The main outputs of this task: elucidation of the effect of helium on deuterium retention in the tungsten wall, analysis of tritium transfer in a Pb–Li liquid breeder, experimental and computational studies on the effects of radiation damage on hydrogen trapping, and modeling of the tritium components and the environment. The common task in the US-J TITAN (Tritium, Irradiation and Thermo-mechanical effects cross-linked considerations in the blanket system modeling on the basis of the material research in each task. In this paper, we review the main outputs of this task: elucidation of the effect of helium on deuterium retention in the tungsten wall, analysis of tritium transfer in a Pb–Li liquid breeder, experimental and computational studies on the effects of radiation damage on hydrogen trapping, and modeling of the tritium barrier in a double-tube heat exchanger.

The blanket of fusion reactors is a multifunctional system that breeds tritium, harvests heat from the burning plasma, and protects the other components and the environment. The common task in the US-J TITAN (Tritium, Irradiation and Thermofluid for America and Nippon) project identifies cross-linked considerations in the blanket system modeling on the basis of the material research in each task. In this paper, we review the main outputs of this task: elucidation of the effect of helium on deuterium retention in the tungsten wall, analysis of tritium transfer in a Pb–Li liquid breeder, experimental and computational studies on the effects of radiation damage on hydrogen trapping, and modeling of the tritium barrier in a double-tube heat exchanger.

The common task creates a self-consistent model by integrating the separate systems of tritium, heat and thermofluid. At the same time, via feedback of important considerations to each task, the validity of our experimental results is assessed in the interfaces between research goals in each task, in order to promote the development of an integrated system modeling methodology.

In this review, we focus on material research in Tasks 1–1; 1–2; and 2–1, 2–2, 2–3 (Table 1). The common critical issue in MFE and IFE in terms of fuel self-sufficiency and environmental safety is tritium mass transfer through the heat exchangers. Therefore, a typical heat-exchanger system, designed to identify appropriate boundary conditions for material researches, is also discussed.

2. Helium (He) Effect on Deuterium (D) Retention in Tungsten

A critical consideration in fusion reactor design is the tritium recycling properties of the first wall of the fusion blanket. The effects of helium on the retention of hydrogen isotopes in tungsten have been extensively reported, but remain contentious. While some studies have reported that retention is enhanced by helium implantation, others have reported the opposite. These discrepancies may be attributed to differences in experimental conditions. The results of several previous studies are shown in Figs. 1 and 2, and numerical data are summarized in Table 2. Results for D retention by energetic ion implantation (open symbols in Figs. 1 and 2) are consistent across studies, with D retention saturating at around $3 \times 10^{20} \text{D}^+ \text{m}^{-2}$, even for He$^+$ fluence as large as $10^{22} \text{He}^+ \text{m}^{-2}$. Given that D retention in the absence of He$^+$ is $\sim 1 \times 10^{20} \text{D}^+ \text{m}^{-2}$, we observe that He$^+$

1. Introduction

Fusion systems of magnetically confined fusion energy (MFE) or inertial fusion energy (IFE) are enclosed within a blanket system that breeds tritium, harvests heat from the burning plasma, and protects the other components and the environment. Thus, the blanket system must be optimized not as a single function but as an integrated multifunctional system incorporating the in-vessel components and the environment. The authors have worked on common-task integrated system modeling under the framework of the Japan–US Joint Research Project TITAN (Tritium, Irradiation and Thermofluid for America and Nippon),¹ In this project, cross linking between tasks was regarded as a multiphysics modeling problem for the optimal design of a fusion blanket, as shown in Table 1.

For each task, tritium transfer, thermofluid mechanisms, and irradiation synergy are investigated under typical reactor conditions: plasma-wall interactions with heat and particles, nuclear and chemical reactions in the blanket material, MHD effects in high magnetic field, heat and mass transfer in each subsystem of the heat exchanger and tritium separation system, and the intermittent effects of intense transient heat loads. The time constants for tritium and material behaviors are separated and evaluated from these tasks, and the characteristics of the system components are verified by an experiment.

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Keywords: blanket, tungsten, tritium, irradiation
Table 1  Task structure and research items in the TITAN project. The common task integrates system modeling by connecting each task under the many boundary conditions existing in the fusion blankets.

