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MOLECULAR DYNAMIC SIMULATION OF PLASMA MATERIAL INTERACTION TO CALCULATE THEORETICAL SPUTTERING YIELD

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In a fusion reaction two light nuclei, Deuterium and Tritium merge to form a single heavier nucleus Helium. However, two positive nuclei repel each other. In order to merge two nuclei they need to have very high velocities. High speed means, high temperature. For the reaction it is significant for a nuclei to keep at 100 million °C temperature. At this temperature D and T atoms form a plasma. In order the reaction to take place, the plasma temperature must be conserved or plasma should not be cooled. Tokamak reactors are designed to confine the plasma in a magnetic field. Thus, the cooling of the plasma is prevented by hitting the reactor walls. Plasma density and temperature must be at a certain level in order to initiate the reaction and to ensure continuity. During the reaction process, positive and negative ions escaping from the magnetic field environment interact with Tokamak walls and cause deformation. This causes the plasma wall to deteriorate over time and the release of neutrons to the environment. Plasma-Wall interaction is one of the most important problems that cause interruption of fusion in Tokamak rectors. The materials which most resistant to ion corrosion in the plasma wall are graphite, beryllium, aluminium and tungsten. In this work, plasma-material interaction is studied theoretically physical and chemical erosion caused by the plasma interactions of different wall material samples (graphite, aluminium and Tungsten) used in the fusion reactor and investigated with the Monte Carlo method with molecular dynamics.

Keywords: Plasma, Nuclear Fusion, Molecular Dynamics, Sputtering Yield, Monte Carlo

Introduction

Today, the increasing world population, rapid industrialization and the need for high-tech have made electrical energy very important. Fossil resources have been used to obtain electrical energy for many years. However, since fossil fuels are depleted over time, alternative energy sources are needed for energy production. In recent years, the issue of utilizing renewable energy sources such as sun, wind, tides, waves, geothermal and biomass has gained importance [1-3]. Although electrical energy can be obtained from sources such as sun and wind, other energy sources are also needed due to problems of cost, continuity and storage. One of solution to generating electricity without using fossil fuels is the nuclear energy. Conventional nuclear power plants are based on the fission reaction. These types of reactors, which are generally based on the decomposition of unstable uranium nuclei into more stable nuclei, are the subject of debate in many aspects; such as both finding nuclear fuel and storing nuclear waste. On the other hand, combining two light elements as a result of a nuclear reaction to form a heavier element is called "fusion". A huge amount of energy is released as a result of fusion, also known as the nuclear reaction. A typical fusion reaction is the reaction between deuterium and tritium, which are isotopes of hydrogen. The following reaction equation is a atomic molecular form to specify the total energy produced in nuclear fusion:

(_1^2) "H + " (_1^3) H → (_2^4) "He" (3.45MeV) + (_0^1) n("14.15MeV") (1)

However, the fusion reaction, which is also a nuclear reaction, is not as easy as a chemical reaction. For the reaction to occur, the repulsive force between the two positively charged nuclei must be overcame. For this issue, isotopes (D and T) must approach close to each other with very high kinetic energies. This energy must be at least 0.7 MeV. A temperature of about 3×109 K is needed for isotopes to have this kinetic energy. If a sufficient number of D and T nuclei are found together and this initial temperature is reached, the fusion reaction then going to be started. This is one of the most important problems in realizing the fusion reaction. On the other hand, scientists have developed two different techniques to overcome this situation. One of them is to confine deuterium and tritium to a small area spatially and initiate the reaction with a high-energy laser, and the other is to carry out the reaction by trapping these isotopes in a magnetic field. A fusion energy reactor can be designed by utilizing the kinetic energies of the neutrons released as a result of this reaction. The most well-known of these reactors is the Tokamak reactor. In the Tokamak reactor, the plasma is trapped in the magnetic field environment to prevent its cooling.

In the Tokamak reactor, the uncharged neutrons, each of which has an energy of 14.15 MeV, are separated from the magnetic field environment. However, these neutrons can be slowed down by a cooling liquid (e.g. water). Electric energy can be obtained by operating turbines with the water vapor obtained as a result of slowing down the neutrons released in a reactor in the liquid. Since neutrons slowed in this way lose most of their energy in the process. Even if they hit the reactor wall, they cannot make the wall radioactive. Some neutrons can be used to create artificial Tritium by interacting with it. On the other hand, He cores, each of which has an energy of 3.5 MeV, are also produced in the Tokamak reactor [4-14]. This energy of helium nuclei can be used to maintain the temperature of the plasma. A Tokamak reactor is a torus (tube) shaped device. As a result of the appropriate arrangement of the magnets, the reaction is ensured by being trapped in the plasma magnetic field environment, and it is prevented from contacting the reactor wall and cooling. However, while the plasma is moving in the magnetic field, some high-energy He ions escape from the magnetic field environment and hit the reactor wall, and some of them escape from the environment due to the secondary magnetic field and hit the reactor wall again. Although most of the He ions are discharged from the diverter, some of them cannot be prevented from hitting the reactor wall. These fugitive He ions sometimes cause the reactor wall to erode and the Tokamak to collapse in the long run. Because of this process the plasma wall to deteriorate over time and the release of neutrons to the environment. This causes neutronic, thermal, radiative and thermomechanic stress load on the walls of the nuclear fusion reactor. Interface management between the plasma and the wall structures of the nuclear reactor is essential.

