithium alloy, which is expected to combine the beneficial properties of its constituent metals. The present study investigates tin-lithium alloy's sorption and desorption characteristics when exposed to hydrogen isotopes under high-thermal stress conditions. Specifically, experiments were conducted using a Sn73Li27 alloy with adsorption and thermally stimulated desorption (TDS) techniques employed to characterize its behavior. The sorption experiments were performed under high-temperature conditions from 450°C to 600°C and at different values of residual deuterium pressure in the device volume. The TDS experiments involved measuring the gas flows released from the tin-lithium alloy into the evacuated chamber under linear heating conditions. The temperature dependence of the effective deuterium solubility constant in the alloy was calculated, revealing the complexity of the interaction mechanisms influenced by experimental conditions. The results provide insights into the interaction dynamics between the tin-lithium alloy and hydrogen isotopes, underlining the material's performance and stability in high-temperature environments.

Keywords: tin-lithium alloy; deuterium; sorption; desorption; fusion reactor; plasma-facing components

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Received 6.02.2025. Revised 28.02.2025. Accepted 28.02.2025. Available online 25.03.2025

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1. Introduction

The quest for efficient nuclear fusion energy [1,2] hinges on managing the immense thermal and mechanical stresses experienced by plasma-facing components (PFC). In this context, understanding how different materials interact with hydrogen isotopes under high-temperature conditions is crucial [3,4].

Liquid metals [5-9], particularly lithium and tin, offer a promising alternative to traditional solid PFC [10] due to their self-regulating liquid surfaces [11]. Investigations with pure tin elements are currently underway [12] and show good prospects for its potential future use in fusion reactors. Tin's low hydrogenic retention and vapor pressure levels make it a very promising candidate, particularly when used in a tin-lithium (Sn-Li) alloy. This combination serves as a hybrid high-low Z material, leveraging the benefits of both tin and lithium: tin's low fuel retention and lithium's favorable plasma performance and compatibility. However, the hybrid nature of this alloy poses a challenge: preferential sputtering, which tends to favor lithium erosion, can alter the bulk properties of the materials. This erosion necessitates periodic replenishment of lithium to maintain the Li-Sn ratio on the exposed surfaces. These materials have the potential to enhance the performance and longevity of fusion reactors by mitigating the severe damage inflicted by high-energy plasma.

Among the various candidates, the Sn-Li alloy [13] stands out for its anticipated synergistic benefits, combining the advantageous properties of both constituent metals. Recent research indicates the potential of the Sn-Li alloy [14] as a new liquid metal for protecting in-vessel components of tokamak reactors from high-energy and high-density particle fluxes [14]. The main hope for this alloy is related to the low vapor pressure of Sn-Li, which raises the upper-temperature limit for using the alloy compared to pure lithium (from 450°C to 500°C) [15] in terms of contamination of the fusion plasma [16,17]. Despite significant advances in fusion research, there remains a notable gap in experimental data concerning the interaction of tin-lithium alloys with hydrogen isotopes.

At present, research on the use of Sn-Li alloys as PFC has been conducted on a limited scale worldwide, and there is limited data from such studies. For example, there are research findings on the interaction of hydrogen isotopes with liquid tin and tin-lithium alloy, which were carried out using both computational-theoretical methods [18] and helium plasma exposure in experimental setups [19]. Additionally, there are data from plasma experiments with Sn-Li alloy in the liquid phase conducted at the ISTTOK tokamak (Lisbon, Portugal) [20,21] and the TJ-II stellarator (Barcelona, Spain) [22,23]. At the FTU tokamak (Frascati, Italy) [24], a limiter was tested with a surface made of a carbon-fiber composite filled with liquid tin.

These foundational studies have paved the way for exploring the behavior of the Sn-Li alloy, which aims to leverage the strengths of both lithium and tin. It is expected that this alloy will exhibit favorable hydrogen isotope retention and desorption properties while maintaining stability under the high temperatures typical of fusion reactors.

Kazakhstaniresearchers also have substantial experience in conducting scientific experiments with Sn-Li alloys, which can be divided into three main areas:

1) studies on the interaction of Sn-Li alloys with stainless-steel and refractory metals [25-27];

2) testing of the Sn-Li alloy under radiation exposure, including plasma [28,29]and reactor irradiation [30];

3) experiments on the interaction of Sn-Li alloys with hydrogen isotopes under thermal loads, which is the focus of this work.

The purpose of the present study is to fill this gap by investigating the sorption and desorption characteristics of a $Sn_{73}Li_{27}$ alloy when exposed to hydrogen isotopes under high-thermal stress. Utilizing adsorption and TDS techniques, this research aims to provide a detailed analysis of the alloy's response to hydrogen isotopes. The findings are expected to offer valuable insights into the alloy's potential as a plasma-facing material, guiding future research and development efforts in the field of controlled thermonuclear fusion. By providing empirical data on the behavior of tin-lithium alloys, this work not only highlights their suitability for fusion applications, but also informs ongoing debates and research directions in the field.

2. Materials and Methods

To examine the behavior of a tin-lithium alloy under thermal conditions in a deuterium environment, an Sn-Li alloy was manufactured, with 73% tin and 27% lithium. This specific ratio was selected based on a review of existing data, which indicated that a composition of 27% lithium and 73% tin may be optimal for enhancing thermal and physical properties, lowering the saturated vapor pressure in the liquid phase, and minimizing lithium loss in the alloy during operation at temperatures above 500°C.

For the alloy fabrication, lithium of grade LE-1 (^6Li of natural enrichment with purity of 99.9%) and tin of grade OVCh (tin purity 99.999%) were used.The alloy fabrication method involves a step-by-step process of mixing tin and lithium in the temperature range of 250–550°C, which ensures the achievement of the required composition and the uniformity of the component distribution. By following the specified stoichiometric ratios and the verified technology, the $Sn_{73}Li_{27}$ alloy was successfully obtained.

