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Simulation of ion irradiation of crystalline and amorphous targets tokamak-reactor first wall materials

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An overview of results concerning simulation of various processes which occur due to atomic bombardment of crystalline and amorphous solids is presented. With the use of original computational codes, the following data were obtained: reflection coefficients, projected energy losses and ranges of ions in solids, channeling data as well as sputtering yield and its dependence on incident angle of bombarding particles for Be−W and Ne−W combinations. Be, C and W targets were studied as these are among the plasma-facing materials in tokamaks, including ITER. The emphasis was made on atom-target combinations which lack reliable experimental data. Experimental data on other materials were used to verify calculations. A significant influence of the interaction potential used on the simulation results is shown. The reviewed results are tied by a common subject a study of interaction of plasma ions and first-wall materials of a tokamak-reactor and also by a common method of study the use of an original computational code.

Keywords: scattering, ion sputtering, interaction potential, energy release.

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Introduction

In the ITER tokamak the first beryllium wall and a diverter made of tungsten will be subjected to intensive irradiation by a flux of neutral atoms and ions leaving plasma. The ITER operation is planned with D−T-plasma, therefor, in our works we considered hydrogen isotope atoms, as well as He atoms — the products of thermonuclear reactions as projectile particles. In addition to beryllium and tungsten the carbon target is of interest, because some tokamaks have carbonic surfaces exposed to plasma effect. Apparently, the phenomenon of atoms reflection from the surfaces in a tokamak-reactor will play a key role in the achievement of key parameters of plasma and determination of thermal load onto materials. Reflection of atoms from materials of the tokamak-reactor is the subject of intensive theoretical studies, whose authors note severe shortage of experimental data [1,2], because there is no experimental data on the reflection indices for Be, and these are scarce for C and W [3,4]. There is also no reliable data on runs of the mentioned atoms in amorphic tungsten. The knowledge of atom runs is required for the assessment of defects formation in structural materials of a tokamak-reactor and accumulation of hydrogen isotopes in the material. Additional study is also required for tungsten sputtering with beryllium ions: there are no experimental data on sputtering, however, according to the studies [5, 6], the tokamak wall bombardment by D and T atoms causes significant ingress of beryllium into plasma. Be atoms in plasma are ionized, accelerated and, in turn, cause diverter sputtering, which is very undesirable, because tungsten ingress into plasma modifies significantly the discharge characteristics [7,8].

The mentioned gaps can be filled by means of computer modeling of the mentioned processes, however, for reliable numeric study a detailed analysis of a set of parameters is required, describing the interaction of atomic particles with a solid body.

1. Modeling methods

Modeling was performed by means of an original code, where two approaches to the description of the atom motion in a solid body are implemented: depending on the task conditions, either a trajectory method, which is a special case of molecular dynamics, or binary collision approximation (BCA) was used. One of the main parameters, whose selection influences the outcome of modeling of atom scattering on the surface, is the projectile atom's potential of interaction with the target atoms. The work [9] demonstrated that the use of the density function theory (DFT) for the determination of the potential for the interaction of atoms gives a result, which is in a better agreement with the experimental data than the widely used ZBL potential [10]. Comparison of the DFT and ZBL is given in Fig. 1. The DFT potential predicts the availability of a drawing well in the interaction potential, meanwhile the ZBL potential is purely a repulsive one. By using the DFT approximation, original interaction potentials were developed for the combinations of H and He atoms with Be,

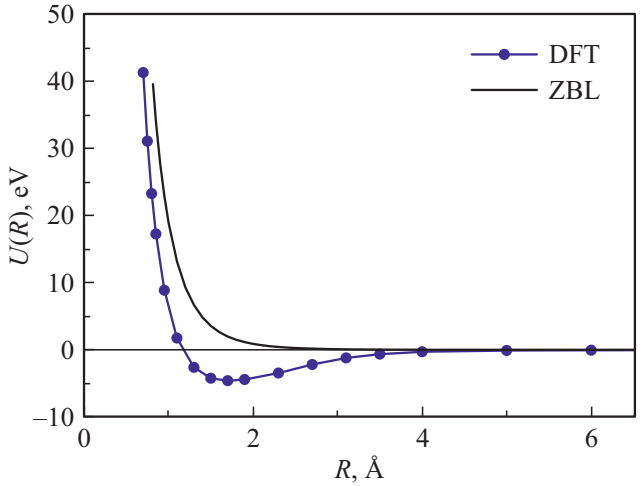

Figure 1. Comparison of the potential obtained by the DFT method, with the ZBL method for the combination of D–W.

