Molecular dynamics simulations of deuterium-beryllium interactions under fusion reactor conditions

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Beryllium (Be) is a strong candidate as plasma-facing material for the main wall of future fusion reactors. Thus, its erosion plays a key role in predicting the reactor's life-time and viability. MD simulations can be a powerful tool to study Be behavior under high plasma particle flux.

In this work, beryllium sputtering due to D bombardment is studied using MD simulations. We have analyzed the fundamental mechanisms for Be erosion considering some important parameters that influence the outcome, such as particle flux and surface temperature. It is shown that the Be erosion yield is strongly dependent on the surface temperature and its dependency on the particle flux is negligible. We also show that different species of Be molecules can be sputtered from its surface, mainly due to swift chemical sputtering mechanism.
Contents

1 INTRODUCTION 2

2 PLASMA-WALL INTERACTIONS 5
  2.1 Nuclear Fusion .............................................. 5
  2.2 Types of fusion reactors ................................. 6
    2.2.1 Stellarator ........................................... 6
    2.2.2 Tokamak ............................................... 7
  2.3 Nature of plasma-wall interactions .................... 9
  2.4 Sputtering .................................................. 11
  2.5 First wall materials ...................................... 13

3 Methods 16
  3.1 Binary Collision Approximation .......................... 16
  3.2 Molecular Dynamics Simulations ........................ 18
    3.2.1 The MD algorithm ................................... 18
    3.2.2 Interatomic potentials .............................. 21
  3.3 Simulation setup .......................................... 25

4 Analysis and Results 27
  4.1 Overview of previous studies on BeD .................... 27
    4.1.1 Experiments and simulations ........................ 27
    4.1.2 Sputtering yield .................................... 27
    4.1.3 Molecule fraction ................................... 28
  4.2 This work’s contribution .................................. 28
    4.2.1 Sputtering .......................................... 28
    4.2.2 Depth profile ....................................... 33
    4.2.3 Surface structure ................................... 34

5 Summary 36

6 References 38


1 INTRODUCTION

One of the most important challenges of 21st century is to find new energy sources that can fulfill the increasing demand of energy caused by the current population expansion. The new energy resources must replace fossil fuels such as coal, heavy crude oil and natural gas, since they are becoming scarce. Further, release of the green-house gas (CO₂) by these energy sources could affect the atmosphere and cause global climate change [1]. During the last decades, few alternatives, such as wind, solar and hydro-power energies are greatly progressing for a safe and CO₂-emission free future.

Fusion power may offer a power plant scale energy production with an almost unlimited fuel supply. Also it is safe; it has no emission of the harmful gas CO₂, no long life radioactive waste and it is independent from the local weather and geographical conditions. Fusion is a process where large amounts of energy are produced by the same process that happens in stars. In fusion, light atoms become so hot that they fuse into new heavier elements and release the excess binding energy as heat. The most suitable fusion reaction for an earthbound fusion is between two hydrogen (H) isotopes, deuterium (D) and tritium (T). D is abundant in seawater and T can be generated from lithium (Li), which is a common element in the Earth’s crust. When these two nuclei combine (Fig. 1.2), on one hand, they form a neutron (n) with an energy of 14.1 MeV. This hot neutron can then be captured, and its energy used just as in a conventional power plant, e.g. to heat a coolant fluid (e.g. water) for producing steam to turn a turbine. On the other hand, a helium nucleus (He) with an energy of 3.5 MeV is produced. Since the helium nuclei are charged, they will stay inside the reactor and transfer their energy to the plasma, keeping it hot.

In thermonuclear fusion, the nuclei must be forced together in spite of the coulomb repulsive force, by heating the fuel up to temperatures around 200 million degrees. At these temperatures atoms are highly ionized and form a plasma. The plasma is surrounded by a vacuum vessel and is confined by a magnetic field, which keeps it away from the fusion reactor walls.

Different devices have been developed for plasma confinement, the furthest developed one being the tokamak (the word is an abbreviation from the original Russian term "toroidalnaja kamera s magnitnymi katushkami" meaning toroidal chamber with
Figure 1.1: The fusion of deuterium with tritium creates helium-4, frees a remaining
neutron, and releases energy. Because $E = \Delta mc^2$, when two atoms are fused, a very
small amount of mass can be converted into a large amount of energy. [2]

magnetic confinement). In a tokamak the plasma is shaped like a torus [3]. The plasma
will interact with the inner surrounding walls of the reactor, the plasma facing com-
ponents (PFCs). The PFCs include the main wall and divertor. Plasma wall interaction (PWI) can harm both the walls and the plasma. The walls get thinner due to erosion. If the eroded particles migrate to the confined plasma, they will cause energy losses by radiation. Radiation losses depend on the atomic
number of the impurity, Z, where heavier elements are more harmful [4]. Moreover,
controlling the erosion is important to maximize the wall lifetime. Examples of suit-
able plasma facing materials (PFMs) are beryllium (Be) for the first wall and carbon
(C) and tungsten (W) for the divertor region.