During the alloy fabrication process, the proportions of components and temperature conditions were carefully controlled, which allowed achieving the required composition homogeneity and even distribution of elements. The characterization of the obtained alloy was conducted using modern analytical methods, presented in [31].

To investigate the behavior of the $Sn_{73}Li_{27}$ tin-lithium alloy in a high-temperature environment with hydrogen isotopes (deuterium), a portable experimental setup [31]was utilized.

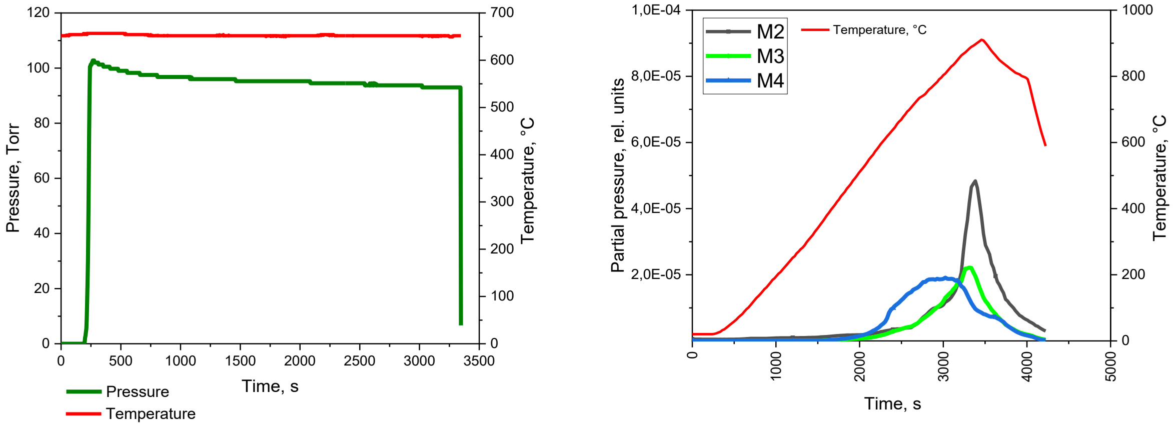
The behavior of the $Sn_{73}Li_{27}$ tin-lithium alloy in a high-temperature environment with hydrogen isotopes was examined using both the adsorption method and thermally stimulated desorption techniques. The adsorption method focuses on analyzing gas absorption by the sample under controlled pressure and temperature conditions. In this study, it was employed to investigate deuterium gas absorption by the liquid tin-lithium alloy, with an absolute pressure sensor continuously monitoring pressure changes in the chamber. The thermally stimulated desorption method measures the gas released from the tin-lithium alloy into a vacuum chamber during linear heating. Here, it was used to generate time-dependent profiles of hydrogen (deuterium) isotope release from the $Sn_{73}Li_{27}$ alloy as a function of the sample's temperature, using the RGA-100 quadrupole mass spectrometer. The experimental results are presented in the following section

3. Results

Sorption-desorption experiments were conducted with the sample of the $Sn_{73}Li_{27}$ alloy within a temperature range of 450°C to 650°C. The experiments were organized sequentially to evaluate the sorption and desorption processes of deuterium over the specified temperature range. This temperature interval was chosen to simulate the operational conditions of the alloy in a fusion reactor, excluding the critical loads associated with plasma disruptions and electromagnetic impulses (ELMs).

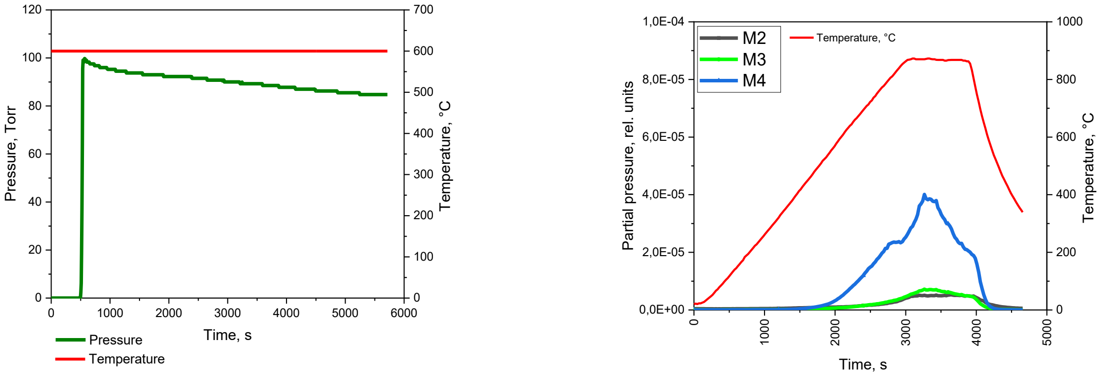
The experimental procedure comprised two stages: initial saturation of the sample with deuterium at a specified temperature, followed by a TDS analysis. The saturation temperatures varied from higher to lower values in 50°C increments.

The summarized data of the sorption and desorption experiments with the sample of the $Sn_{73}Li_{27}$ alloy are presented in Figure 1.