C, and W atoms [11]. Position and depth of a potential well obtained by means of DFT for these pairs agree with the experimental and calculation parameters of corresponding diatomic molecules. When modeling the atom motion inside a target, slowdown at an electron component of a solid body was taken into account — for this purpose the experimental data from the NDS data base of the International Atomic Energy Agency were used [15].

2. Reflection of atoms from amorphic surface

As a result of modeling of the H, D, and T atoms scattering on the amorphic surfaces of Be, W, and C, a suddenly high impact of the drawing well on the value of reflection indices was found, which is manifested in case of slippery fall of atoms ($< 20°$ from the surface) with the energy of about hundreds of eV (Fig. 2, *a*). The figure clearly demonstrates transition from virtually one hundred percent reflection manifested during modeling with the use of the ZBL potential to considerable particles absorption by the surface, which takes place when using the DFT potential. At the energies over 2 keV this difference becomes insignificant.

Comparison with the experimental data was possible only for the combination of D–C (Fig. 2, *b*): a good agreement with the experiment results was demonstrated [4]. There are no experimental data for other combinations within the range of energies in question, however, comparison with the results of independent calculations of the reflection indices [2,13,14], which is possible at the energies of > 1 keV, when selection of the potential has a low impact on the result, has shown satisfactory agreement with the obtained values. The verifications have provided the ground for the use of the DFT potential in calculations of the reflection indices: the reflection indices were calculated for

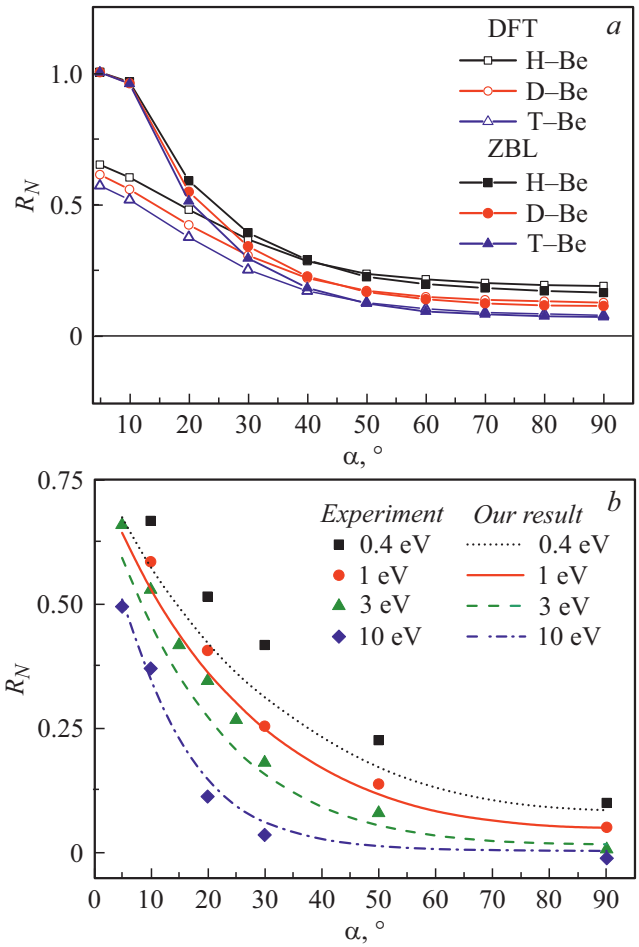

Figure 2. *a* — reflection indices of different hydrogen isotopes with the energy of 100 eV from the Be target depending on the angle of incidence (counted from the surface) in case of the use of the DFT and ZBL potentials; *b* — the comparison of reflection indices calculated by using the DFT potential with the experimental data [4] for the combination of D–C.

the H, D, T, He atoms during bombardment of the amorphic targets of Be, C, W [11, 15] at various angles within a wide range of energies 100 eV–10 keV, which corresponds to typical energies of the plasma particles.