The behavior of these materials can be studied with experimental fusion devices.
The roadmap towards a future fusion power plant is built based on knowledge gained
various devices. Due to their first wall material choice, the most relevant devices for
the present work are: JET, its successor ITER and a demonstration reactor called
DEMO. JET represents a pure scientific experiment aiming to test different materials
and plasma configurations for ITER. The reactor scale experiment ITER is designed to
deliver ten times the power it consumes, demonstrating heat ignition can be achieved.
The next foreseen device, DEMO, is expected to be the first fusion power plant to
reliably provide electricity to the grid [6]. However, computer simulations are an essential and complementary tool to achieve a
theoretical understanding of the experimental systems and predict the following steps
more accurately.

The purpose of this study is to improve the knowledge of the behavior of fusion reactor first wall materials when subjected to energetic particles. In greater detail, the first wall material, Be, under irradiation by the main plasma component, D, has been modeled in this work. These results will provide more accurate data for further plasma-wall interaction studies and will help in the interpretation of experiments.
2 PLASMA-WALL INTERACTIONS

Plasma-wall interaction (PWI) effects are among the most important problems to be solved along the way towards fusion as an energy source. PWI issues in fusion devices are expected to have a strong impact on plasma performance, and affect the operation of devices as well as the availability of them. As a result, a discussion of PWI effects is related to the discussion of the general building of a device. It also affects the choice of PFM [7].

2.1 Nuclear Fusion

Nuclear fusion is the main source of energy in the universe as it is the energy source of the stars. Fusion energy is generated in the sun when the nuclei of light elements, such as hydrogen, fuse together to form heavier elements. As given by Einstein’s famous formula, \( E = \Delta mc^2 \), energy (E) is gained because of the change in the nucleus mass (\( \Delta m \)) where c is the speed of light.

However, because of the strong Coulomb repulsion of the nuclei, the fusion reaction happens at high temperatures. The nuclei collide at high kinetic energies and a small fraction of them join together, releasing a large amount of energy. For example, this is the reaction of choice in ITER [8]:

\[
\begin{align*}
2D + 3T &\rightarrow n + 4He + 17.6MeV.
\end{align*}
\]

Due to momentum conservation, most (80%) of the energy of the D-T fusion is carried away by neutrons (n). Some of these neutrons can be trapped in a blanket containing lithium (Li), leading to [9]

\[
\begin{align*}
6Li + n &\rightarrow 3T + 4He + 4.78MeV.
\end{align*}
\]

According to these reactions, \( ^2D \) and \( ^6Li \) are the ultimate fuels for fusion. Since the fusion reaction is not a chain reaction, a fusion reactor is safe from nuclear explosion and the lifetime of the only radioactive component, T, is short, 12 years. As mentioned in the introduction, the other neutrons will be used for heating the coolant, thus extracting the fusion energy.
2.2 Types of fusion reactors

As the plasma particles are ionized, the plasma can be confined in toroidally closed magnetic surfaces [10]. The two main categories of magnetic fusion devices are tokamaks and stellarators. However, in each category there are many variations in design, with both benefits and disadvantages.

2.2.1 Stellarator

The stellarator is a helically symmetric system based on a torus-shaped vessel. Its performance depends on accurately designing coils for producing the helically shaped magnetic field needed to confine the plasma. One of the major advantages of the stellarator is not needing a current in the plasma, which makes it an ideal concept for a fusion power plant. In addition, the stellarator should be able to keep the plasma in steady-state [11].

One of the challenges in a stellarator is producing the helically shaped magnetic field. This demanding design issue, along with the costs of realising such complex designs have made stellerators less common than tokamaks.

At the moment, the advanced stellarator Wendelstein 7-X is under construction in The Max Planck Institute for Plasma Physics in Greifswald, Germany. Its magnetic coils are engineering masterpieces, bent elaborately to create the required magnetic field and also to fulfill the requirements for confining the plasma. In the 7-X stellarator, the magnetic coils are superconducting in order to achieve intense magnetic fields [6].

With the progress of 3D imaging and construction techniques, interest in stellarators has increased, becoming the main competitor to the tokamak for fusion energy [12].

![Schematic of a stellarator.](image-url)
2.2.2 Tokamak

The most developed design for magnetic confinement plasma is the *tokamak*. This method is also the basis for the design of near future fusion reactors. The magnetic coils create a toroidal magnetic field. Fig. 1.2 illustrates the tokamak configuration. This magnetic system consists of superconducting toroidal and poloidal field coils, a central solenoid and a set of correction coils that magnetically confine, shape and control the plasma inside a vacuum vessel [3].

