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RESEARCH REPORT
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Simulation study on retention and reflection from tungsten carbide under high fluence of helium ions*

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Abstract

We have studied, by a Monte Carlo simulation code ACAT-DIFFUSE, the fluence-dependence of the amount of retained helium atoms in tungsten carbide at room temperature under helium ion bombardment. The retention behavior may be understood qualitatively in terms of irradiation-dependent diffusion coefficient assumed and range. The emission processes from tungsten carbide under helium ion irradiation derived were compared with each other. We have discussed the retention curves for incident energy of 5 keV at incident angles of 0° and 80° and of 500 eV at 0°. The energy spectra of helium atoms reflected from tungsten carbide for incident energy of 500 eV at 0° and 80° were compared with those from graphite and tungsten.

Keyword: retention, irradiation-dependent diffusion coefficient, reflection, helium, tungsten carbide, Monte Carlo simulation

1. Introduction

In fusion devices of a reactor grade, high-Z materials and their composites are planned to be used to avoid severe erosion due to heavy particle and heat load[1-3]. In particular, tungsten materials are being considered to be promising candidates because of high-melting temperatures, high thermal conductivities and strong resistance for erosion due to high threshold energies for sputtering. Tungsten and carbon materials are expected to be used simultaneously as a divertor plate and a first wall armor in future fusion devices, respectively. The mutual redeposition of the sputtered materials may modify the surface layers of the materials into tungsten carbide under plasma irradiation at high temperatures for long-term operation.

In the case of a burning plasma, plasma facing materials are exposed to the helium ash produced through fusion reactions. Thus, the plasma facing walls may retain the ash. The amount of helium ash in a core plasma increases when the retained helium is emitted by sputtering or thermal desorption and the shielding of a scrape-off layer is not effective.

To estimate the helium emission from the walls, the helium retention properties of them have to be investigated. There are not sufficient data on helium retention. We will discuss, in the following, the helium retention properties of tungsten carbide derived with a simulation code ACAT-DIFFUSE[4], as well as the energy distributions of reflected helium from that material.

2. Simulation method

Since ACAT-DIFFUSE code has been described in detail elsewhere [4], a simple outline of the code necessary to the following discussions is only sketched here. The code handles an amorphous composite material. The ACAT part of the code simulates, on the basis of a Monte Carlo method, atomic collisions in a target material to a binary collision approximation. To be capable of dealing with a large total dose Φ within the framework of the

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divided into smaller dose increments $\Delta\ \Phi$ during which a target composition is not varied appreciably by incident ions. The ions corresponding to $\Delta\ \Phi$ are assumed to hit a target material simultaneously and to be slowed down instantaneously. The ions' slow-down, together the associated vacancy and range distributions are calculated by the ACAT part. The collided atoms diffuse during the time interval of $\Delta\ \Phi/J$ (J being the ion flux). The DIFFUSE part copes with diffusion processes by solving the diffusion equations numerically. These two routines are iteratively repeated n times where $n=\Phi/\Delta\ \Phi$.

3. Numerical results and discussions

We have calculated, with ACAT-DIFFUSE, the amount of the helium atoms retained in tungsten carbide, tungsten, and graphite under helium ion bombardment as shown in Fig. 1. The incident energy of helium ions considered was 5 keV and the incident direction was normal to the surface. The flux chosen was $1\text{x}10^{18}$ ions/m^2 sec and the target materials were assumed to be at room temperature. We have adopted, for our calculations, a model that the diffusion coefficient in the region shallower than the range is enhanced five times as great as that in the deeper region and that the former diffusion coefficient is proportional to the energy deposition, which we will explain below. The calculated curves for graphite and tungsten agree well with the experimental results [5]. The curve for tungsten carbide derived lies between those for graphite and tungsten, and it is very close to that for tungsten. Thus, we think that the calculated retention curve for tungsten carbide is almost reasonable. After increasing up to the maximum with the increase of helium ion fluence, it then saturates approximately. This tendency of the retention may be understood qualitatively in terms of diffusion coefficients and ranges. The region, located closer to the surface than the range, is exposed to helium ion irradiation, which may well give rise to the increase of the diffusion coefficient there for high ion fluence, compared to that in the nonirradiated region. If we take such a situation for the diffusion coefficients, the difference in the diffusion coefficients works to trigger stronger backward diffusion of implanted ions from the range, which, in turn, may produce the saturation of helium retention. The saturation level of helium retention depends approximately on the product of the number of interstitial sites and a range. The ranges of helium ions with 5 keV are approximately 22 nm, 30 nm and 20 nm in tungsten carbide, graphite and tungsten, respectively. The fluence values of the three materials at which the retention curves start to saturate reflect partly those range values. The ratio of the concentration of carbon to that of tungsten at the tungsten carbide surface is about 0.25 at the saturated level as a result of preferential sputtering.