3. Runs of atoms in amorphic targets

The impact of a drawing well in the interaction potential on the results of modeling was also assessed for the modeling of atomic particles passage through an amorphic solid body. Fig. 3 shows comparison of the values of atom runs in tungsten, calculated by using the potential with and without the well. The values of runs obtained by using the DFT potential exceed the values obtained with the ZBL potential, wherein the difference is decreased as far as the initial energy of projectile particles is growing. This can be explained by the dependence of the nuclei slowdown capabilities on the interaction potential; these capabilities are

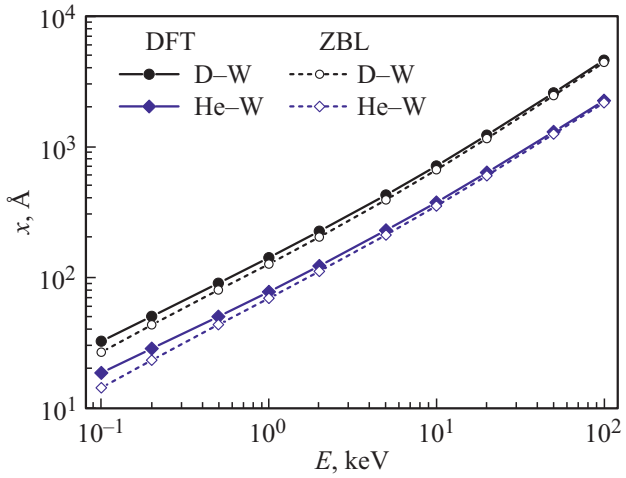

Figure 3. Comparison of calculation dependences of the average run on the energy of projectile particles for the combinations of D−W, He−W obtained by using the DFT and ZBL potentials.

several orders lower than the electron slowdown capabilities. Contribution of the electron slowdown capabilities into the atomic particle slowdown in a solid body is growing with the energy increase.

Due to the absence of experimental data on the runs of atomic particles in tungsten, the check of applicability of the used methods and parameters was performed by means of additional modeling of the hydrogen atoms passage through amorphic silicon. A good agreement was demonstrated in [16] with the experimental data [17,18].

The distributions of runs were calculated by depths for combinations of H−Si and D−W at the initial energy of bombardment particles of 100 eV−10 keV. The obtained distributions [16] are described by characteristics allowing to build the run distributions by depths without calculations.

4. Energy release in amorphic targets

Modeling of passage of atoms H, D, T through amorphic targets allowed to make a conclusion on the energy release distribution by depth in materials of a tokamak-reactor. It is shown that at the energies of projectile particles of $\lesssim 100$ keV the maximum of energy release is within the area near to the surface. Dynamics of change of the energy release curves nature during further increase of the energy of projectile particles for the combination of H−W has shown that the Bragg peak starts considerably manifesting only within the area of energies of ~ 500 keV [19]. Comparison of distributions of the energy release by depth for different hydrogen isotopes has shown their similarity at the same value of initial energy (Fig. 4, *a*). At a low depth the energy release in case of H is higher than in case of D and T, which can be explained by a high value of electron slowdown capabilities of a lighter isotope.

The analysis of distribution of the energy release in materials of the first wall in case of irradiation by a bunch