In order to prevent the entry of impurities from the air outside and the escape of the fuel from inside the chamber, as well as to protect the magnetic coils, the vessel of a tokamak is vacuum-proof. The vacuum vessel is around the divertor and the main wall. The size of the vacuum vessel imposes the volume of the fusion plasma; the larger the vessel, the greater the amount of power can be produced. The interior surface of the vacuum vessel in ITER is covered by a Li blanket, where part of the fuel is produced.

The limiter is a material surface within the tokamak vessel which defines the edge of the plasma and thus avoids contact between the plasma and the vessel. The divertor is also a separate region in the reactor, where the exhausted ions leave the reactor, but divertors show several important advantages over limiters. Limiters are easier to design, but they cannot handle appropriately heat and sputtering in reactors with higher power and particle flux densities [14]. Thus, choosing a proper material for divertor and limiter for future fusion reactors is highly critical. ITER planned to begin operations with a divertor target made of carbon fiber-reinforced carbon composite (CFC). CFC is a material that has high thermal conductivity. However, the CFC has recently been discarded as divertor material due to excessive fuel retention (see section 2.3). Thus, the divertor in ITER will be entirely made of tungsten (W).

Both the main wall and divertor are facing the edge plasma. The hot plasma might have the leakage of energetic and radioactive particles which could damage both the main wall and the divertor. One of the best candidate for the first wall material is beryllium (Be) because of its low atomic number and high thermal conductivity. Finally, there is a wall between the blanket and the plasma.
History of tokamaks

Experiments in tokamaks devices have been ongoing for decades, improving their design. The first international collaboration device was named T-3, and it was built in the Kurchatov Institute, Moscow, Soviet Union in 1963 [15]. Its larger version, T-4, was tested in 1968 in Novosibirsk, conducting the first ever quasi-stationary thermonuclear fusion reaction, a big achievement for reaching electron temperatures of over 1000 eV in a tokamak device [16].

Many tokamaks have been built ever since all around the world. Some of them had been operated more than 10 years like the Tokamak Fusion Test Reactor (TFTR Princeton University, USA), with operation from 1982 until 1997. It was followed by the PDX (Poloidal Diverter Experiment) and PLT (Princeton Large Torus) devices [17].

Today, there are plenty of devices which are currently in operation. The Joint European Torus (JET) is the largest tokamak in the world. This is the only operational fusion experiment capable of producing fusion energy. Its construction started in 1978 in Oxfordshire, UK. There are also other devices such as JT-60 (JT stands for Japan Torus) that was launched in the middle of the 1970s by the Japan Atomic Energy Research Institute [18]. JT-60 is a typical Tokamak with a D-shaped poloidal cross-section, similar to JET and its construction was due to very encouraging scientific
results and a significant increase in the budgets attributed to research on controlled fusion.

In the near future, ITER (means "the way" in Latin) will start its operation. It is an international project being built in Cadarache, France, and its construction began in 2010. It will be capable of producing 500 MW of fusion power. ITER is a step towards the first power-plant scale fusion reactor DEMO (DEMONstration Power Plant), which will be built upon the expected success of the ITER. According to the preliminary timetable, the construction of DEMO is expected to begin in 2024 and DEMO’s aim is to produce 2000-4000 MW of fusion power [19].

2.3 Nature of plasma-wall interactions

Plasma-wall interactions issues are among the most important challenges along the way to constructing a future fusion reactor. In a fusion reactor, a very hot plasma (200 million degrees Celsius) is kept away from the wall of the chamber by using a strong magnetic field. However, this confinement cannot be perfect so that the exhausted particles can leave the reactor. Thus, the ions from the plasma will hit the plasma-facing materials (PFMs). These interactions may cause problems as they involve high heat and particle fluxes from plasma. Therefore, the best candidates for PFMs are ones that are heat-resistant, thermally conductive, resistant to physical and chemical erosion and show low fuel retention.

These three crucial issues are the main PWI concerns [20]:
1. Lifetime of PFMs.
2. Dust production from eroded PFMs.
3. Tritium (T) inventory in the vacuum vessel.

The PFMs may erode because of sputtering, melting, sublimation and brittle destruction [21]. The damage to the wall materials is caused by the impact of plasma fluxes and erosion of materials. This results in both reduction of material lifetime and plasma contamination. Fig. 2.3, shows a basic process that happen at the plasma-surface interface. Details about different types of erosion in PFMs are discussed in the following section (2.4).

In fusion science, dust represents all erosion outputs which are due to PWI processes. Dust are particles in the nanometer (nm) or micrometer (µm) size range inside
the vacuum vessel. Dust particles can result from various erosion processes. Also the size of dust particles is important. Some of them are too heavy to be moved by the plasma and tend to remain at the bottom of the vacuum vessel. They can be removed by vacuum chamber cleaning during the shutdown period. In contrast, smaller dust particles usually have a high sticking coefficient, making them to stick chemically on the reactor walls, which makes the cleaning procedure harder. Since carbon (C) was removed from the divertor, dust production plays a relatively minor role in fusion devices and it seems not to be an operation hazard in comparison with the two other PWI issues.