<table>
<thead>
<tr>
<th>Task</th>
<th>Subtask</th>
<th>Facilities</th>
<th>Research items</th>
</tr>
</thead>
<tbody>
<tr>
<td>Task 1 Tritium and mass transfer blanket</td>
<td>1–1 Tritium and mass transfer in first wall</td>
<td>STAR/TPF/PISCES</td>
<td>Tritium retention and transfer behavior and mass transfer in first wall</td>
</tr>
<tr>
<td></td>
<td>1–2 Tritium behavior in blanket systems</td>
<td>STAR</td>
<td>Tritium behavior through elementary systems of liquid blankets</td>
</tr>
<tr>
<td></td>
<td>1–3 Flow control and thermofluid modeling</td>
<td>MTOR</td>
<td>Flow control and thermofluid modeling under strong magnetic fields</td>
</tr>
<tr>
<td>Task 2 Irradiation synergism</td>
<td>2–1 Irradiation-tritium synergism</td>
<td>HFIR STAR</td>
<td>Irradiation effects on tritium retention and transfer behavior in first wall and structural materials</td>
</tr>
<tr>
<td></td>
<td>2–2 Joining and coating integrity</td>
<td>HFIR</td>
<td>Synergy effects of simultaneous production of tritium and helium on joining and coating integrity</td>
</tr>
<tr>
<td></td>
<td>2–3 Dynamic deformation</td>
<td>HFIR</td>
<td>Effects of irradiation and simultaneous production of tritium and helium on dynamic deformation of structural materials</td>
</tr>
<tr>
<td>Common Task System integration modeling</td>
<td></td>
<td>MFE/IFE system integration modeling</td>
<td>Integration modeling for mass transfer and thermofluid through first wall, blanket and recovery systems of MFE/IFE</td>
</tr>
</tbody>
</table>

Table 2  Summary of conditions of various He⁺ and D⁺ implantation and plasma exposure experiments.

<p>| Ion energy: | Ion flux: | Ion fluence: | Implantation temperature |</p>
<table>
<thead>
<tr>
<th>He</th>
<th>D</th>
<th>( \phi_{D^+}/m^2 \cdot s^{-1} )</th>
<th>( \phi_{D^+}/m^2 \cdot s^{-1} )</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>○ Y. Oya</td>
<td>3.0 keV</td>
<td>( (2.0–1.8) \times 10^{18} )</td>
<td>( (0.2–1.8) \times 10^{22} )</td>
<td>R.T.</td>
</tr>
<tr>
<td></td>
<td>3.0 keV</td>
<td>( 1.0 \times 10^{18} )</td>
<td>( 1.0 \times 10^{22} )</td>
<td>R.T.</td>
</tr>
<tr>
<td>◇ S. Nagata</td>
<td>10 keV</td>
<td>—</td>
<td>( 4.2 \times 10^{16}–6.0 \times 10^{16} )</td>
<td>R.T.</td>
</tr>
<tr>
<td></td>
<td>1 keV</td>
<td>—</td>
<td>( 3.0 \times 10^{19} )</td>
<td>R.T.</td>
</tr>
<tr>
<td>☆ H. Iwakiri</td>
<td>8 keV</td>
<td>—</td>
<td>( (0.1–2.0) \times 10^{18} )</td>
<td>R.T.</td>
</tr>
<tr>
<td></td>
<td>4 keV</td>
<td>—</td>
<td>( 10^{17}–10^{19} )</td>
<td>R.T.</td>
</tr>
<tr>
<td>△ Y. Sakoi</td>
<td>3 keV</td>
<td>( 5.0 \times 10^{10} )</td>
<td>( 1.0 \times 10^{21} )</td>
<td>R.T.</td>
</tr>
<tr>
<td></td>
<td>3 keV</td>
<td>( 1.0 \times 10^{10} )</td>
<td>( 1.0 \times 10^{21} )</td>
<td>R.T.</td>
</tr>
<tr>
<td>◆ B. I. Khripunov</td>
<td>4 MeV</td>
<td>—</td>
<td>( (1.0–3.0) \times 10^{22} )</td>
<td>373 K</td>
</tr>
<tr>
<td></td>
<td>250 eV</td>
<td>—</td>
<td>( (0.27–1.3) \times 10^{26} )</td>
<td>373 K</td>
</tr>
<tr>
<td>☆ H. T. Lee</td>
<td>500 eV</td>
<td>( 10^{14–10^{19}} )</td>
<td>( 10^{21–10^{23}} )</td>
<td>300 K</td>
</tr>
<tr>
<td></td>
<td>500 eV</td>
<td>( 1.0 \times 10^{10} )</td>
<td>( 0.5–2.0 \times 10^{21} )</td>
<td>300 K</td>
</tr>
<tr>
<td>▲ M. Miyamoto</td>
<td>120 eV</td>
<td>( 5.0 \times 10^{10} )</td>
<td>( 2.5 \times 10^{24} )</td>
<td>573 K</td>
</tr>
<tr>
<td></td>
<td>120 eV</td>
<td>( 1.0 \times 10^{10} )</td>
<td>( 5.0 \times 10^{25} )</td>
<td>573 K</td>
</tr>
<tr>
<td>▼ D. Nishijima</td>
<td>20–25 eV</td>
<td>( (0.25–4.8) \times 10^{22} )</td>
<td>( (1.8–9.0) \times 10^{21} )</td>
<td>700–1600 K (He)</td>
</tr>
<tr>
<td></td>
<td>80 eV</td>
<td>( 4.0 \times 10^{21} )</td>
<td>( 3.0 \times 10^{25} )</td>
<td>550 K (D)</td>
</tr>
<tr>
<td>□ Y. Sakoi</td>
<td>10 eV</td>
<td>( 1.0 \times 10^{11} )</td>
<td>( 3.0 \times 10^{22} )</td>
<td>573 K (He)</td>
</tr>
<tr>
<td></td>
<td>3 keV</td>
<td>( 1.0 \times 10^{11} )</td>
<td>( 1.0 \times 10^{21} )</td>
<td>R.T. (D)</td>
</tr>
</tbody>
</table>