The integrated emission processes of helium from tungsten carbide, which control the amount of helium retained in the material, are shown in Fig. 2. Except at very low ion fluence where thermal desorption is comparable to reflection, it is clear from Fig. 2 that thermal desorption is always much stronger than reflection and sputtering. In particular, thermal desorption is about two orders of magnitude higher than sputtering at the saturation level of retention.

We compare, in Fig. 3, the retention curves for incident energy of 5 keV at incident angles of 0° and 80° and of 500 eV at incident angle of 0° to the surface of tungsten carbide. For the two cases with 5 keV, the saturation level of retention for oblique incidence is several times smaller than that for normal incidence. This fact is explained qualitatively by noting that the range is shallower and that reflection increases for glancing incidence than for normal incidence, both of which work to decrease the saturation level for glancing incidence. The low saturation level for incident energy of 500 eV is also understood because of those effects. In addition, the fact that the curve for 500 eV increases with increasing ion fluence indicates that the difference between the diffusion coefficient in irradiated region and that in nonirradiated region is small because of low energy deposition. On the other hand, the tendency that the curve for 5 keV decreases with increasing ion fluence means that the difference of the diffusion coefficients in the two different regions is large because of strong energy deposition for this comparatively large energy.

We show in Fig. 4 the normalized energy spectra of helium atoms per eV reflected from tungsten, graphite and tungsten carbide for incident energy of 500 eV,where E_0 is the incident energy of helium ions. The energy spectra for tungsten carbide were those obtained at the saturation level. Fig. 4(a) and Fig. 4(b) correspond to the incidence of normal and 80° to the surface of the materials. The spectrum for tungsten carbide is similar to that of tungsten. This indicates that the surface of tungsten carbide has been changed to be rich in tungsten as pointed out above. The small hump at very low energies can be ascribed to collisions with helium atoms accumulated in tungsten carbide. The difference in the features of the spectra for tungsten carbide and for graphite reflects the difference in the mass ratios of helium to the target atoms. All spectra shown in Fig. 4(b) increase with increasing incident energy and have maximum near E_0. The peaked region of the spectra indicates that sequential distant collisions are a main process.

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4. Conclusion

We have calculated, with a Monte Carlo simulation code ACAT-DIFFUSE, the fluence dependence of the amount of retained helium atoms in tungsten carbide under helium ion bombardment. The calculated retention curves for graphite and tungsten were shown to agree with experimental results. The retention curve obtained for tungsten carbide resembles to that for tungsten. To get the retention curves, we have adopted a model that the diffusion coefficient in the irradiated region be enhanced five times as great as that in the nonirradiated region. The saturation level of retention could be qualitatively accounted for in terms of range. The main emission process, which controls the retention feature of helium in tungsten carbide, is thermal desorption at saturated retention. The amount of retained helium is stronger for normal incidence than for oblique incidence. This fact may also be understood in terms of the diffusion coefficient model assumed. The energy distributions of reflected helium atoms from tungsten carbide are similar to those from tungsten because of tungsten rich surface at the saturated retention. A small hump was found for the spectra at very low energies, which can be ascribed to reflection from helium atoms accumulated in tungsten carbide. The hydrogen retention of tungsten carbide is under study.