The main results of the confinement, like H mode is based on efficient management of the controlled interface. There are many mechanisms occur in the wall structures of the nuclear fusion reactor, for instance adsorption of large quantities of gas particles issued by the plasma, fast particles in the plasma cause erosion and heat flux on the surface of the walls. These mechanisms result plasma radiation to lose large amount of temperature and type of impurities that affect the plasma. This process creates the plasma wall to deform over time to release neutrons into the environment [15-16]. Interaction between the reactor walls and plasma is important factor in designing a fusion reactor. Since plasma induced erosion can seriously shorten the life time of the reactor wall components [17-18].

The interaction of the plasma with the reactor walls has been one of the critical issues in the development of the fusion energy reactor, as plasma-induced wear can severely limit the lifetime of the wall components. There are many interactions that cause plasma with reactor walls. One of them is the divertor segment of the Tokamak fusion reactors. Generally nuclear fusion reactor such as Tokamak type of geometry has a output door called divertor to take of the He out of the plasma. Innovation on the material fusion wall materials research is progressing day by day and understanding the plasma and wall interaction are the central topics in nuclear fusion research under the plasma diagnostic and plasma material interaction literature. Produced fusion artifacts such as fusion ash from He must be cleaned out of plasma. As the He cleans off then the He contacts the divertor walls of the nuclear fusion reactor wall. This mechanism cause divertor and the nuclear fusion walls deform over time and to release neutrals into the environment. Graphite, Beryllium, Moybdenum, Steel and Tugsten are resistant materials against the erosion processes in Tokamak reactors. Tungsten is the most resistant material against plasma with high atomic number and melting point [19-20].

In experimental reactors such as ITER or DEMO, He ash accumulation measurements are stated in recent studies. Observations shows that the effects of the alpha particle concentration on plasma process is studied and the computations are done as in zero dimensional power and particle balance equations so that the He fusion reactions and they reach to the optimal condition. Literature observations stated that He as the as of the deuterium-tritium reaction cannot be avoided in Tokamak fusion reactors. Experimental reactors such as ITER and DEMO shows the low activation materials such as steels SiC ceramic composites and vanadium alloys are tried in nuclear wall materials. There are many new investigations related to diagnostic tools and measurement techniques to measure the deformation amount in the wall materials existed in research. The measured value of the affect of the plasma material interactions is mainly found by the energy (temperature) of the plasma, the charge density of the plasma and the mass density of the material. Since the plasma material interactions are all concentrated on various complex and multifaceted atomic and plasma processes. For instance, materials crystal structures physiology affects the molecular bounds of the plasma particles to create new artifacts during the nuclear fusion operation. During the plasma material interaction nuclear fusion reactor complex processes are existed such as neutralization, desorption, reflection, dust, cavities, sputtering, H/He trapping, interstitials, vacancies inside the material crystal structures, bubbles, dislocations, co-depositions and neutron damaging. These mechanisms must be simulated separately to understand the physics behind the system. Modeling and simulating the plasma material interaction in Tokamak reactors are easy and cheap way to design and build fusion reactors by linking the experimental gaps. Extrapolation of plasma material interaction in literature experiments to the relevant duration of operations in commercial fusion reactors and plasma material interaction results on fusion performances to commercial fusion reactors must be shown. Plasma material interaction in Tokamaks involve complex material and plasma interaction which exists on time and space scales spanning over several orders of magnitude. It is also comprehensive to model and simulate the plasma material interactions in Tokamak to solve a hierarchy of material and plasma models coupling. In order to solve the complex occasions fast computers to compute high performance calculations. In literature multiscale modelling, continuum fluid model, quantum mechanics model, lattice Boltzmann, Brownian Dynamics, Kinetic Monte Carlo and Molecular Dynamics with Monte Carlo are existed as a context in plasma material interactions [21].

In this study, physical erosion, chemical erosion and sputtering rates of Be, Al, C and W used to meet plasma in Tokamak reactor against neutron and He ions were calculated using molecular dynamic Monte Carlo simulation model. This method is effective and efficient when compared with the above mentioned methods. It is easy to establish the borders of the modelling context and time efficient in calculations in the molecular structure when performing the executions in the computer simulation. For this, Python-based OMFIT (One Modeling Framework for Integrated Tasks) and ASE (Atomic Simulation Environment) programs were used. In this context, the open code software ASE Monte Carlo simulation package program was used to examine the interaction of neutron (H+) and He(+) with Be, Al, C and W. As a result of the study candidate materials of the reactor wall, physical sputtering yields, chemical sputtering yields, back scattering yield and total sputtering yield and radiation enhanced sublimation (RES) were calculated.