Fig. 1  D retention in ion-implanted or plasma-exposed tungsten, as a function of He⁺ fluence.

Fig. 2  D retention in ion-implanted or plasma-exposed tungsten, as a function of D⁺ fluence.
implantation enhances D retention by two- to three-fold. Above a fluence of $1 \times 10^{19} \text{He}^+ \text{m}^{-2}$, He exerts no further enhancing effect on D retention. While He bubble formation and radiation damages create potential D trapping sites, higher density and larger He bubbles may enhance desorption of D by suppressing its diffusion toward the bulk tungsten. The lack of annealing effects in ion implantation experiments would have reduced the ion flux, thereby contributing to D retention in the implant region. In different plasma exposure experiments, D retention is quite scattered even at the same D$^+$ fluence, as shown in Fig. 1. A strong mediator of D retention in tungsten is the formation of He bubbles and occupation of trap sites by He atoms. As previously mentioned, tungsten exposed to He plasma at a high temperature (1600 K) exhibits reduced He retention capacity, while additional exposure to D plasma exposure induces D trapping. However, exposure to lower-temperature He plasma enhances the formation of He bubbles and He retention, leading to reduced D retention.

Under Task 1–1, the effects of He on D retention of tungsten were clarified in D + He mixed plasma exposure experiments, conducted in the Plasma Interaction with Surface and Components Experimental Simulator (PISCES) facility at the University of California, San Diego. Complementary ion irradiation experiments were performed at Shimane University. Transmission electron microscopy (TEM) observations of prethrown W samples exposed to mixed D + He plasma in PISCES revealed the formation of high-density nanosized He bubbles in the near surface region, accompanied by suppression of blister formation and significantly reduced D retention. The volume fraction of bubbles, estimated from TEM cross-sectional observations and ellipsometric measurements, exceeds the percolation threshold, beyond which bubbles interconnect at the near surface region. The percolating bubble clusters provide a diffusion path to the surface for D atoms exposed to the plasma, allowing them to escape. D retention is similarly reduced under the sequential irradiation of helium and deuterium ions. Preirradiation of 3 keV He$^+$ at high fluence (above $1.0 \times 10^{22} \text{He}^+/\text{m}^2$) results in a drastic reduction of D retention. On the other hand, at lower He fluences (up to $1.0 \times 10^{22} \text{He}^+/\text{m}^2$), retention increases with increasing He fluence. This suggests that defects induced by He irradiation may trap D atoms at lower He fluences, where He bubbles are not yet interconnected.