Fuel retention is related to the fuel particle deposition or implantation in the PFCs. Retention becomes more important when radioactive tritium (T) is used as fuel. Only a limited amount of the T will be allowed in a fusion reactors for safety reasons. For example the legal limitation for tritium content in ITER is 700 grams between shutdowns. Figure 2.4 shows the estimation of tritium retention in ITER for the all-C (blue line) and all-W options (red line) compared to the initial material choice CFC/W/Be (magenta). In addition, retention values for the option of a full-W divertor and Be first wall are included (black line). The assessment was performed assuming different particle fluxes to different divertor and wall areas [22]. It is also economically not feasible to retain the fuel on the wall, where it is unavailable to the burning plasma.

There are different mechanisms for T retention, such as co-deposition or implantation as shown in Fig. 2.3. Co-deposition is the simultaneous deposition of fusion fuel and impurity particles on the surface of the PFCs. Co-deposition of T with materials
that eroded from the PFCs is expected to be the main process of T accumulation in the vessel. Tritium can move deep inside the walls and be trapped in remote areas, which can makes dust removal harder. For example the erosion of carbon leads to the production of hydrocarbons and eventually their re-deposition on the wall and in remote area by trapping T. Co-deposition also occurs in beryllium Be as the main wall of the reactor.

T retention also happens by an implantation mechanism where ions can go through the material and implant there. It is the main retention mechanism in tungsten.

2.4 Sputtering

The erosion of the PFCs surface is also a highly critical issue [23]. Sputtering of materials is a process in which atoms or molecules are ejected from the material surface, for example, by plasma ions bombardment. Sputtering depends on a number of parameters such as mass ratio of incident particles to surface atoms, particle energy and flux, as well as surface temperature [24]. There are three main sputtering mechanisms: physical, chemical and electronic sputtering.
Electronic sputtering is due to energetic electrons such as in a transmission electron microscopy or due to very high-energy ion bombardment, where the electronic excitation can cause sputtering [23]. However, the electronic sputtering yields are low in fusion reactor conditions and hence the focus of this work is on chemical and physical sputtering.

Physical sputtering can happen in all materials independent of their structures. It results from the transfer of kinetic energy of the incoming particle to the target atoms on the surface layers [37]. Bond breaking and therefore sputtering will be take place if the energy received in the direction normal to the surface is sufficient to overcome the surface binding energy $S_E$. Three regimes exist in this process: 1. If the energy is not enough to produce collision cascades, the sputtering occurs as a single knock-off event. 2. A linear cascade event can happen when a few cascades, but no sub-cascades are created. 3. When the incoming ion is heavy enough, the collisions occur very close to each other. In this case the binary collision approximation (BCA) is not valid anymore (neither at low energies) and the collisional process should be understood as a complicated process of many-body interactions between thousands of atoms. This causes what is known as heat spike [23].

Chemical sputtering occurs when the incoming particles form chemical compounds with the surface atoms by breaking and forming new bonds. Therefore, chemical sputtering is highly dependent on the surface materials and on surface temperature, leading to processes such as thermal desorption and evaporation. To prevent such processes, a cooling system should be designed in the reactor’s first wall to control the wall temperature to be always safely below a critical temperature. The erosion of hydrocarbons in fusion reactors is an example of the chemical sputtering. One well understood way by which molecules can form at the surface of certain materials by swift chemical sputtering (SCS). In the SCS process, an energetic particle penetrates between two substrate atoms, causing their bond to break, which release a surface atom together with any other atom bound to it. For example beryllium surfaces can also form and sputter BeD molecules when exposed to D plasma. The SCS in Be is illustrated in Fig. 2.5. The figure shows sputtering of a BeD and a $D_2$ molecule due to 10 eV D ion bombardment of Be surface. The D ion enters between the Be pairs causing their bond to break and bind with a Be atom [23].

The erosion rate of a surface is defined as the sputtering yield $Y$. It is defined as
Figure 2.5: (a)–(f) A sequence of molecular dynamics simulation results showing the chemical sputtering of Be during low-energy deuterium (D) ion irradiation. (a), (b), and (c) show the impact of the 10 eV D ion between Be atoms (large blue spheres), while (d) and (e) demonstrate the local rearrangement and rotation that breaks several Be–Be bonds prior to the chemical sputtering of a BeD molecule in (f) [23].

the average number of atoms ejected from the surface per incident ion. Y depends on several factors such as type of the surface atom, binding energy of surface atoms, relative mass of the ions and atoms, incident ion energy and angle of incidence of ions. Measurement of sputtering yields can be done by different experimental techniques such as mass loss measurements, detection of sputtered particles on a collector, field-ion microscopy and spectroscopy. Because of low-energy many-body interactions in the PWI relevant systems, modeling must be used for studying chemical sputtering, such as molecular dynamics (MD).