1 Methods

1.1 Calculation of Total Sputtering Yield

One of the most important concepts in plasma-wall interaction is sputtering yield. Sputtering yield can be defined as the number of particles removed per particle falling on the wall.

$$Y=\frac{\text{NumberofParticlesRemoved}}{\text{NumberOfIncomingIons}} \tag{2}$$

Incoming ion atoms interact with the target atom and cause it to break, as well as being held by the target. Therefore, sputtering depends on both the properties of the incoming ion (energy, mass and kinetic energy) and the properties of the target atoms (atomic mass, surface binding energy, surface texture, crystal orientation). If the kinetic energy of the bombardment particle is greater than the lattice displacement energy of the target atoms, surface damage will occur. The lattice displacement energy is the energy required to move the target atom one atomic distance from its original position.

The above yield of sputtering yield is a very general statement. When evaluated more comprehensively, the sputtering yield also depends on the bombardment energy (E0), the angle of incidence of the incoming ions. A series of elastic scattering is also possible if the electronic stimulation of the target is neglected. Sputtering yield, taking into account elastic collisions and recoil atoms in the target

$$Y(E_0,\theta_0)=\beta\alpha N S_n(E_0) \tag{3}$$

It can be expressed as Here, β is a factor that defines the properties of the target (such as surface binding energy, crystal orientation). N is the atomic density at the target, α is the correction factor defined as the ratio of the mass of the target atoms to the mass of the incoming ions, and Sn is the nuclear arrest cross section is expressed as [22]. From the literature Yamamura to calculate the sputtering yield under normal incoming conditions is given as:

$$(E) = 0.42\frac{a^{*}QKS_n(\epsilon)}{U_s[1+0.35U_sS_e(\epsilon)]}\left[1-(E_{th}/E)^{1/2}\right]^{2.8} \tag{4}$$

1.2 Molecular Dynamics and LAMMPS Method

As part of the simulation studies, Molecular Dynamics calculations were performed using the Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) open source code package program. Molecular Dynamics consists of solving classical Newton's equations for N atoms in a predefined simulation cell. According to classical Newton's equations i. force acting on the atom and the position of the atom is defined as:

$$F_i(t_0)=m_i\ddot{r}_i(t_0) = \frac{\partial U}{\partial r_i(t_0)} \quad (5)$$

$$r_i(t_0+\Delta t)=r_i(t_0) + \dot{r}_i(t_0)\Delta t+\frac{1}{2}\ddot{r}_i(t_0)[\Delta t]^2 + \cdots \quad (6)$$

The interaction potential (U) between atoms was calculated with the embedded-atom model (EAM).

The surface of the simulation cell (100) was bombarded with an ion beam of 1-5 keV. The ion beam was placed 10 Å above the top layer (on the z-axis) and an initial kinetic energy was given. The bombardment simulation was repeated for 2000 times steps with 0.01 fs time steps, and the bombardment simulation was repeated 60 times as a function of the kinetic energy of the ions. Physical sputtering yield values were calculated by counting neutral atoms 5 Å above the target surface. In numerical application, physical sputtering yield and chemical erosion yield are calculated with the generalized equations obtained by using data obtained as a result of Monte Carlo simulation with empirical equations.

1.3 Monte Carlo Method

Monte Carlo Method is a simulation method that determines the state of a system consisting of N particles and in a constant volume V at any temperature T. The Monte Carlo method is based on the numerical solution of a problem that models the motion of objects interacting with their surroundings, taking into account the body-body or body-environment interactions. Partition function in classical physics, is defined as [23]:

$$Q=c\int dp^N dr^N \exp[-H(r^N,p^N)/k_N T] \quad (7)$$

Here, rN is the coordinates of the N particle, and pN is the momenta. is the Hamiltonian of the system. By using Monte Carlo technique in plasma surface interaction, physical sputtering yield and chemical erosion yield are calculated numerically. Then, analytical expressions are fitted to the numerical data obtained for practical applications. Physical sputtering yield based on experiment and Monte Carlo numerical data:

$$Y^{fiz}(E_0)=QS_n(\varepsilon)\left[1-\left(\frac{E_{th}}{E_0}\right)^{\frac{2}{3}}\right]\left(1-\frac{E_{th}}{E_0}\right)^2(\cos\alpha)^{-f}\exp\left(f[1-(\cos\alpha)^{-1}]\cos\alpha_{opt}\right) \quad (8)$$

It is given with Here, Q and threshold energy are feet parameters. E0 is the energy of the incident particle.