To verify the abovementioned experimental observations, we consider that multiscale modeling, combined with various simulation techniques (e.g., molecular dynamics simulation and finite element method), is required. Multiscale modeling can capture a wide range of spatial and temporal phenomena occurring in real-time fusion reactors. For example, energy is transferred from implanted D to target W atoms in a femtosecond timeframe, while He bubbles are expected to form and migrate over a much longer period, given that the implantation depth of D in W and the diffusion distance of D in W are on the order of several millimeters.

3. Tritium Absorption and Diffusion in Pb–Li

Task 1–2 of the TITAN project is the quantitative analysis of tritium absorption and diffusion in a promising blanket cooling material (Pb–Li). First, the solubility of T in Pb–Li must be determined. Previous data of H isotope solubility in Pb–Li eutectic alloys are highly scattered. Therefore, in our study, solubility measurements were carried out by two different methods: (1) a constant volume method at the Idaho National Laboratory (INL) and (2) a transient permeation method at Kyushu University. The former experiment determined T solubility in Pb–Li, while the latter determined the solubility and diffusivity of H and D in Pb–Li. The results are presented in a separate Task 1–2 paper of the special issue: "Clarification of tritium behavior in Pb–Li blanket system." The second task is system design integration, with the application of a Pb–Li breeding material to the fusion reactor systems. Pb–Li is proposed as a test blanket module (TBM) in ITER, although other candidates, such as He-cooled lithium lead (HCLL) and dual coolant lithium lead (DCLL), have been proposed by the European Union and United States. In Japan, a water-cooled ceramic ($\text{Li}_2\text{TiO}_3$) breeder blanket is used as the ITER–TBM. Blanket designs using Pb–Li as coolant and breeder of magnetic fusion have not been considered previously. On the other hand, a wet-wall Pb–Li design is proposed for the Koyo-fast commercial fusion reactor. A schematic of this design, with a list of design parameters, is shown in Fig. 3. Pb–Li flows into the top of the reactor chamber to protect the metal chamber from damage by heavy neutron irradiation. Besides its role as a tritium breeder, Pb–Li receives heat from particles created by D-T fusion and the $n^4$Li reaction within the blanket. The energy conversion and tritium recovery systems in the external Pb–Li flow for IFE are essentially same as those for MFE, except that the flowing Pb–Li directly comes in contact with the high-temperature plasma on the wet wall of the vacuum chamber. Tritium concentration in the Pb–Li flow is controlled by the tritium generation rate in the chamber and by the Pb–Li flow rate. The Pb–Li temperature is maintained between 300 and 500°C. Majority of the tritium is recovered by a Pb–Li–He counter-current flowing system, but a small portion escapes from the outlet of the recovery system into the heat exchanger. Tritium balance and permeation rate through heat-exchanger tubes were initially estimated as 255 Ci/day. We consider that this comparatively high tritium permeation rate can be mitigated by coating the heat exchanger tubes with ceramic. A 1000-fold reduction in permeation implies a tritium leakage rate below 1 Ci/day, which complies with the safety standards. Experimental verification of permeation reduction is presented in the Task 1–2 section of the above mentioned paper.

4. Effect of Radiation on Tritium Retention in Tungsten Exposed to Ion and Neutron Irradiations

The effect of radiation on tritium accumulation in tungsten (a promising candidate for the first wall of fusion blankets) has attracted much attention since radiation damage is likely to increase tritium retention. Most previous research has focused on ion irradiation rather than neutron irradiation; however, the formation of radiation damage structures depends on the irradiation conditions. Hence, accurate
prediction of tritium retention in fusion reactors requires careful analysis and interpretation of these experimental results, which has not necessarily been accomplished to date. In Task 2–1, the effects of neutron and ion irradiation were investigated by computer simulations as well as by irradiation experiments with neutrons and ions.