2.5 First wall materials

Plasma facing components (first wall materials) in fusion reactors are exposed to extreme conditions such as high thermal and particle loads and thus, they have several requirements. First they must be able to tolerate high temperatures, which can even exceed 1000 degrees Celsius in certain locations of the reactor. Secondly, the wall
materials must be able to withstand bombardment by high-energy neutrons produced by the fusion reaction, which can damage the material’s crystal structure. Furthermore, tritium fuel retention and transmutation of elements is a major concern for the operation of fusion reactors. Atoms of one element can transform into another element by transmutation [29]. In addition chemical, as well as physical sputtering, which leads to erosion and re-deposition processes of mixed layers (see section 2.3), has to be taken into account. Finally, if an eroded particle enters the plasma core, its electrons will be excited, loosing the plasma energy by irradiation. Further, these impurities dilute the fuels in the plasma, leading to a lower reaction rate. Thus, a particle entering the core plasma should be as light as possible. Because of the above mentioned requirements, the number of candidate materials for high thermally loaded plasma facing components is limited.

In current reactors, carbon is the most popular wall material, because it resists extremely high heat loads and as a light atom, it does not harm the plasma performance. In fact, sputtered carbon is even beneficial for cooling the edge plasma at the divertor. The benefits of carbon-fiber composites (CFC) and silicon carbide based materials for fusion reactors have been discussed for decades, primarily due to their inherently low induced radioactivity [30,31]. However, as carbon has high tendency to react with and bond to hydrogen atoms, in a reactor carbon leads to fuel (T,D) retention which makes this material unacceptable for future fusion reactors [6].

Another candidate material for the first wall of a reactor is tungsten (W), a heavy metal. The important advantage of W is its high melting point (3422 degrees Celsius). It also shows a high physical sputtering threshold and low chemical reactivity with H-isotopes. Moreover, W has a high thermal conductivity and a low tritium retention potential. Thus, W is used for the divertor, where the PWI are most intense. However, it has a high atomic number so sputtered W particles under the confined plasma, would be very harmful for the operation of a reactor.

The best candidate material for the main wall of a reactor is beryllium (Be). Be is a metal with a low atomic number. It has a hexagonal closed packed crystallographic structure in equilibrium. Its melting point is not as high as tungsten’s, but it is sufficiently heat resistant to provide a light alternative material for those parts of the wall that do not suffer the highest heat loads [6], as they do not come into direct contact with the plasma. It also has a high thermal conductivity. Further, Be is able
to remove oxygen from the plasma due to its oxygen affinity [32]. However, Be can be sputtered by the SCS mechanism.

In this thesis, the behavior of Be as main wall material in fusion reactor at different temperatures and irradiated by different deuterium (D) fluxes is studied.

Figure 2.6: An artist’s view of ITER [33].
3 Methods

To study the behavior of materials under irradiation in fusion reactors, several experimental devices exist, such as small fusion and linear plasma devices. However, the experimental studies cannot always explain the exact mechanisms participating in the PWIs. Therefore modeling can be used to complement the study of PWIs, mediating between theory and experiments. Therefore, computer modeling has a very distinguished role in fusion research besides the experimental studies [6]. The present study at the atomic scale is done to complement the understanding of materials erosion in a fusion reactor’s main wall.

In this section, the computer simulation methods that have been used in this work are described.

3.1 Binary Collision Approximation

One of the widely accepted techniques employed for sputter erosion and for studying ion irradiation induced damage at surfaces, which is important at higher energies, is the Binary Collision Approximation (BCA) [34]. In BCA it is assumed that the collisions between atoms can be approximated by elastic binary collision. In this technique a single collision between the incoming ion and a target atom is treated by solving the classical scattering integral between two colliding particles. Solution of the integral results in both scattering angle of the incoming ion and its energy loss to the target atom. The scattering angle between the ion and the target atom is calculated as

$$\theta = \pi - 2 \int_0^{\frac{1}{2}} \left( \frac{1}{p_2^2} \left[ 1 - \frac{v(u)}{E_1} \frac{(m_1 + m_2)}{m_2} \right] - u^2 \right) \frac{1}{u} du$$  \hspace{1cm} (3.1)

The interatomic potential is usually a screened coulomb potential of the form [9]

$$V(r) = \frac{1}{4\pi\epsilon_0} \frac{Z_1 Z_2}{r} \phi\left(\frac{r}{a}\right)$$  \hspace{1cm} (3.2)

where $Z_1$ and $Z_2$ are the magnitudes of the charges, the scalar $r$ is the distance between the charges and $\epsilon_0$ is the dielectric constant. The Ziegler-Biersack-Littmark (ZBL) screening function is often used for $\phi\left(\frac{r}{a}\right)$ where $\frac{r}{a}$ is a screening length [35].