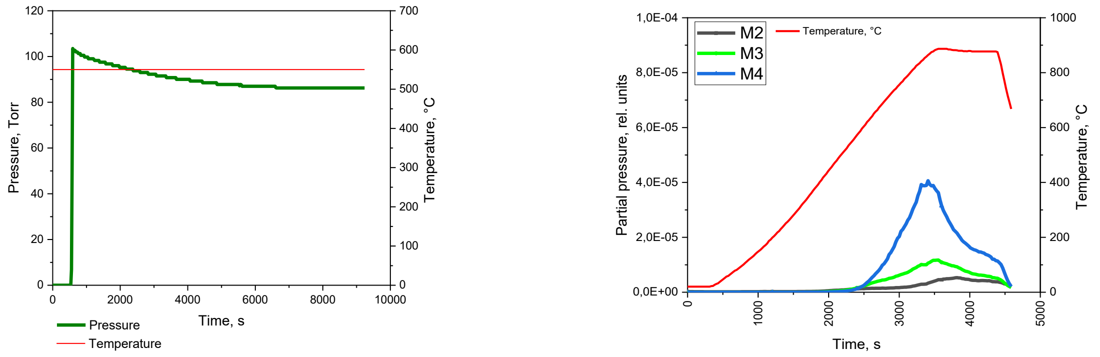
1 series of sorption

1 series of desorption



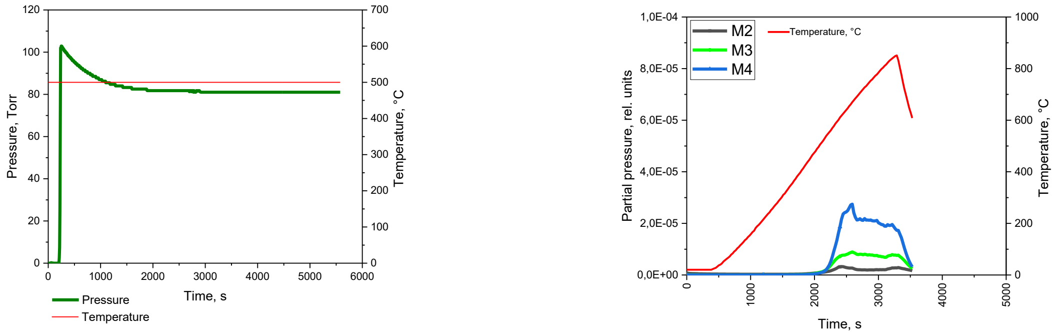
2 series of sorption

2 series of desorption



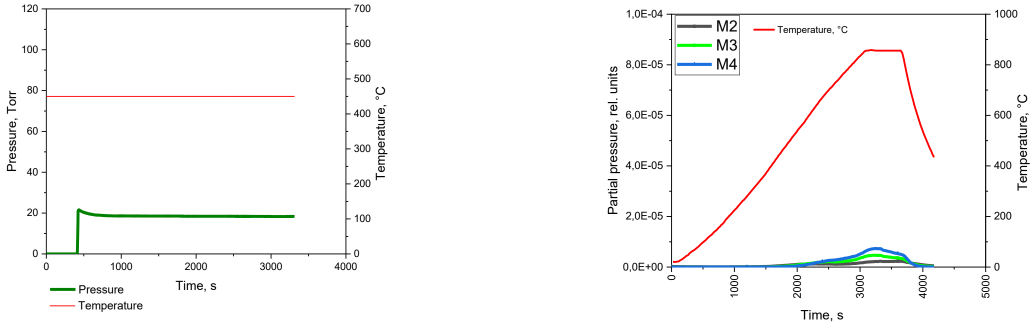
3 series of sorption

3 series of desorption



4 series of sorption

4 series of desorption



5 series of sorption

5 series of desorption

Figure 1. A series of experiments on deuterium sorption/desorption with a $Sn_{73}Li_{27}$ sample: (a) Sorption series; (b) Desorption series

Details of the experiments are outlined below:

First Series: Saturation was performed at 650°C for 3300 s. By the end of saturation, the pressure level in the ampoule continued to decrease significantly. During the TDS, a desorption peak was observed at approximately 845°C, with deuterium release beginning in the range of 300°C to 350°C.

Second Series: Saturation was conducted at 600 °C for 5200 s. The pressure level in the ampoule also continued to decrease notably by the end of the saturation period. The desorption peak was observed at around 875°C (after a hold time of approximately 500 s). Deuterium release commenced in the range of 350 °C.

Third Series: Saturation took place at 550°C for 8600 s. At the end of the saturation period, the pressure level in the ampoule continued to decrease slightly. The desorption peak appeared at the beginning of the maximum temperature plateau, approximately 890 °C. Deuterium release started in the range of 500°C to 550°C.

Fourth Series: Saturation was performed at 500°C for 5300 s. By the end of the saturation period, the pressure level in the ampoule had nearly stabilized, with saturation entering a quasi-equilibrium state after approximately 2000 s. The desorption profile exhibited a broad superposition of peaks, with gas release occurring between 600°C and 875°C. Deuterium release began around 500°C.

Fifth Series: Saturation was conducted at 450°C for 2900 s. The pressure level in the ampoule continued to decrease slightly by the end of saturation, and the saturation reached a quasi-equilibrium state after approximately 1200 s. The desorption peak was observed at the maximum temperature plateau, around 855°C (after a hold time of approximately 250 s). Deuterium release began in the range of 500°C.

During the sorption process at 650°C, the pressure in the ampoule decreased significantly, indicating that deuterium was primarily dissolved in a free state. Desorption was observed in the temperature range of 300-350°C, with the main peak recorded at 845°C.

At 600°C, during the sorption process, a steady decrease in pressure was observed, indicating a change in the ratio of free to bound deuterium concentration. Desorption began at 350°C, with the main peak recorded at 875°C.

At the end of the saturation stage, the rate of pressure decrease slowed down at 550°C, but full equilibrium was not reached. Desorption began in the temperature range of 500-550°C, with the main peak around 890°C.

During the saturation process at 500°C, the pressure stabilized after approximately 2000 seconds, indicating the achievement of equilibrium. Desorption began at 500°C, with the extended peak observed in the range of 600-875°C.

During the sorption process at 450°C, the pressure stabilized rapidly, indicating that the alloy absorbed a limited amount of deuterium. Desorption began at 500°C, with the main peak recorded at 855°C.