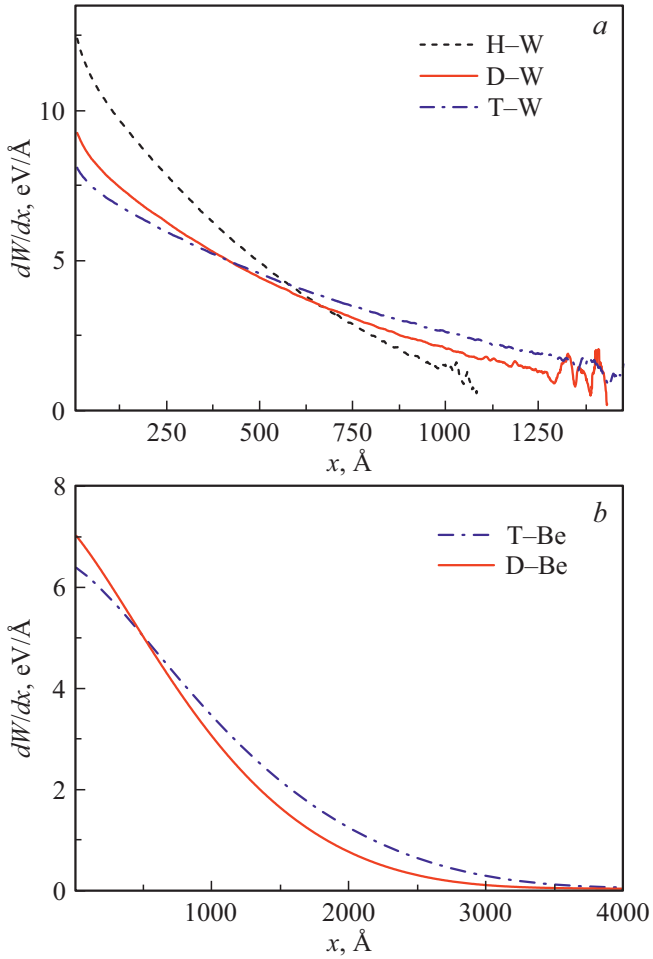

Figure 4. *a* — the distribution of energy release by depth in case of H, D, T passage with the energy of 5 keV through W. dW/dx — linear losses of energy (average losses of energy by the particle within the interval of dx); *b* — distribution of energy release by depth in Be exposed to the ITER tokamak-specific spectrum of atoms of D and T leaving plasma normalized for one projectile particle.

of particles with the energies corresponding to the typical spectrum of D and T atoms leaving plasma (calculation of spectrum was performed by using the DOUBLE-MC software) has shown [20] (Fig. 4, *b*) that during bombardment of the studied targets by atoms with angular and energy distribution as expected in the ITER tokamak plasma conditions, the atoms of T ingress into material about 20% deeper than the atoms of D, which lead to a hazardous accumulation of tritium in the first wall.

5. Atoms passage through a crystal — channeling mode

In addition to the study of the atoms passage through amorphic targets, the channeling phenomenon modeling was also performed in crystals. The distributions of runs of the D atoms in W(100) were also calculated at different

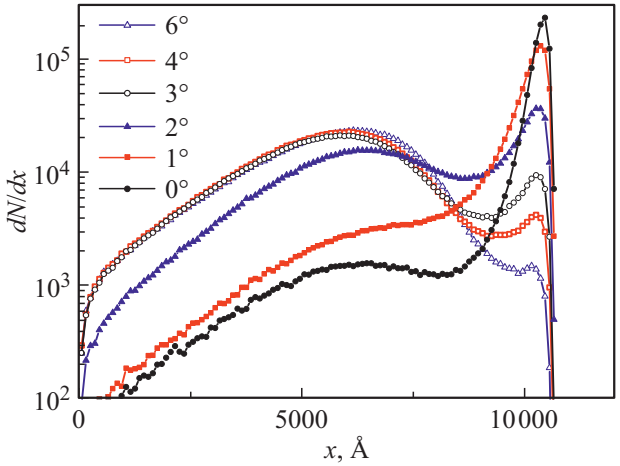

Figure 5. Distributions of runs by depth of material for the combination of D−W(100) at various incidence angles relative to a normal to the surface; energy of projectile particles 100 keV.

initial energies [21] and angles of incidence. Fig. 5 shows how the portion of particles captured in the channels changes in case of the bunch incidence angle change by several degrees relative to the normal: with the angle increase the runs distribution is transformed by reflecting the decrease of a portion of particles captured into the channel. It can be seen that in case of deviation by 6° a portion of particles in the channel is $\sim$ 1%. The result agrees with theoretical assessment of the critical channeling angle in tungsten [22].

The analysis of evolution of the spatial distribution of a bunch of D atoms captured into the W(100) crystal channel. For this purpose, modeling was performed for the passage of the D atoms bombarding the surface within one cell of crystalline grid through the W(100) target. At the depth of 1000, 3000, 7000 and 9000 Å the spatial distribution of particles within the irradiated channel and in the neighboring channels was registered. Fig. 6 shows the dynamics of change of the atomic particles distribution in the channel. Formation of a clear structure in the spatial distribution of particles was found, and its preservation up to the depth of about 90% of the run of particles. The shape of the formed structure agrees with independent analytical prediction [23] and is determined by the distribution of total potential in the channel, which enables to suggest an experiment for determination thereof based on the angular distribution of particles released from crystal after passage of 30−60% of the penetration depth.