2 Results and Discussion

Using the equations given in Method section, the total sputtering yield of H, He and D ions from Be, C, W and Al surfaces, which are the materials used as plasma countering materials in the Tokamak reactor, were calculated. Sputter yield calculated as a function of the kinetic energy of H, He and D ions are given in Fig 1, Fig 2 and Fig 3. In the H, D and He-wall interactions, the atom sputtering yield of W was lower than that of Be, C (Graphite) and Al. W is used as wall material in the Diverter part (the part where He and excess heat are discharged) in Tokamak reactors. Although the probability of splitting atoms from W for these isotopes seems very low from the figures, it is thought that H and He ions are held on the W surface, and even high-energy H ions penetrate into the W and cause diffusion. The solubility of H in W is very low and it occupies the tetrahedral crack regions. He atoms, on the other hand, have self-trapping properties as they settle in these regions of W. In this way, the accumulation of H and He ions in W affects all mechanical and physical properties of W. On the other hand, atom sputtering yield from Be was found to be the highest in the 0-1000 eV kinetic energy range.

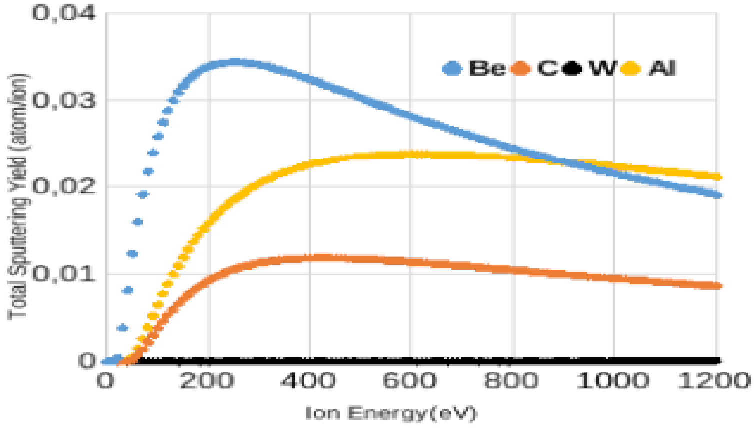

Fig 1. Atom sputtering yield of H from Be, C (Graphite), W and Al surfaces

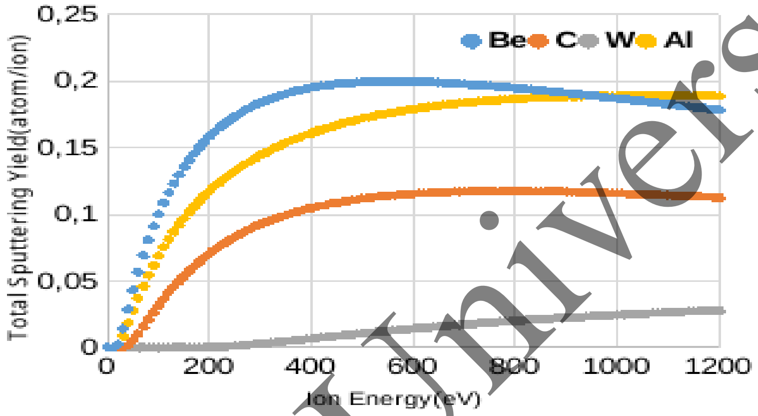

Fig 2. Atom sputtering yield from He's Be, C (Graphite), W and Al surfaces

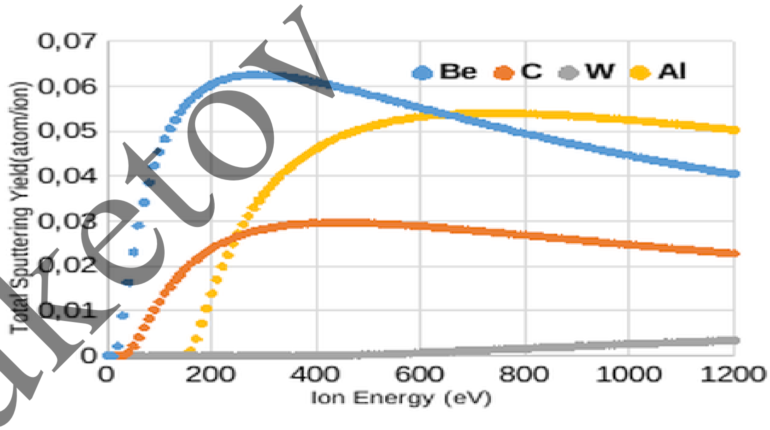

Fig 3. Atom sputtering yield from D's Be, C, W and Al surfaces

From the plotted graphs of the theoretical calculation resultant graphs between Fig-1, Fig-2 and Fig-3 most minimum sputtering yield affected atom can be seen as the bombardment of Ion Energy increased of H, He and D is determined as W. This fact is also similar in the experimental studies of the [24], W is selected as the main wall material in the design of the ITER demo reactor. Since the design of the ITER is now build as monoblock W plates that is placed in the reactor wall. It is already tested to the hot plasma and W gave the most resistive material among the other materials. As the heat in the plasma increases as can be seen in the Fig-1, Fig-2 and Fig-3 sputtering effects which is calculated as total sputtering yield already provide W is the most featured material.