The temperature decrease mode was chosen considering the characteristics of the experimental equipment, which included an external heater and a thermocouple with some inertia. This approach allowed for more precise temperature control and prevented overheating of the sample.

4. Discussion

4.1. Analysis of Experiments

The comprehensive and complete analysis of the experiments must include detailed information such as:

The composition of impurities in deuterium during the saturation experiments.

The history of pumping, annealing, and preparation of the setup with the sample for experiments, including the condition between saturation/desorption cycles.

Even with such data, it is impossible to evaluate the complex factors affecting the experiments (e.g., the degree of sample sputtering during a series, surface contamination of the sample at different stages of the study, etc.).

Therefore, we will focus on a qualitative assessment of the results using possible mechanisms of interaction between deuterium and the tin-lithium alloy sample.

Let us assume that at a certain temperature, deuterium can exist in the alloy in two states: as a so-called "free atom" not trapped (e.g., lithium deuteride form) and as a "trapped deuterium atom" (located in a trap). A transition of deuterium atoms from one state to another is observed, with the ratio of equilibrium concentrations of deuterium atoms in both states being determined by a temperature-dependent constant. Let us further assume that there may be several "traps" for deuterium in the alloy with different parameters, but for convenience, we will consider one bound state of deuterium in the alloy:

$$\mathrm{D+trap} \rightleftarrows \mathrm{D\text{-}Trap}$$

There will be a shift to the left in the equilibrium expression above for deuterium in the alloy with increasing temperature. Then, at a qualitative level, the obtained series of experiments can be explained as follows:

At the highest saturation temperature of 650°C, deuterium dissolved in the alloy is primarily in a free state. Upon cooling and subsequent heating, a release peak resembling a peak caused by the migration (transfer) processes of these free atoms is observed.

At a lower saturation temperature of 600°C, deuterium is present in both free form and in traps. Therefore, the desorption peak is a superposition of the peak caused by the transfer of free deuterium atoms and the peak caused by the transfer of deuterium released from traps (by the activation mechanism during heating).

At an even lower saturation temperature, deuterium is mainly present in the traps. Accordingly, the release peak during heating is largely determined by the release of deuterium from the traps, has a symmetric shape, and is shifted to the right on the temperature scale (compared to the "diffusion peak"). This is also evidenced by the significant shift of the deuterium release onset towards higher temperatures.

The fourth cycle of experiments significantly differs from the first three, presumably due to the influence of surface non-metallic films on the sample. Firstly, changes in the saturation kinetics are observed: the rapid achievement of equilibrium saturation likely indicates the closure of the sample surface by such films, and a rapid decrease in the number of sorption centers is observed accordingly. During desorption, a sharp closure of the surface at 650°C is also observed, and the deuterium release trend acquires a monotonically decreasing, practically unanalyzable character.

The last cycle of experiments conducted at the lowest temperature (450°C) was carried out at significantly lower pressure and short saturation time, which presumably resulted in the sample's saturation being more than uneven and non-equilibrium compared to other experimental cycles. The rapid equilibrium pressure change during saturation also indicates surface saturation closure. At the same time, the type of deuterium desorption appears as a superposition of two deuterium release peaks from two different bound states, suggesting that deuterium is present in two types of traps at 450°C.

4.2. Numerical Modeling of Deuterium Release Processes

Within the proposed interaction mechanism, the temperature dependences of the effective solubility constant of deuterium in the tin-lithium alloy were initially calculated. The calculation was based on both sorption and desorption experiments. The integral amount of absorbed (released) deuterium for each saturation temperature was determined. The results of the calculations are presented in Figure 2.

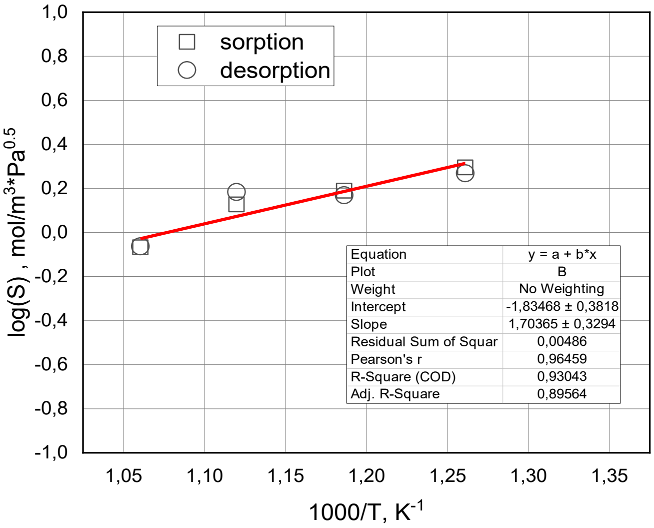


Figure 2. Temperature dependence of the effective solubility constant

As can be seen from Figure 4, there is a good agreement for the solubility values calculated from different experiments, with a significant deviation from the trend for the solubility value obtained at 450°C. This is because the sample did not reach equilibrium saturation (as mentioned earlier). The activation energy of solubility turned out to be positive, indicating that lithium deuteride formation occurs during saturation (such processes are usually exothermic).

For further analysis of the experimental data, a model was used that considers both diffusion and deuterium release from traps (i.e., bound states) during heating. Convective mixing-driven transport was not considered, and thus the diffusion coefficient obtained during modeling is effective (i.e., qualitatively determining the mobility of free deuterium atoms in the alloy).

Equations for the Diffusion Model in the Presence of Gas Sources in Traps:

$$\frac{\partial C}{\partial t} = D(t) \cdot \frac{\partial^2 C}{\partial x^2} + k_1 \cdot \mathrm{C}_{trap}.$$

$$\frac{\partial \mathrm{C}_{trap}}{\partial t} = -k_1 \cdot \mathrm{C}_{trap}$$

Where C is the deuterium concentration; C_{trap} is the concentration of deuterium sources; k_1 – constants of deuterium release from traps.