6. Sputtering of an amorphic target

A software for the study of tungsten sputtering by ions of beryllium was developed on the molecular dynamics (MD) principle and optimized for the specifics of the task. The target was an amorphic solid body, the interaction between its atoms was described by means of the multiparticle potential under the model of a submerged atom [24]. Due to the absence of experimental data on the sputtering coefficients for the combination of Be−W additional modeling was performed for the combination of Ne-W. Dependences of the reflection index on the energy of projectile particles (Fig. 7) and on the angle of incidence were obtained for both combinations. In case of tungsten sputtering by neon ions the agreement with experimental data was demonstrated [25]. For comparison, the results of calculation by widely used SRIM software were presented [26] — it is seen that it exceeds the value of sputtering threshold. For the combination of Be−W, the agreement was achieved with molecular-dynamic calculation by using the LAMMPS software given in the work [27].

We suggested a model allowing to calculate the tungsten sputtering coefficients by light ions bombarding a target. For the application of this model it is required to know the energetic and angular distribution of backscattered primary particles bombarding the near-to-the-surface layers of a target. Using the formula

$$Q = \frac{4M_1M_2}{(M_1+M_2)^2} \cdot E_1 \cdot \sin^2\left(\frac{\chi}{2}\right)$$

the energy is determined that was transferred by ion with the mass of M_1 and the energy of E_1 to the resting atom of the target with the mass of M_2, which belongs to the superficial layer. χ is the angle of scattering in the mass center system. The sputtering condition is determined as follows: the component of the energy Q, transferred to the tungsten atom along the axis perpendicular to the surface must exceed the energy of sublimation, which is equal to 8.45 eV for tungsten. In accordance with this condition, threshold values of E_1 and χ (E_{th} and χ_{th} accordingly) are determined, at which the scattering of superficial layer of the target takes place. From the data on back scattering of ions a number of cases is selected, when the energy is transferred that exceeds the energy of sublimation in case of surface-perpendicular collision of an atom of the material. By dividing the number of sputtered atoms by the number of initial projectile particles, we can determine the sputtering coefficient. The result obtained by using this model is shown in Fig. 7 (BSS — Back Scattering Sputtering). It can be seen that the calculation by using our model agrees with the molecular-dynamic calculation, and with the experimental data for Ne−W.

In Fig. 8 the coordinates show coefficients of tungsten sputtering by ions of D, He, Be, Ne, obtained by using the developed model. Our model demonstrates versatility of the dependences of sputtering coefficients on the energy in the near-to-threshold area. It can be seen that the curves for ions with similar mass are close to each other. There is an option for the extrapolation of the results for the cases beyond the study.