In applications of material development mechanisms given in [24] also states the diamond can be used with W by mixing them to resist against the hot plasma. This is because diamond (C) or graphite is the highest melting point after W. However, since it is low atom numbered material it cannot be used alone. As

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can be seen from sputtering yield graphs H, He and D ion plasma energies, C showed the most resistive case as in sputtering yield when compared to the W.

When we consider Be, it is a candidate material for good thermal loading and minimize radiation losses of the sputtered plasma atoms from H, He or D. However, from the graphics of the sputtering yield theoretical works it is third material with the highest sputtering yield in Fig-1, Fig-2 and Fig-3. In [24] states the experimental works show that Be has low melting point and its high toxicity. This means it cannot be used purely in the long run in the plasma facing material for future. For this reason Be is mixed with other metals such as Titanium and Vanadium. The last material Al is the soft metal crystal which has the higher sputtering yield in Fig-1, Fig-2 and Fig-3 with the minimum atomic number. It is affected by H, He and D plasma ions. Al is not used alone in the nuclear fusion reactors. It is mixed with different alloys. It has the lowest melting point when compared to Be and W. It is specified in [24] studies and Bronze is mixed with Al to be used ITER blanked design experiments. Since pure Al cannot resist against the hot plasma in the long duration process of nuclear fusion.

In the literature, there are several open-coded computer programs that examine the plasma-wall interaction in Tokamak reactors. In the research study, the current package programs and the related literature were examined in detail. Especially Python-based OMFIT (One Modeling Framework for Integrated Tasks) and ASE (Atomic Simulation Environment) programs have been found to be suitable for the purposes of the study. In this context, the ASE package program, which is an open source code software, was modified to examine the H-W interaction and it was determined whether the Lennard Jones and Morse potentials were suitable for the H-W interaction with test studies. Fig 4 and Fig 5 show the minimum energy paths and diffusion barriers calculated by the Nudged elastic band (NEB) method using these potentials for the H-Al interaction. It has also been observed that the diffusion barrier for the Morse potential is high and there is a potential well on the minimum energy path. A high diffusion barrier means that it is difficult for incoming ions to eject atoms from the target up to the diffusion threshold.

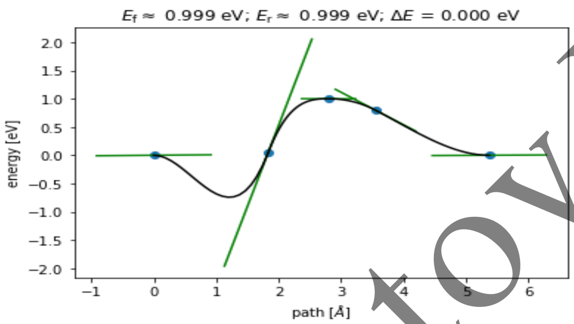

Fig 4. Diffusion barrier obtained by NEB method using Morse potential in H-Al interaction

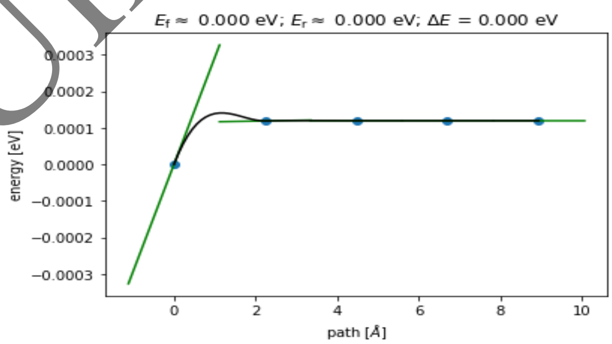

Fig 5. Diffusion barrier obtained by NEB method using Lenard-Jones potential in H-Al interaction

Nudge Elastic Band of the H and Al interaction is also computed in Fig 4 and Fig 5 by using the Lennard Hones and Morse Potentials. It can be seen that the potential threshold energy to eject an atom a high diffusion barrier energy need to be passed for each candidate material that will be used in the nuclear fusion reactor design. That means if the candidate materials are studied in [24], it must be also known the barrier energies also a criteria for selecting the plasma facing materials.

For graphite bombarded with H, D, T and He ions, the physical sputtering yield values calculated using the sputtering yield calculation using Molecular Dynamics, LAMMPS and Monte Carlo processes stated in Method section as a function of kinetic energy, incidence angle and plasma temperature are given in Fig 6, Fig 7 and Fig 8, respectively.

Fig 9 gives the change of chemical erosion yield depending on ion energy. In studies in the literature on graphite, the chemical erosion yield is generally calculated only for the low energy region. Therefore, no peak around 300 eV was observed. This peak indicates that the chemical erosion of the target material is maximum at this energy. It was observed that the chemical erosion caused by deuteron at an energy value of 300 eV was the highest. As can be seen from the figures, the physical sputtering yield increases as the mass of the bombardment ion increases in all four cases. For physical sputtering, this is to be expected.