The energy loss of an incoming ion to target electrons can be handled separately as an inelastic energy loss. This energy loss process reduces the energy of the incoming
Figure 3.1: Schematic illustration of binary collision between atoms [36].

ion, but does not change the direction of that. A target surface layer atom is considered to be sputtered if its energy normal to the surface is larger than the surface binding energy [37].

The advantages of BCA is its speed, which is 4-5 orders of magnitude faster than MD (see next section) [9]. This approximation is reasonable for high-energy recoils where the surface binding energy is small compared to the recoil energy of the atoms. Therefore BCA is based on some assumptions and limitations. This approximation can arise at low ion energies, in very dense materials, or when chemical effects play a role in materials.

There are many computer simulation programs based on BCA dealing with crystalline and amorphous targets. A static Monte-Carlo program which is known as transport of ions in matter TRIM is one of the programs dealing with amorphous targets. The reciprocal dynamic version of that is TRIDYN which can describe not only collision effects but also compositional changes in solids [38]. SDTrimSP (where S stands for static, D for dynamic, the end S stands for serial and P for parallel) is the combination of two mentioned programs with all possible output facilities provided, such as sputtering, backscattering and transmission.

The basic physics in the new program SDTrimSP is the same as in the former versions. It assumes an amorphous target structure at zero temperature and infinite side size and treats the bombardment of incident ions on different target structures [39]. Stopping and Range of Ions in Matter SRIM code is another program which can calculate interaction of ions with matter. The core of SRIM is TRIM.
### 3.2 Molecular Dynamics Simulations

Molecular dynamics (MD) is a simulation method based on solving classical equations of motion for each atom in the system. Currently, MD can be used on systems with millions of atoms. The popularity and applications of MD has been increasing since its first usage in the 1950's with increasing computational power [40]. In MD simulations, the computational time is for finite-ranged interatomic interactions and it is a linear function of number of atoms in system.

#### 3.2.1 The MD algorithm

MD solves Newton’s equation of motion for atoms. It can be based on quantum-mechanical interactions, but the simulation used in this work is the classical MD method, based on the Born–Oppenheimer approximation. This approximation states that the dynamics of electrons is so fast that they reach the equilibrium well before the nuclei do. Thus, the two subsystems may be treated separately. The forces acting between atoms are given by so a called *interatomic potential*. The effect of the electrons is approximated as a single potential energy surface and electronic effects like the formation of atomic bonds, are implicitly included in the interatomic potential that is used.

Figure 3.2 describes the algorithm for an atomistic MD simulation. The algorithm starts with setting initial positions \( \mathbf{r}_i \) and velocities \( \mathbf{v}_i \) of the atoms \( i = 1 \ldots N \). Then, Newton’s equations of motion for this system are solved

\[
\mathbf{F}_i(\mathbf{r}_i, t) = m_i \ddot{\mathbf{r}}_i = m_i \mathbf{a}_i(t) = -\nabla_{\mathbf{r}_i} V(\mathbf{r}_i)
\]

where \( m_i, \mathbf{r}_i(t), \mathbf{a}_i(t) \) and \( \mathbf{F}_i(\mathbf{r}_i, t) \) are the mass, position, acceleration and force acting on the atom \( i \) at a time \( t \), respectively, determined by the interatomic potential \( V(\mathbf{r}_i) \). The accelerations for the atoms can be calculated from this equation.

This equation is solved at each time step to calculate the new atomic configurations. In all simulations, the timestep must be much smaller than the inverse of the fastest vibrational frequency in the system. When the timestep gets smaller the number of steps needed to reach the final time, increases and the modeling becomes computationally less efficient. In most MD-simulations the timestep is a few fs.
The integration of Eq. 3.3 is done numerically, using an accurate and efficient integrator algorithm. For example, the Gear 5 predictor-corrector algorithm [41] is employed in the MD code PARCAS [42] used in this thesis. In a predictor-corrector method, first a prediction for the result is made and then this result is corrected in a second step. The corrector step can use different methods to refine the result by using the old data.

After computing the accelerations, the new positions for the atoms can be calculated. With the given timestep ($\Delta t$) the new position can be calculated as

$$\mathbf{r}_{i+1} = \mathbf{r}_i + \mathbf{v}_i \Delta t + \frac{1}{2} \mathbf{a}_i \Delta t^2$$  \hspace{1cm} (3.4)

where $\mathbf{r}_i$ and $\mathbf{v}_i$ are the old position velocity, respectively, and $\mathbf{a}_i$ is the calculated...
acceleration. The new velocity of the atom is determined by

\[ \mathbf{v}_{i+1} = \mathbf{v}_i + \mathbf{a}_i \Delta t \]  

(3.5)

However, these equations are rather inaccurate numerically, and much better accuracy can be achieved by adding a few more terms to the expressions [59]. After calculation of new positions and velocities, the list of nearby atoms for each atom in the system must be updated, usually done every \( \sim 10 \) simulation steps.