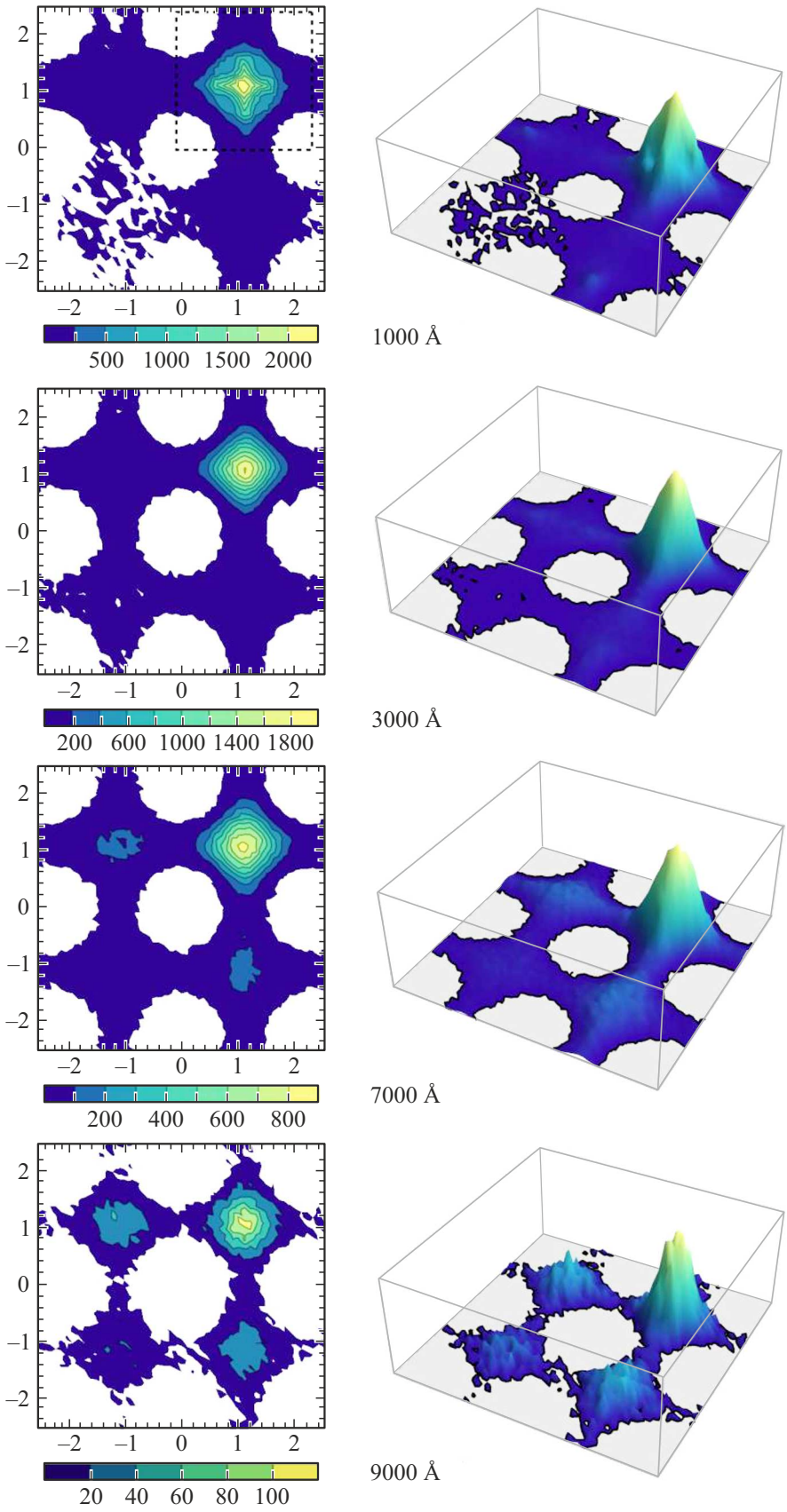

Figure 6. The spatial distribution of particles captured into the channel at the depth of 1000, 3000, 7000 and 9000 Å for the combination of D−W(100), initial energy 100 keV. On the axes, the distance in Å. Color scale shows the number of particles registered at each point of space. Dashed square refers to the area of irradiation by the bunch of D, corresponding to one channel of crystal.