Moreover,

$$D(t) = D_0 \cdot exp\left(-\frac{E_D}{RT}\right),$$

$$k_1(t) = k_{10} \cdot ex\,p\left(-\frac{E_T}{RT}\right),$$

Where T – is the sample temperature *(K); E_D, E_T* – activation energies of diffusion and deuterium release from the trap, respectively *(kJ/mol); R* – universal gas constant; k_1 – constants of deuterium release from the bound state in the sample.

Initially, for the first desorption cycle experiments, diffusion parameters were obtained based on Equation (1), assuming no deuterium sources C_{trap}=0.

Then, the classical diffusion equation for the initial condition when the diffusant concentration in the metal $C_0(x, t=0)$ is known was solved. (This value was obtained based on normalization relative to the total amount of deuterium in the sample).

As a model approximation, the following boundary conditions were applied that satisfy the conditions of continuous diffusant pumping:

(x=0, t)=0 (the deuterium flow at the alloy-stainless steel boundary is 0)

C(x=l, t)=0, wherel – sample thickness *(desorption from the alloy surface into a vacuum occurs very quickly).*

Modeling was carried out using the finite element method with licensed the COMSOL Multiphysics program. As initial data in the model, the experimental temperature dependence on time was also used (it was introduced as a segmented curve where the corresponding sample temperature was chosen for each time measurement range). An example of the distribution of free deuterium atoms in the sample obtained during modeling is presented in Figure 3. The curve closest to the experimental data for deuterium release from the sample is shown in Figure 4. It was obtained for the temperature dependence of the diffusion coefficient:

$$D = 15 \cdot 10^{-3}\ (m^2/s) \cdot exp(-110\ (kJ/mol)/(R \cdot T)).$$

It should be noted that satisfactory agreement between the experimental and model curves was also achieved when varying the values of the pre-exponential factor D_0 in the range of $(2 \cdot 10^{-11}$ - $10^{-9})$ m^2/s and diffusion activation energies in the range of (100 - 120) kJ/mol.

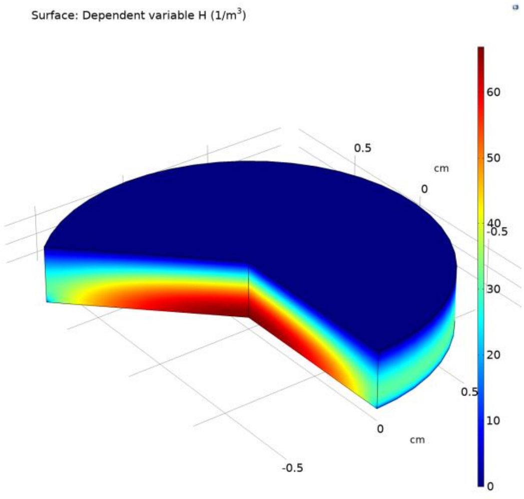


Figure 3. Distribution of free deuterium atoms in the sample at 4191 seconds of the experiment

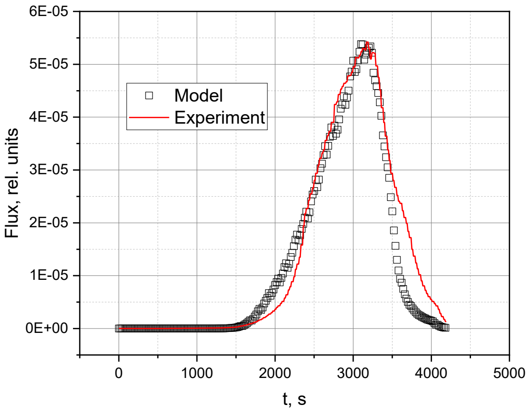


Figure 4. Simulation result of deuterium release from the sample during the first desorption cycle

The modeling of deuterium release for subsequent experiment cycles was conducted using the calculated deuterium diffusion coefficient and allowed for determining the rate constant of deuterium release from traps.

$$K = 150\ (1/s)\cdot\exp(-90\ (kJ/mol)/(R\cdot T)).$$

This constant was used to describe the change in deuterium concentration in the traps (see Figure 5) and accurately represent the experimental dependencies observed in desorption experiments (see Figure 6).

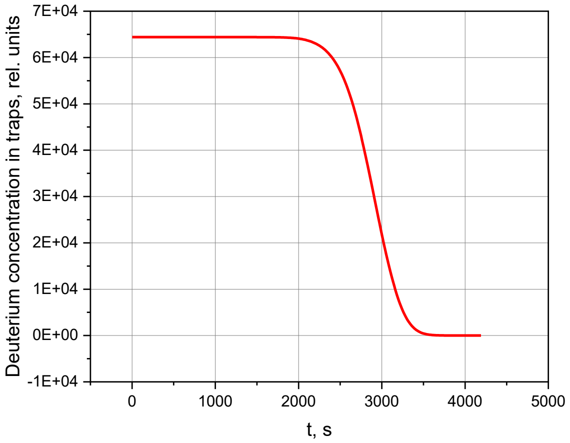


Figure 5. Time dependence of deuterium concentration in traps

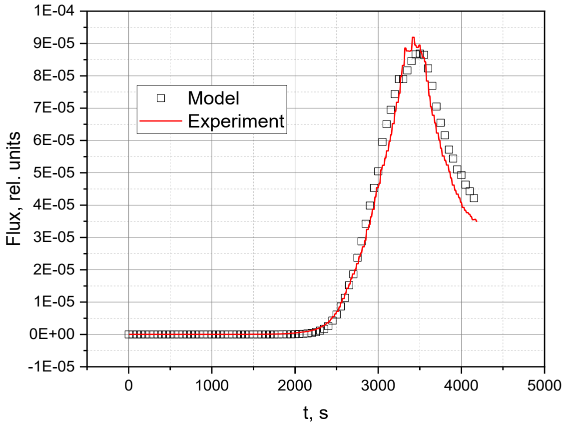


Figure 6. Simulation result of deuterium release from the sample during the third desorption cycle

As seen from the calculations, the obtained diffusion coefficient values are quite low, and the transport of deuterium due to diffusion is significantly less (by more than 5 orders of magnitude) than the transport caused by convective mixing during the heating of the liquid alloy (here, the average transfer speed through the sample volume can exceed 1 mm/s). Thus, as expected, the calculated values represent effective constants and can be used for comparative characterizations of the process kinetics, model selection, and mechanism evaluation, etc.