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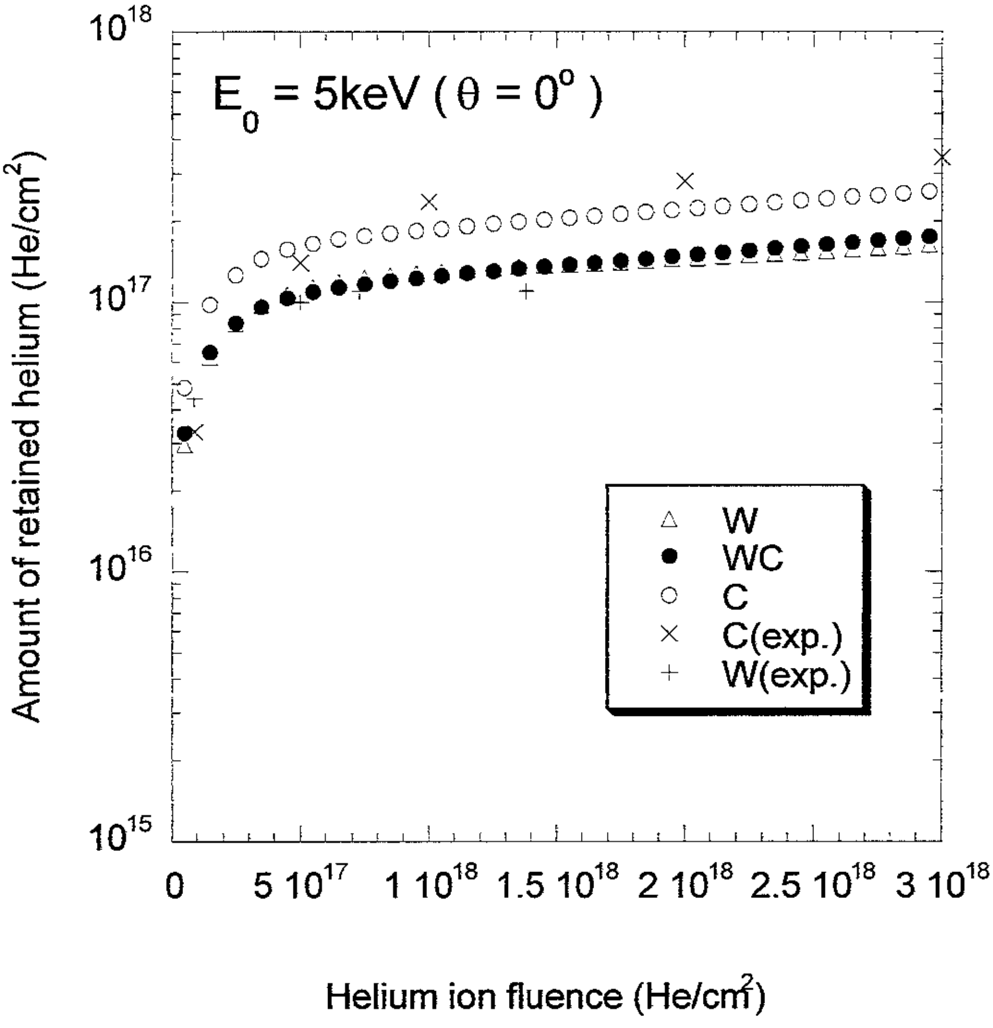

Fig. 1 : Amount of helium retained versus helium ion fluence in tungsten carbide (filled circle), tungsten (open triangle), graphite (open circle) for incident energy of 5 keV at normal incidence. The experimental results for graphite (x) and for tungsten (+) [5] are also shown.