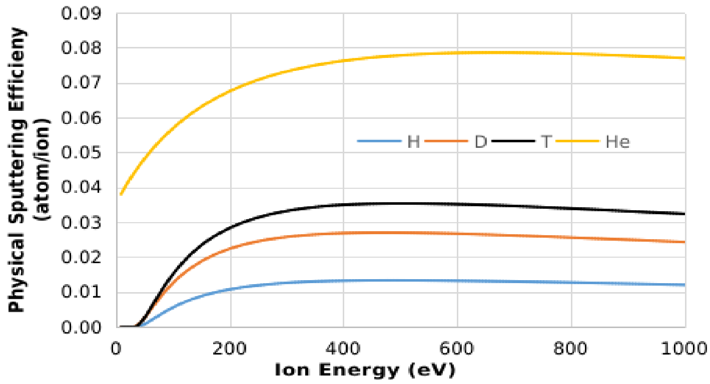

Fig 6. Variation of physical sputtering efficiency depending on the energy of H, D, T and He ions

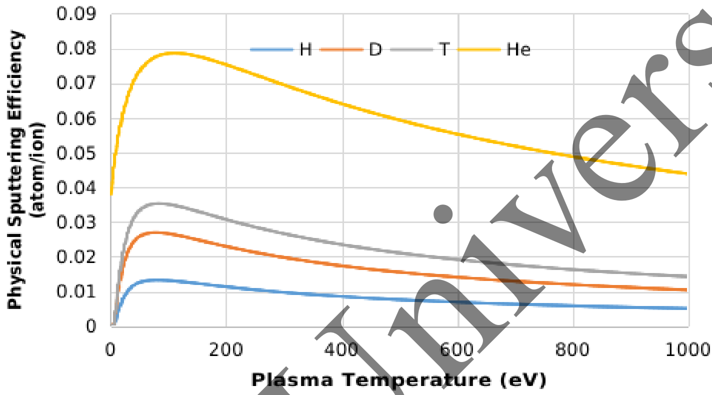

Fig 7. Variation of physical sputtering efficiency depending on the plasma temperature

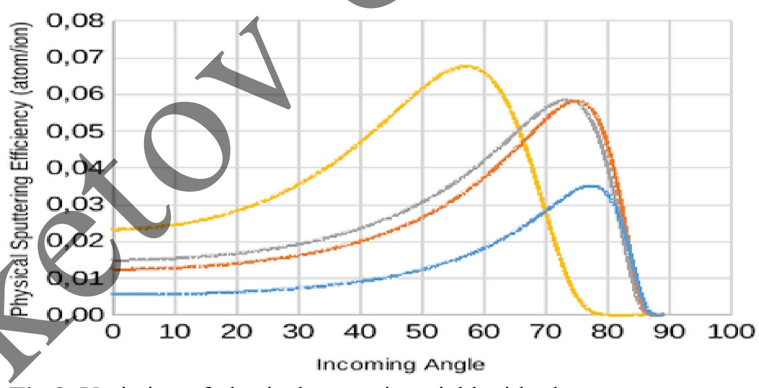

Fig 8. Variation of physical sputtering yield with plasma temperature

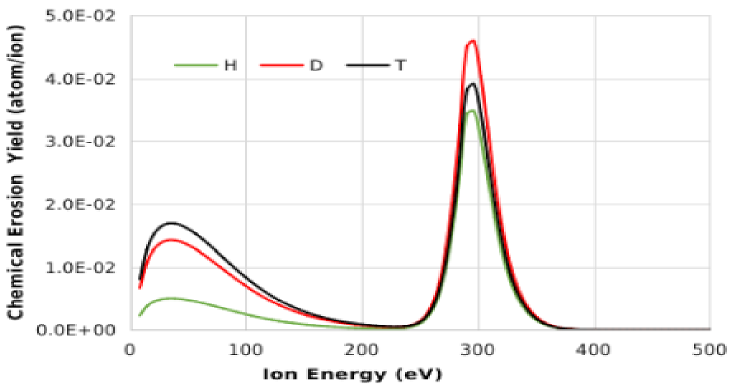

Fig 9. Variation of physical sputtering yield with the angle of incidence of ions

On the other hand, the maximum of the physical sputtering yield was observed for all three hydrogen isotopes at the same location, while the maximum sputtering yield for the He ion was observed at a lower angle. From the graphs depending on the energy and temperature, it was observed that the target material was subjected to a strong physical sputtering up to a certain energy value and then the physical sputtering became stable. When evaluated according to the angle of incidence, it is seen that the physical sputtering yield is maximum when the ions come to the target surface at an angle of 50-80 degrees.

While the physical sputtering yield was generally calculated in the literature studies, in this study, chemical erosion, back scattering, RES (Radiation Enhanced Sublimation) yield and thermal evaporation yield were also calculated using the PSI open source code based on the Kinetic Monte Carlo simulation method. For this purpose, an ion beam consisting of 1013 ions was sent to the graphite surface and chemical erosion, back scattering yield, RES yield and temperature increase in the target material were calculated using the Yamamura technique. Fig 10 The variation of the back scattering yield depending on the ion energy is given. Since low energy ions can be back scattered by ESP (electron stopping power), it is expected that the back scattering yield is high at low temperatures of the plasma and decreases with increasing temperature.