4.3. Proposed Mechanism

At this stage of analysis, we developed another, more plausible mechanism for the deuterium release process from the alloy in the experiments conducted. The mechanism is as follows (see Figure 7):

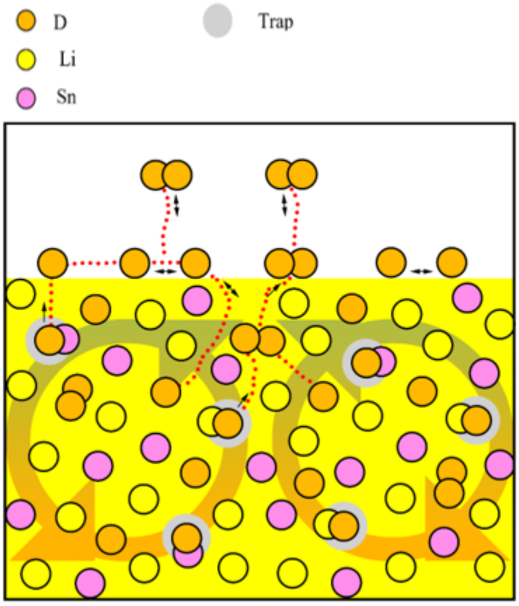


Figure 7. Mechanism of deuterium release from the sample in the presence of free deuterium atoms and deuterium release sources from traps, with active convective mixing and deuterium atom association into molecules throughout the sample volume

After conducting sorption experiments, wehave a lithium-tinalloy with a certai-ninitial concentration of deuteriumatoms (CD) for the desorption experiments. Deuteriume-xistsin two forms: "free" (CF) and "bound" (CT), with the total concentration being CD = CF + CT. During desorption, free deuterium a tomsaretrappedat a much slowerrate comparedtotheir-release from traps. The high convection rateinthemoltentin-lithiumalloyensures a uniform-deuterium concentration through out the sample. Inthis sample, D2 molecules can form from the association of freed euteriumatoms, and their concentration, which is proportion al to the deuterium flux from the sample, rapidly reaches the surface and release with out further activation. The refore, the deuterium flux from the sample is gover ned by the associationrate of free deuteriumatoms, which follows as $Ka=Ka_0 \cdot exp(-E_a/RT)$ an Arrhenius-type rateconstant.

Based on the above, we can establish the following differential equations:

For the deuterium flux from the sample: $J_{D2}(t)=Ka^* C_F^2$ (Polanyi-Wigner law)

For the change in the concentration of free deuterium atoms and trapped deuterium atoms:

$$\frac{dC_F}{dt} = -Ka * C_F^2 + k_1 \cdot \mathrm{C}_{trap}$$

$$\frac{\partial \mathrm{C}_{trap}}{\partial t} = -k_1 \cdot \mathrm{C}_{trap}$$

Initial conditions are defined base don the experimental curve aftercal culating the total amount of releas eddeuterium. These equations can be effectively solvedusing a recursive approach to compute the concentration of free deuteriumatom sin the sample. For example, in the case with outtraps (first experimental cycle), with a time interval of Δt, the concentration of free deuteriumatoms can be calculatedas:

$$\mathrm{C}_{Fi} = \left(\frac{1}{C_{F0}} + \Delta t * \sum_{k=0}^{i-1}\left(Ka0 * e^{-\frac{E_a}{R*T_k}}\right)\right)^{-1}$$

Modeling has successfully described the experimental curves and determined the parameters for the rate constant of the association of free deuterium atoms in the conducted experiments. The values for Ka0 are in the range of (5000; 33000) m4/(mol·s), and Ea ranges from (105; 133) kJ/mol. Recent studies have provided in-depth evaluations of tin-lithium alloys, shedding light on their interactions with hydrogen isotopes and implications for fusion reactors.

E. Oyarzabal et al. [32] conducted laboratory experiments to examine the uptake and release of hydrogen isotopes in liquid lithium. Their study, performed at temperatures of 200°C and 400°C, identified two distinct absorption phases. In the initial phase, hydrogen quickly dissolves into lithium to form a solution, reaching a saturation point at which a secondary phase begins, characterized by slower absorption and the likely formation of polycrystalline lithium hydride (LiH). At 400°C, the absorbed hydrogen percentage reached 1% H/Li, aligning well with existing literature on the saturation solubility in lithium. At 200°C, the solubility was higher than previously reported data, suggesting temperature-dependent variations in hydrogen uptake. The study revealed preferential absorption of deuterium (D_2) over hydrogen (H_2) in clean lithium. Interestingly, pre-deuterated samples showed a faster absorption rate for H2, indicating that previous deuterium absorption alters the surface properties of lithium, possibly through modifications in the LiD layer. TDS results exhibited desorption peaks at approximately 485°C, significantly lower than the decomposition temperature of LiH. This suggests that the desorption process is not solely reliant on LiH decomposition but may involve hydrogen dissolved in lithium or the breakdown of a superficial LiH layer. Dynamic experiments with samples pre-implanted with H_2 and D_2 showed no significant isotope exchange at temperatures up to 500°C, indicating a high stability of the absorbed isotopes in molten lithium within this temperature range.