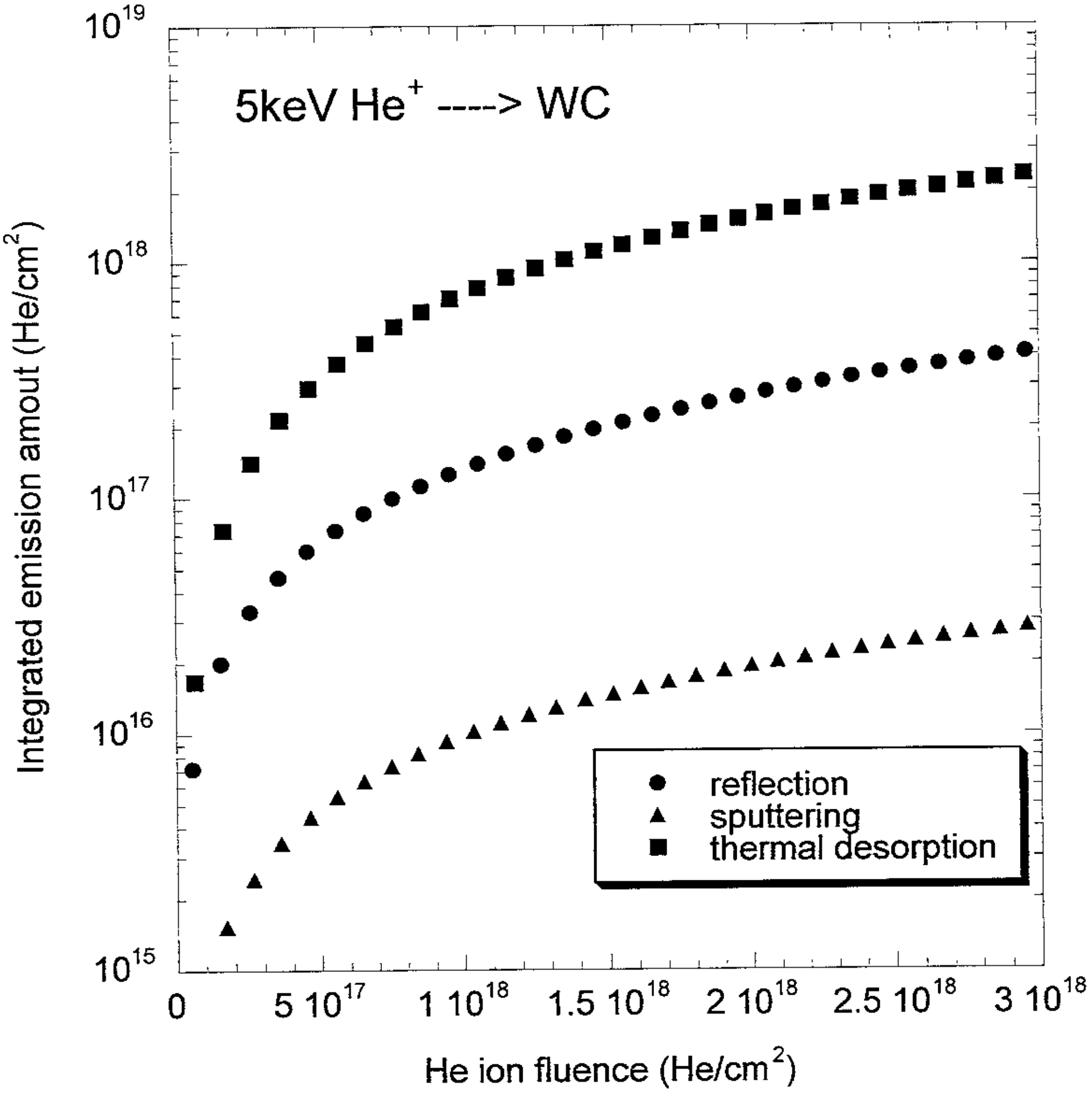

Fig. 2 : Emission processes versus helium ion fluence for tungsten carbide bombarded with 5 keV. Reflection (filled circle), sputtering (filled triangle), and thermal desorption (filled square) are shown.