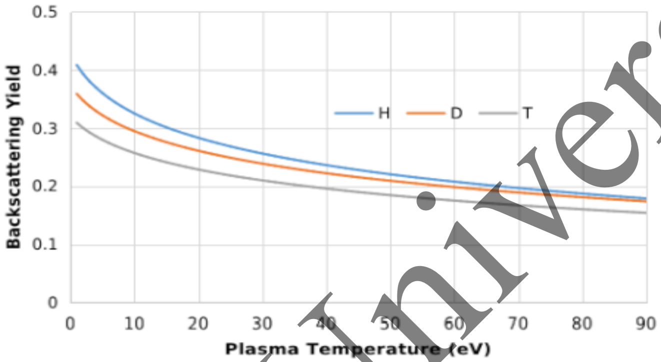

Fig 10. Variation of back scattering yield with temperature of H, D and T ion plasma

The variation of RES yield with the temperature of the graphite target is given in Fig. 11. Radiation enhanced sublimation (RES) is unique to the graphite material and is the result of increasing the ratio of the number of graphite (C) atoms emitted to the number of ions in the plasma beam when graphite reaches high temperatures.

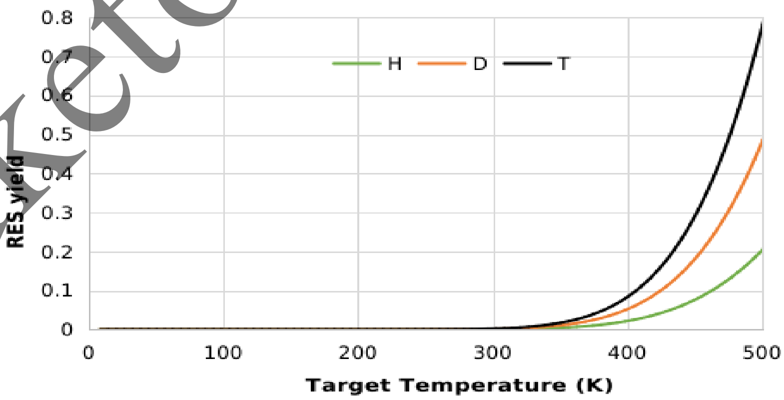

Fig 11. Variation of RES yield with temperature of graphite target

Fig 12 shows the temperature change in the graphite target depending on the energy of the ions. As seen in the figure, the increase in the energy of the plasma beam causes a non-linear increase in the temperature of the target material. In addition, it can be seen that the increase in the number of ions is very important in increasing the temperature of the target material. In the case of 1012 ions, the temperature increase on the target surface is in the range of 300-500 K, while in the case of 1013 ions, the temperature increases up to 3000K.

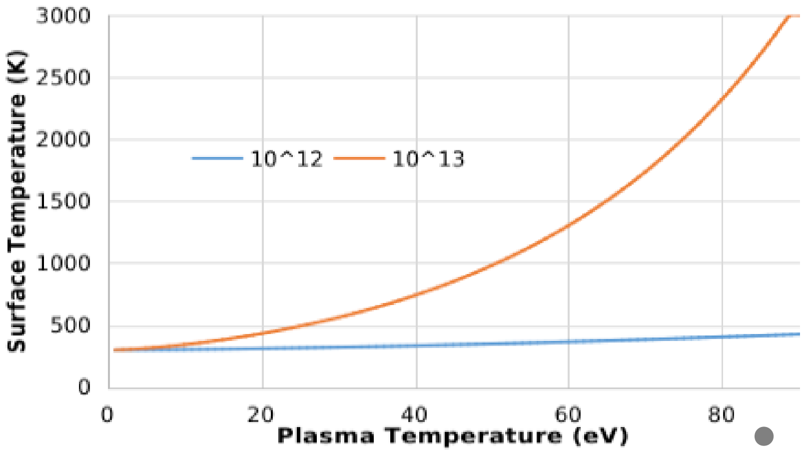

Fig 12. Variation of back scattering yield with temperature of H, D and T ion plasma

Fig. 13 shows the evaporation flux depending on the increase in ion energy. As can be seen from the figure, while the evaporation flux for all ions up to 430 eV is quite low, it is seen that after this energy the flux increases again after a significant peak. Evaporation flux is the number of atoms ejected from the target surface. In the study, it was planned to experimentally measure the ion density in the tube and the number of atoms detached from the target. For this, it is planned to use Langmuir probe. However, due to the increase in the exchange rate, the Langmuir probe was abandoned and it was decided to calculate it by simulation. As seen in the figure, while no atoms were removed from the surface until the threshold energy of 430 eV, atoms began to be snatched from the surface due to this threshold temperature. Especially after this energy value, the sudden rupture of more than 1014 atoms from the surface shows that a rapid erosion starts in the material after this energy.