M.J. Baldwin and colleagues [33] took a closer look at the surface chemistry involved in the recombination of deuterium atoms on molten Li-LiD alloys. They measured the recombination rate constant across a temperature range of 573-873 K using thermal desorption techniques. The recombination rate followed an Arrhenius-type temperature dependency, which is characteristic of surface-limited processes. However, the experimental rates were found to be significantly lower than theoretical predictions for a clean lithium surface. This discrepancy is attributed to surface contamination, particularly by oxides, which reduce the availability of surface sites for recombination. The study highlighted that even minute amounts of surface contamination could drastically alter the recombination dynamics. Surface oxides, such as Li_2O, appear to create an energy barrier for chemisorption, thus reducing the overall recombination rate of deuterium. The data aligned reasonably well with the hydrogen release model of Pick and Sonnenberg when accounting for surface impurities, demonstrating that surface cleanliness is crucial for controlling hydrogen isotope behavior in liquid lithium systems.

Richard Schumacher and Alarich Weiss [34] extended the understanding of hydrogen interactions by investigating the solubility of hydrogen in liquid lithium alloys, specifically Li-In, Li-Pb, and Li-Sn. Their research explored the behavior of these alloys at various hydrogen pressures and temperatures, extending up to 1220 K. Hydrogen solubility in the alloys followed Sieverts' law at low concentrations, indicating that the dissolved hydrogen existed as atoms in solution. However, strong deviations were observed in certain alloys, indicating potential alloy decomposition and the formation of hydrides at higher hydrogen concentrations. The study found that the addition of elements like indium, lead, and tin altered the hydrogen absorption behavior of lithium, reducing its overall hydrogen solubility. This could be due to changes in the electronic structure and atomic arrangement within the alloy, affecting how hydrogen atoms interact with the metal matrix.

Beatriz G. del Rio and colleagues [35] used first-principles molecular dynamics simulations to explore the behavior of deuterium in liquid Li-Sn alloys. This study is crucial for understanding the impact of deuterium addition on the alloy properties and its implications for fusion reactor applications. The simulations showed that when deuterium concentration (β\betaβ) in the alloy exceeded 22.5, D_2 gas bubbles formed. These bubbles caused lithium atoms to segregate towards them, reducing the overall retention of deuterium within the alloy matrix. Thermodynamic analyses indicated that for alloys containing less than 82% lithium, most of the added deuterium would form D_2 molecules rather than bonding with the alloy. This suggests a tendency towards the formation of molecular deuterium gas rather than stable hydrides, making the alloy less prone to isotope retention. Deuterium addition significantly increased the viscosity of the alloy, a behavior like that observed in pure liquid lithium. This viscosity increase is attributed to interactions between lithium and deuterium, affecting the alloy's diffusion properties and potentially influencing its performance in a plasma environment. The tendency of Li-Sn alloys to form D_2 gas and limit deuterium retention is promising for their application as PFCs, offering a pathway to reduce tritium retention in fusion reactors. This characteristic could help maintain plasma purity and enhance reactor safety by minimizing the accumulation of tritium within the PFCs. Understanding the changes in diffusivity and viscosity with deuterium addition is vital for predicting the alloy's behavior under reactor conditions, ensuring that the material properties remain within acceptable limits during operation.

The collective insights from these studies highlight the nuanced behavior of hydrogen isotopes in liquid lithium and its alloys. The preferential absorption and complex desorption kinetics of hydrogen and deuterium in liquid lithium indicate a strong interaction with the metal, influenced by temperature, surface conditions, and prior isotope exposure. Alloying lithium with metals like tin reduces hydrogen solubility and promotes the formation of molecular hydrogen, mitigating the risk of isotope retention.

In the context of fusion reactors:

Pure Liquid Lithium: Offers high hydrogen isotope absorption but also poses challenges in managing tritium inventory due to hydride formation and strong isotope retention.

Li-Sn Alloys: Show promise in reducing hydrogen isotope retention by facilitating the formation of molecular hydrogen rather than stable hydrides. These alloys may serve as more effective plasma-facing materials with reduced tritium retention risks.

Building on these comprehensive studies, our investigation focuses on the $Sn_{73}Li_{27}$ alloy, evaluating its sorption and desorption behavior in high-temperature hydrogen isotope environments. By doing so, we aim to contribute to the development of PFCs that combine the beneficial properties of both tin and lithium, offering reduced retention, thermal stability, and effective recycling in fusion applications.

5. Conclusion

The present investigation provides a detailed analysis of the sorption and desorption behavior of the $Sn_{73}Li_{27}$ alloy in high-temperature hydrogen isotope environments, focusing on its interactions with deuterium. The study employed sorption and thermally stimulated desorption (TDS) techniques over a temperature range of 450°C to 650°C to simulate operational conditions of plasma-facing materials in fusion reactors.

The results demonstrated that deuterium is present in both free and trapped states within the alloy, with distinct temperature-dependent release behaviors. At higher saturation temperatures (e.g., 650°C), deuterium is predominantly in its free atomic state, leading to a higher and earlier release during desorption. As the saturation temperature de-creased, the proportion of trapped deuterium increased, resulting in delayed and more complex desorption peaks due to the activation of release mechanisms from bound states.

The numerical modeling of the desorption process, considering both diffusion and release from traps, revealed effective diffusion coefficients and rate constants for deuterium release. The effective diffusion coefficient for deuterium was found to be $D = 15\cdot10^{-3}$ $(m^2/s)\cdot\exp(-110$ $kJ/mol/(R\cdot T))$, with a good match between experimental and simulated data. The analysis suggests that convective mixing plays a significant role in enhancing deuterium transport within the liquid alloy, complementing the diffusion-driven release.