Moreover, periodic boundary conditions (pbc) can be used to simulate bulk materials and infinitely long wires without having to simulate too many atoms.

Often the temperature must be controlled throughout the simulation. There can be a variation of the initial temperature, a cooling of the system to release the excess of energy introduced by a recoil, heating up to relax the system or the system is kept at constant temperature during the whole simulation. In this method, the initial temperature is achieved by using Maxwell-Boltzmann distributed temperatures for all atoms, so all atoms will not have exactly the same kinetic energy.

In PARCAS, the temperature is controlled by using the Berendsen thermostat method [43]. Here the system temperature \( T \) is controlled by coupling it to an external heat bath at a temperature \( T_0 \). Thus, the system’s temperature will relax exponentially to the desired \( T_0 \) with a time constant \( \tau \),

\[ \frac{dT}{dt} = \frac{T_0 - T(t)}{\tau} \]  

(3.6)

where \( T(t) \) is the temperature of the system at time \( t \). In MD, this is implemented as a friction term in the equation of motion (Eq. 3.3), since the temperature of the system is defined by the velocities of the atoms in it,

\[ m_i \mathbf{a}_i(t) = \mathbf{F}_i(\mathbf{r}_i, t) - m_i \gamma (T_0/T - 1) \mathbf{v}_i \]  

(3.7)

where \( \tau = (2\gamma)^{-1} \) is the time constant

\[ \lambda = \sqrt{1 + \frac{\Delta t}{\tau} \frac{T_0}{T} - 1} \]  

(3.8)

In a similar way to the temperature control, the pressure control can be achieved by scaling the positions instead of the velocities of atoms. Depending on the simulation
setup, it is desired to maintain the system at constant pressure and let the volume \( V \) of the simulation box fluctuate.

The Berendsen pressure control \cite{44}, scales the atom coordinates and the simulation cell dimensions by multiplying them by,

\[
\mu = \sqrt{1 - \frac{\Delta t}{\tau_P} (P - P_0)}
\]  

(3.9)

where \( P_0 \) is the average pressure of the system, \( P \) the desired pressure and \( \tau_P \) is the time constant that determines the pressure scaling rate, as in the temperature control.

### 3.2.2 Interatomic potentials

The result of an MD simulation depends on the forces acting on the atoms. Thus, the most critical part of the MD simulation algorithm is the calculation of these forces (see Eq. 3.3) from the interatomic potential \( V(r_i) \). So, developing desired potential models that can describe the interaction between atoms in a solid well, is vital. These potentials depend on different parameters. In general, they consist of attractive and repulsive terms, to account for the attractive and repulsive interactions between electrons and nuclei, due to the different charge signs, at different interatomic distances. Although these potentials are classical, their formalism is usually derived from quantum mechanical principles.

**Brenner-Tersoff-like analytical bond-order potentials**

An analytical bond-order potential (ABOP) was used to model the PWIs in the Be–C–W–H system \cite{45}. The ABOPs are able to describe variations of the local chemical environment, such as bond-breaking. Examples of ABOPs include the Tersoff potential \cite{46} and the Brenner potential \cite{47}. Examples of only analytical potentials but not bond-order potentials are the Finnis-Sinclair potentials \cite{48}, ReaxFF \cite{49} and the second-moment tight-binding potentials \cite{50}.

The ABOPs were initially developed by Tersoff to describe covalent solids, but it was shown by Brenner \cite{51} to be extendable to metals.

For a Brenner-Tersoff like potential, the bonding strength between two atoms depends on the number of neighbors around, where more neighbors results in a weaker bond.
Moreover, the reactivity of ABOPs can describe breaking and formation of bonds. This is important in any system with chemical reactions. Although, this can result in computationally expensive simulations. The total energy in a Brenner-Tersoff like ABOP is expressed as a sum over individual bond energies:

\[ E = \sum_{i>j} f_{ij}(r_{ij}) \left[ V_{ij}^R(r_{ij}) - \frac{B_{ij} + B_{ji}}{2} V_{ij}^A(r_{ij}) \right]. \]  

(3.10)

where \( r_{ij} \) is the distance between the atoms i and j, and \( V_{ij}^R(r_{ij}) \) and \( V_{ij}^A(r_{ij}) \) are the repulsive and attractive terms of the potential, respectively. These are pair potentials given by Morse-like terms,

\[ V^R(r) = \frac{D_0}{S-1} \exp \left( -\frac{\beta \sqrt{2S}}{\mu} (r - r_0) \right), \]  

(3.11)

\[ V^A(r) = \frac{S D_0}{S-1} \exp \left( -\frac{\beta \sqrt{2S}}{\mu} (r - r_0) \right), \]  

(3.12)

where \( D_0 \) is the dimer binding energy, \( r_0 \) is the equilibrium bond distance and \( S \) is an adjustable parameter. The parameter \( \beta \) can be determined by the ground state oscillation frequency of the dimer.