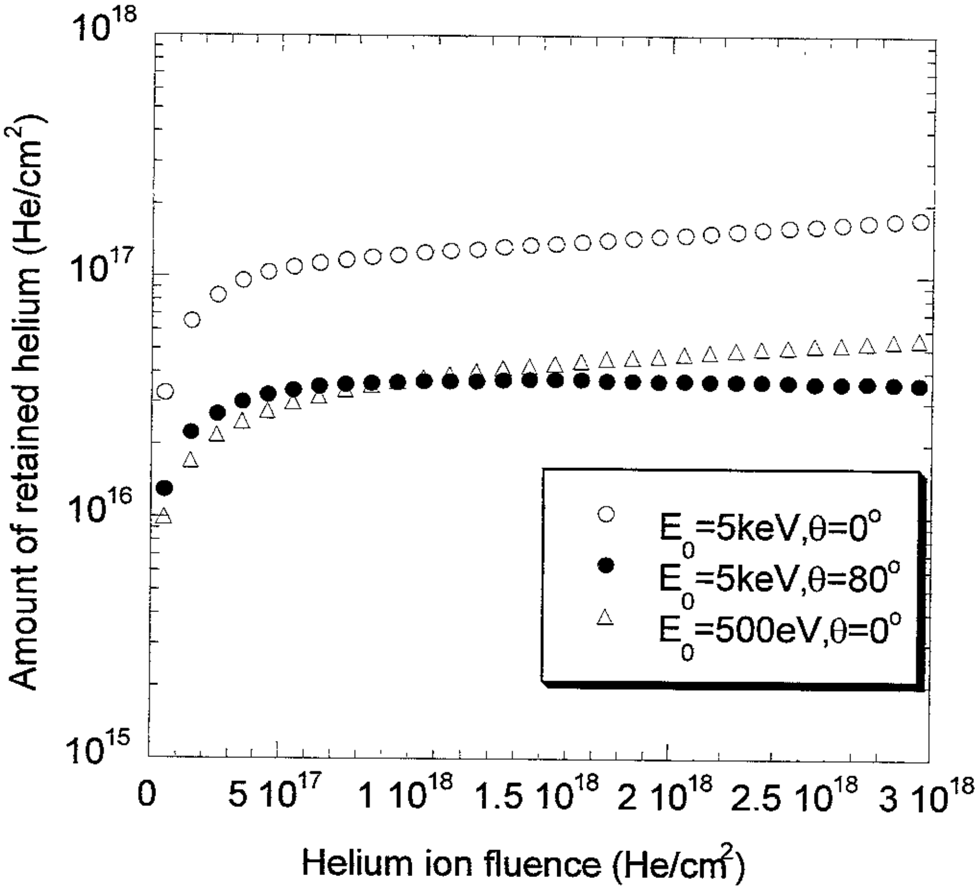

Fig. 3 : Amount of retained helium in tungsten carbide versus helium ion fluence. The amounts for incident energy of 5 keV at normal incidence (open circle), of 5 keV at incident angle of 80° (filled circle) and of 500 eV at normal incidence (open triangle) are shown.

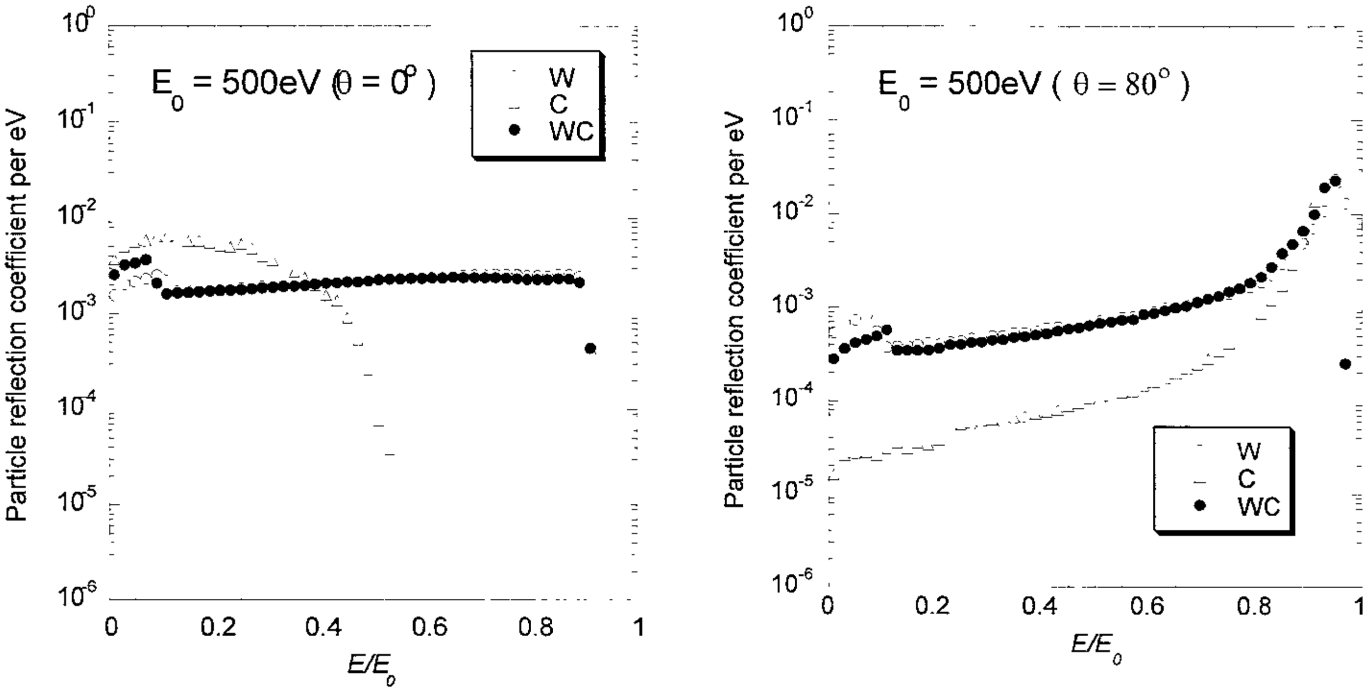

Fig. 4(a), 4(b) : Energy distributions of reflected helium atoms from tungsten carbide for 500 eV at normal incidence (a) and at incident angle of 80° (b) compared with those for other materials. The target materials are tungsten (open circle), graphite (open triangle) and tungsten carbide (filled circle).

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