These findings are critical for understanding the thermal and hydrogen isotope retention properties of Sn-Li alloys, particularly in fusion reactor environments, where plasma-facing materials are subjected to extreme thermal stresses. The $Sn_{73}Li_{27}$ alloy exhibited promising characteristics for use in next-generation fusion reactors, offering a balance of low deuterium retention and efficient release at elevated temperatures. Future investigations should focus on further refining alloy compositions and optimizing operational parameters to enhance the alloy's performance in fusion reactors.

In conclusion, this study advances our understanding of Sn-Li alloy behavior in hydrogen isotope environments, providing essential data for the development of liquid metal-based plasma-facing components in fusion energy systems.

Authors' contributions

I.E. Kenzhina – conducting experiments, working out the modes of obtaining alloys, characterizing samples.

T.V. Kulsartov – conducting experiments, interpreting results of experiments, general analysis, determining the kinetics of material degradation.

Ye.V. Chikhray – conducting experiments, interpreting the obtained data, analyzing the state of the problem, processing the obtained results.

A.L. Kozlovskiy – conducting experiments, general analysis, determining the kinetics of material degradation

Zh.A. Zaurbekova – general analysis, determining the kinetics of material degradation.

A.B. Yelishenkov – conducting experiments, general analysis, determining the kinetics of material degradation.

S.K. Askerbekov – conducting experiments, general analysis, determining the kinetics of material degradation.

A.U. Tolenova – conducting experiments, general analysis, determining the kinetics of material degradation.

Acknowledgment

There search was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan with Program number BR21882237.

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Жоғары температурада сутек изотопы ортасындағы қалайы-литий қорытпасының әрекетін зерттеу: сорбция және десорбцияанализі

Аңдатпа. Басқарылатын термоядролық синтездің тиімділігі едәуір дәрежеде бірінші қабырғаға, әсіресе плазмофизикалық қондырғылардағы диверторға әсер ететін қарқынды энергетикалық жүктемелерді басқаруға байланысты. Өзін-өзі реттейтін сұйық бетінің арқасында литий және қалайы сияқты сұйық металдар плазмаға қаратылған қатты материалдарға перспективалы балама болып табылады. Перспективалы кандидаттардың бірі оның құрамына кіретін компоненттердің пайдалы қасиеттерін біріктіретін қалайы-литий қорытпасы болып табылады. Осы зерттеуде жоғары температура жағдайында сутегі изотоптарының әсер етуі кезінде қалайы-литий қорытпасының сорбциясы мен десорбциясының сипаттамалары зерделенеді. Атап айтқанда, сутегі изотопы ортасындағы $Sn_{73}Li_{27}$ қорытпасының әрекетін зерттеу үшін адсорбция және температуралық-индукцияланған десорбция (ТДС) әдістерін қолдану арқылы эксперименттер жүргізілді. Сорбция бойынша эксперименттер 450°С-ден 600°С-ге дейінгі жоғары температуралық жағдайларда және құрылғы көлемінде дейтерийдің қалдық қысымының әртүрлі мәндерінде орындалды. ТДС бойынша эксперименттер қалайы-литий қорытпасынан сызықтық қыздыру жағдайында камерада бөлінетін газ ағындарын өлшеуді қамтыды. Қорытпадағы дейтерийдің тиімді ерігіштік констан-тасының температураға тәуелділігі есептелді, бұл тәжірибе жағдайларына байланысты өзара әрекеттесу механизмдерінің күрделілігін орнатуға мүмкіндік берді. Нәтижелер қалайы-литий қорытпасы мен сутегі изотоптары арасындағы өзара әрекеттесу динамикасы туралы түсінік берді және материалдың жоғары температуралы ортадағы өнімділігі мен тұрақтылығын көрсетті.

Түйін сөздер: Қалайы-литий қорытпасы; дейтерий; сорбция; десорбция; синтездік реактор; плазмаға түрлендірілген компоненттер

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Исследование поведения оловянно-литиевого сплава в условиях высокотемпературной среды с изотопами водорода: анализ сорбции и десорбции

Аннотация. Эффективность управляемого термоядерного синтеза в значительной степени зависит от управления интенсивными энергетическими нагрузками, воздей-ствующими на первую стенку, особенно на дивертор в плазмофизических установках. Благодаря своей саморегулирующейся жидкой поверхности жидкие металлы, такие как литий и олово, представляют собой многообещающую альтернативу твердым материалам, обращенным к плазме. Одним из перспективных кандидатов является оловянно-литиевый сплав, который, как ожидается, будет сочетать в себе полезные свойства компонентов, входящих в его состав. В настоящем исследовании изучаются характеристики сорбции и десорбции оловянно-литиевого сплава при воздействии на него изотопов водорода в условиях высоких тепловых нагрузок. В частности, были проведены эксперименты с использованием сплава $Sn_{73}Li_{27}$ с применением методов адсорбции и температурно-индуцированной десорбции (ТДС) для изучения его поведения. Эксперименты по сорбции выполнялись в высокотемпературных условиях от 450°C до 600°C и при различных значениях остаточного давления дейтерия в объеме устройства. Эксперименты по ТДС включали измерение газовых потоков, выделяющихся из оловянно-литиевого сплава в откачанную камеру в условиях линейного нагрева. Была рассчитана температурная зависимость эффективной константы растворимости дейтерия в сплаве, что позволило установить сложность механизмов взаимодействия, зависящих от условий эксперимента. Полученные результаты дают представление о динамике взаимодействия между оловянно-литиевым сплавом и изотопами водорода, а также подчеркивают эффективность и устойчивость материала в высокотемпературных средах.

Ключевые слова: Оловянно-литиевый сплав; дейтерий; сорбция; десорбция; термо-ядерный реактор;плазма-обращенные компоненты

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