We developed a simulation code based on the Monte Carlo technique for modeling the accumulation and release behaviors of hydrogen isotopes interacting with vacancies in tungsten. The code utilizes the results of first-principle calculations as well as data obtained in previous experiments. It can integrate systems containing vacancies from external sources, for example, from TRIM code. We then evaluated the behavior of hydrogen loaded by plasma exposure or ion irradiation. The results are presented as depth profiles in tungsten and thermal desorption spectra. From the simulation results, hydrogen introduced by plasma exposure was found to be localized in a region of high defect density created by ion irradiation of tungsten. In contrast, in neutron-irradiated tungsten, hydrogen was spread over a wide region (Fig. 4). Thermal desorption behavior of introduced hydrogen also differed between ion-irradiated and neutron-irradiated samples, consistent with the experiment. These differences are attributed to a difference in the vacancy distribution between ion-irradiated (localized distribution) and neutron-irradiation (uniform distribution) systems. In future work, the accuracy of simulation results will be improved by (1) balancing long-time irradiation processes with a rapid diffusion process, (2) preventing unrealistic accumulation of hydrogen, and (3) modeling the release of hydrogen forcibly loaded into a region already containing high hydrogen density.

5. Multiscale Modeling of Microstructural Change in SiC during Irradiation

The main component of SiC/SiC composites, used as blanket structural materials for nuclear fusion reactors, is cubic silicon carbide (β-SiC). Fusion reactor materials are subject to various point defects such as vacancies (V), self-interstitial atoms (SIAs), and those induced by helium and hydrogen atoms displaced by high-energy incident neutrons from the fusion core plasma. These processes occur on picosecond-order timeframes and across nanometer-order distances. The resulting defects thermally migrate and form defect clusters (SIA clusters, V clusters and cavities) over submicrosecond times and across submicrometer distances. The microstructural changes caused by defect clusters degrade the performance of the material; therefore, such changes should be accurately predicted and controlled. Material response to irradiation is inherently a multiscale phenomenon, as described above, and should be modeled by multiple complementation of experimental and computational techniques over appropriate time and distance scales.

To understand the microstructural changes in β-SiC during irradiation, a variety of transmission electron microscopy experiments have been conducted on material test fission
reactors and ion accelerators. While these experiments have elucidated the species and sizes of defect clusters under various irradiation conditions,25,26 the formation mechanism of defect clusters remains poorly understood. In the present study, the kinetics of defect cluster formation in β-SiC were numerically evaluated through a multiscale modeling approach, focusing on the nucleation and growth processes of SIA clusters. We note that SiC is a binary compound comprising silicon and carbon atoms; therefore, defect clusters of various chemical compositions could be formed, depending on the irradiation conditions. Modeling defect cluster formation in a compound material requires special care, as discussed below.

First, the formation, binding and migration energetics of β-SiC defects were investigated by classical molecular dynamics (MD) and molecular statics (MS), combined with the method of Gao–Weber empirical interatomic potential,27 which employs not only experimental observations but also ab-initio calculations. In the MD and MS calculations, the formation energy of the most energetically favorable SIA clusters was derived as a function of size and chemical composition (Fig. 5). Knowledge of the formation energy is crucial for evaluating binding energy between defects since the binding energy corresponds to the thermal stability of the defects. Migration energies of isolated silicon and carbon interstitials (SIAs) were also derived.28

On the basis of the defect energetics obtained from the atomistic calculations, the nucleation and growth processes of SIA clusters were then investigated by the kinetic Monte Carlo (KMC) method. Here the KMC model constructed allows for statistical fluctuations in the inflow/outflow of isolated SIAs into/from an SIA cluster. In the KMC simulations, the ratios of the diffusion fluxes between silicon and carbon interstitials ($D_{Si}^{C_{Si}}$, $D_{C}^{Si}$) were set as 1:1, 1:10 and 1:100, while the total diffusion flux ($D_{Si}^{C_{Si}} + D_{C}^{Si}$) was kept constant at 1.0 x 10^{19} m^2/s. The formation kinetics of SIA clusters in β-SiC during irradiation were roughly classifiable into two temperature-dependent classes.29 At relatively high temperatures, the thermal stability of an SIA cluster is crucial, and the chemical composition of the cluster is almost stoichiometric (i.e., Si/C = 1), as shown in Fig. 5(a). In contrast, at relatively low temperatures, where cluster thermal stability is no longer crucial, the composition of SIA clusters can deviate markedly from stoichiometric (Fig. 5(b)). Such information is very important for prediction of the microstructural changes in compound materials during irradiation. As such, it will form the basis of a model incorporating reaction-rate-theory analysis and phase-field method, for evaluating microstructural changes over a prolonged time and length scales.