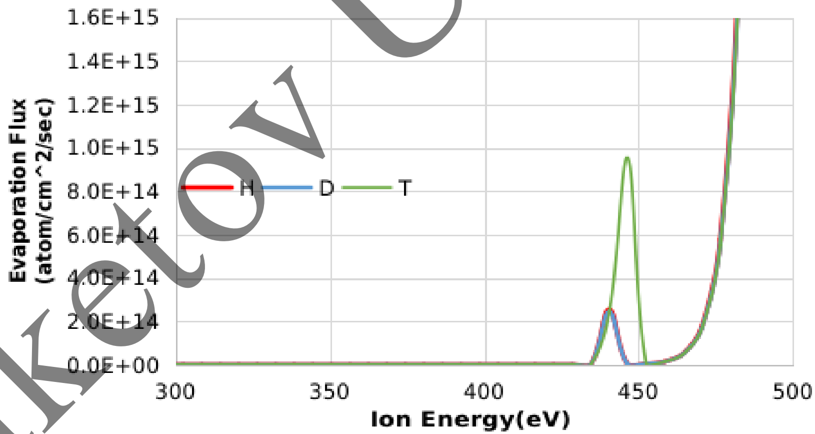

Fig 13. Variation of the evaporation flux in the target due to the change in ion energy

Calculations made within the scope of the study were performed on the Dell Power Edge R740 Rack Server. Chemical sputtering is observed in the materials which is known for the best graphite/diamond (C) atoms. Beside graphite/diamond (C) atoms are affected by the hot plasma H, He and D ions by physical sputtering, it is also known that graphite/diamond (C) atoms are also affected in chemical sputtering path too. In the next part of the theoretical studies, graphite/diamond (C) atoms are bombarded with H, He, D and T plasma ions. Plasma temperature, incoming angle, ion energy, backscattering graphics are calculated in Fig 6 to Fig 13. In study [24] diamond or graphite is mentioned with the highest melting point. However, it has the lowest atom number. That means barrier energy of graphite/diamond (C) material is very low to eject from its crystal structure. Especially H, D and T plasma ions can make chemical bounds with the ejected graphite/diamond (C) atom. In order to prevent this phenomena, graphite/diamond (C) materials are alloyed with other materials such as W to increase the resistance to the hot plasma interaction.

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Conclusion

In the study, the interactions of H, D and He ions and Al, C, Be and W, which are used as plasma meeting materials in Tokamak reactors, were investigated using molecular dynamics and Monte Carlo simulation techniques. From the molecular dynamics simulation results, it was seen that the material with the lowest total sputtering yield was W. This result shows that the material with the highest radiation resistance that can be used in the reactor is Tungsten (W). Calculations of physical sputtering yield, chemical erosion yield, radiation-enhanced sublimation calculations were performed as a result of the interaction of H, D, T and He ions with graphite (C). The results showed that the physical sputtering yield and chemical erosion yield of He cores were the highest. It has also been observed that the surface temperature changes depending on the plasma density (ion number) and the number of atoms detached from the surface increases very rapidly after a threshold value of the plasma energy (approximately 450 eV). For instance, research in Joint European Torus (JET) experiment Be and W mix is used in the vacuum reactor wall. In that occasion researchers observe Be has good heat conductivity, strong gettering, high tolerance for plasma impurity and low nuclear activation. However, as the experiments progress erosion and tritium retention based on H is observed. Because of this plasma purity is also affected. In some of the experimental reactors Graphite is also used as first wall material. But Graphite adsorbs and traps too much H fuel from the plasma into its crystal structure. Generally, engineers use Tungsten material as a selection because it has the highest melting point and extremely resistant to heat because of melting point is high. Inner reactor wall of the tokamak is upgraded from graphite to beryllium. Graphite makes new molecular bounds with the H and test in JET reactor in 2011. Beryllium is excellent in thermal and mechanical properties for the fusion reactor. In ITER reactor it is considered to be Tungsten material on the wall material and Beryllium in the divertor regions of the Tokamak reactor walls. Aluminum is selected as a replacement against the Beryllium in the divertor regions of the Tokamak reactors. It is cheap and easy to supply to the reactor designers. However, its metal structure is affected by He highly in its crystal structures. All of the body of the crystal structure in the Al is transform into the cheese type of formation after the He interaction. Its melting point is also low when compared to all three materials Be, C and W. These observations are also made in the molecular dynamic models of the study. Tungsten showed low sputtering yield affection in the model, then Be and after Al and C showed the similar graphic values. When the calculation results are evaluated together, it has been concluded that Tungsten (W) is the most suitable material for facing with H, D and He ions in Tokamak reactors, but Tungsten (W) has high Tritium retention and it is appropriate for the components to face Tritium to be made of Aluminum (Al) or Graphite (C).

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