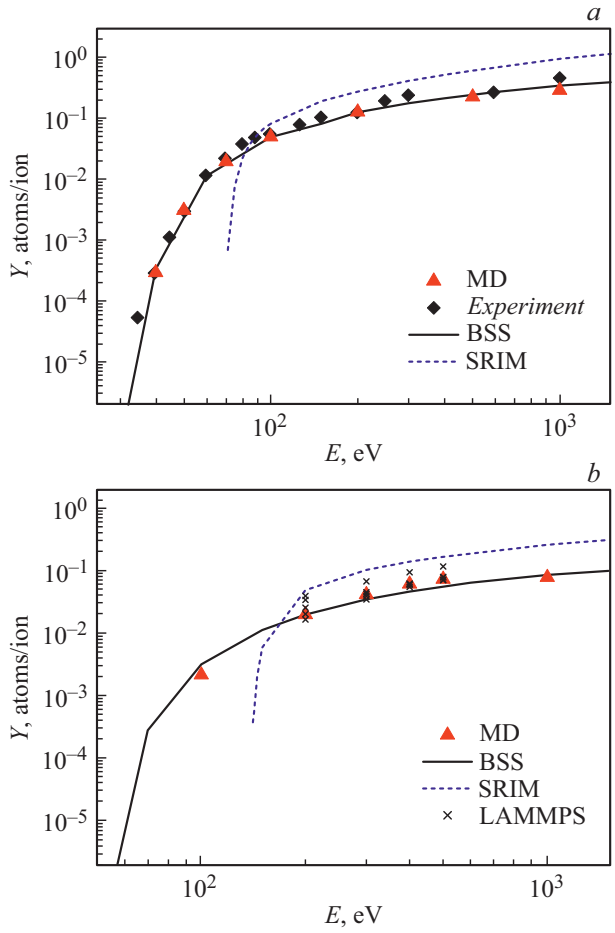

Figure 7. *a* is the dependence of the sputtering coefficient Y on the energy of projectile particles for the combination of Ne–W: our molecular-dynamic calculation, the calculation by using the BSS model, experimental data from the work [25] and calculation by using the SRIM software [26]; *b* is the dependence on the sputtering coefficient Y on the energy of projectile particles for the combination of Be–W: our molecular-dynamic calculation, the calculation by using the BSS model, LAMMPS calculation from the work [27] and calculation by using the SRIM software [26].

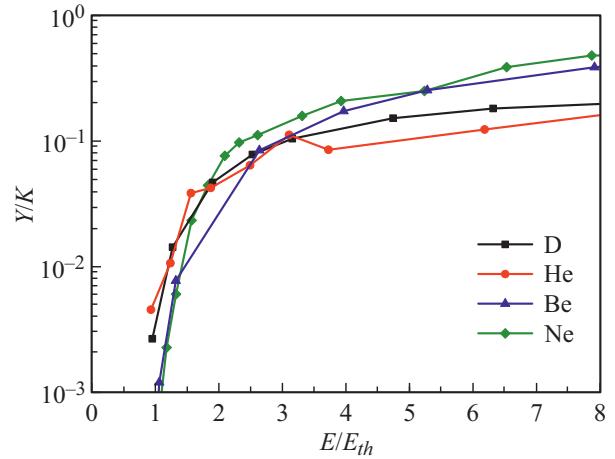

Figure 8. Dependence of the W sputtering coefficient by ions of D, He, Be, Ne in the given coordinates. $K = \sigma(\chi_{th})/d^2$ at $E/E_{th} = 4$, where d is the average distance between the layers of W.

Conclusion

The main results of the works performed refer to the following:

1. Numerical software was developed for modeling the interaction of bunches of ions and atoms with a solid body. Comparison of the obtained results with the experiment for the processes of particles reflection, particle runs in crystalline and amorphic targets, sputtering at ion bombardment allows to confirm the reliability of the obtained data.

2. The reflection indices are obtained for all combinations of H, D, T, He atoms and amorphic surfaces of Be, C, W within the range of energies from 100 eV to 10 keV at various incidence angles of the projectile particles. A suddenly strong impact of the drawing well in the potential on the result at the energies of about hundreds of eV was found.

3. The runs of atoms of H, D, He in amorphic Si and W were calculated. The formulas were suggested for the description of the obtained results.

4. As a result of modelling of the channeling phenomenon in crystalline targets the runs of atoms H and D in W(100) were calculated and the change of the nature of runs distribution by depth depending on the atoms energy was shown. The analysis of evolution of spatial distribution of the channeled bunch in W(100) was performed that shows the formation of a clear spatial structure of the channeled bunch preserved on the 90% of the particles track in the channel.

5. Predominance of the energy release near to the target surface was shown in case of bombardment of the amorphic surfaces of Be, C, W by isotopes of hydrogen with the energies of 100 keV. Based on the obtained distributions, the energy release per one projectile particle was calculated in case of irradiation of these materials by atoms with the ITER tokamak-specific spectrum of energies. Accumulation of tritium in the first wall of a tokamak-reactor was predicted.

6. Dependences of sputtering coefficients W by ions of Ne and Be on the energy and angles of incidence of the projectile particles were calculated. A model of tungsten sputtering by back scattered light ions was developed to explain the universal nature of dependences of the sputtering coefficients on the energy within near-to-threshold area.

As shown in the work, application of computer-aided modeling in combination with clarification of our concepts on the potentials of particles interaction allows to successfully fill the gaps in cases when there is no experiment. The obtained data are highly relevant for modeling of various processes in the near-to-the-wall plasma of a tokamak-reactor.

Conflict of interest

The authors declare that they have no conflict of interest.

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