6. Leakage Control of Tritium through Heat Cycles of Fusion Reactor

Tritium leakage by diffusion through heat exchangers occurs in both MCF and IFE. While retaining the system efficiency, the tritium leakage must be reduced by a factor of 1/10^{10} to reach that of a current fission plant. To reduce tritium permeation from the primary liquid metal or sodium loop into the secondary water loop, a heat exchanger incorporating small-diameter tubes containing an oxidizer was proposed.30 An inert gas containing a small amount of oxidizer flows through the tubes, oxidizing tritium intercepted from the primary liquid metal coolant. The tritiated water was conveyed to a tritium recovery system, minimizing leakage into the secondary water loop. Evaluation of this design indicated that the tritium leakage through the heat exchanger was reduced by 1/10^{5}, with an acceptable increase in the size of the heat exchanger. This scheme is compatible with the coating technique, using compounds such as Er_2O_3 and ZrO_2, which may further reduce permeation by a factor of 1/10^{4.31}

The permeation rate and chemical form of tritium after permeation are known to depend on surface conditions and temperature. Figure 6 shows a simplified model of tritium permeation through the wall of a heat exchanger. A virtual gap with zero thickness between the wall and the liquid LiPb is assumed. The tritium concentration in metals and the tritium partial pressure in the gap are assumed to be related by Sieverts’ law. Following the permeation of wet surfaces,
almost all of the tritium atoms form HTO through isotope exchange reactions. However, some tritium forms T2 when the surface is dry and the temperature is high. Henry's law is assumed to relate the tritium concentration in pressurized water to the T2 in the vapor phase.

Figure 7 shows cross sections of the steam tube proposed in this study. The thick walls of the tube are fitted with small-diameter tubes filled with an oxidizer and carrier gas. Tritium permeating from the outer LiPb will be oxidized on the surfaces of the small tubes and conveyed to the tritium recovery system, thereby reducing the amount of tritium reaching the inner surface of the steam pipe.

In the following calculations, the partial pressures of tritium in the outer and inner virtual gaps are assumed as 1 Pa and zero, respectively. The permeation rate is $8.3 \times 10^{12}$ atoms m$^{-2}$ Pa$^{1/2}$ s at 745 K. The solubility and thermal conductivity are $7 \times 10^{21}$ atoms/m$^3$ Pa$^{1/2}$ and 20 W/mK, respectively. The apparent thermal conductivity and permeation of tritium from outer to inner surfaces are calculated using a commercially available finite element code (ANSYS).

Figure 8 shows the normalized tritium permeation through a heat exchanger equipped with different configurations of double pipes. The heat flow through the exchanger is constant.

be designed for the second loop. Almost all of the injected tritium can be recovered and reused as fuel after isotope separation.

7. Summary

The common task in the US-J TITAN project identifies cross-linked considerations in the blanket system modeling on the basis of the material research in each task. The results are summarized as follows:

(1) The helium effects on hydrogen isotope retention in tungsten were investigated by reviewing the results of previous studies and by conducting D + He mixed plasma exposure experiments in PISCES. These results reveal that D retention is reduced by high-density He bubbles forming in the near surface region.

(2) Research into permeability, diffusivity and solubility of hydrogen isotopes in a Pb–Li alloy as a tritium breeder is summarized. The blanket design must achieve a low tritium leak to the outside and high tritium recovery from a breeder loop.

(3) A simulation code to model the accumulation and release of hydrogen isotopes interacting with vacancies in tungsten was developed using a Monte Carlo technique. Simulation results revealed that the behavior of hydrogen isotopes depends strongly on the mode of irradiation (i.e., whether the specimen is ion- or neutron-irradiated).

(4) Multiscale modeling of microstructural changes in a binary compound material during irradiation has elucidated the nucleation and growth processes of defect clusters.

(5) Tritium permeation through a heat exchanger equipped with double tubes filled with an oxidizer can be reduced to $1/10^4$ that of bare stainless tubes, without degrading the heat exchange rate.

Acknowledgment

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