The cut-off function \( f_{ij}(r_{ij}) \), defines the interaction range, which is usually restricted to the nearest neighbor and given by,

\[ f(r) = \begin{cases} 1, & r \leq R - D, \\ \frac{1}{2} - \frac{1}{2} \sin \left[ \pi (r - R)/(2D) \right], & |R - r| \leq D, \\ 0, & r \geq R + D, \end{cases} \]  

(3.13a)

(3.13b)

(3.13c)

where \( R \) and \( D \) are parameters determining the cutoff range and interval. The bond-order parameter \( B_{ij} \) in Eq. 3.12, introduces the three-body interactions and angular dependence to the potential,

\[ B_{ij} = (1 + \chi_{ij})^{-\frac{1}{2}}, \]  

(3.14)

where

\[ \chi_{ij} = \sum_{k(\neq i,j)} f_{ik}(r_{ik}) g_{ik}(\theta_{ijk}) \exp[2\mu_{ik}(r_{ij} - r_{ik})]. \]  

(3.15)

Here, \( \mu_{ik} \) is a fitting parameter and again the cutoff function is included, while the indexes monitor the type dependence of the parameters, which is important for the
description of compounds. The angular function \( g_{ijk} \) is of the form

\[
g(\theta_{ijk}) = \gamma \left( 1 + \frac{c^2}{d^2} - \frac{c^2}{[d^2 + (h + \cos \theta_{ijk})^2]} \right).
\] (3.16)

where \( \gamma, c, d \) and \( h \) are adjustable parameters. In the case of \( c = 0 \), where the angular function becomes a constant, the total potential resembles an embedded atom method (EAM) potential, used to model the pure metal interaction.

**The embedded atom method**

The embedded atom method (EAM) is a model that is suitable for metals, where atoms are treated to be planted in a sea of electrons [52]. The energy in EAM is expressed as a function of the electron density,

\[
E = \sum_i F_i(\rho_i)
\] (3.17)

where \( F_i \) is the embedding energy, and \( \rho_i \) is the electron density of an atom at the site \( i \).

To determine the term \( F \), the Finnis-Sinclair solution can be derived from second-momentum approximation of the tight-binding theory in solids,

\[
F_i(\rho_i) = -A \sqrt{\rho_i}
\] (3.18)

where \( A \) is a fitting parameter.

Practically, a correction term to represent the pair potential must be added to the total energy for the short-range repulsive interaction. The total energy of a system is given by,

\[
E = \sum_i F_i \left( \sum_{j \neq i} \rho_j(r_{ij}) \right) + \frac{1}{2} \sum_{i,j \neq i} V_{ij}(r_{ij}).
\] (3.19)

**Be-H potential**

The ABOPs are suitable for studies regarding plasma–wall interactions in fusion reactors, since they are able to model non-equilibrium phenomena such as particle irradiation, sputtering and the formation of mixed materials.
Beryllium (Be) is a metal with hexagonal close-packed (hcp) structure in its ground state. The value of its $\xi/a$-ratio is much smaller than the ideal hcp one, 1.5677 (compared to 1.63) [53].

If the interactions of atoms are restricted only to the nearest neighbors, the energy per bond, $E_b$, can be expressed by the Pauling relation which is a function of the equilibrium bonding, $r_b$ distance,

$$E_b = -D_0 \exp[-\beta \sqrt{2S}(r_b - r_0)].$$

(3.20)

with the same parameters as described before.

For the Be–C–W–H system, two Be potential versions (Be-Be I and Be-Be II) were parameterized [45]. Version I was developed for pure Be simulations and the second version works well together with the Be-C and Be-H descriptions [45]. However, differences exist between these two potentials, e.g. in the cohesive energy, elastic constants, thermal expansions and melting temperatures [54].

Because of completely filled subshells ($1s^22s^2$) in a Be atom, the $Be_2$ dimer is very weakly bonded and has a large bond length.

The properties of bulk Be in hcp structure are well described within both potential versions. The Be-H potential was fitted to properties of $BeH_x$ molecules and to H as an interstitial defect in bulk Be.
3.3 Simulation setup

In this work, the Be sputtering by D bombardment was simulated under fusion relevant conditions: impact energy of 50 eV, different particle fluxes and within a surface temperature range 320 - 2400 K (see the note and modeled temperatures at the end of this section).

A box of dimensions $x = 20$ Å, $y = 24$ Å, and $z = 29$ Å, represented a tiny part of a Be wall in the simulations. This cell consisted initially of 1728 Be atoms.

The substrate cells were created by thermalizing the desired structure (hcp for Be), which acts as a bulk structure and thus, the pbc are applied in three ($x$, $y$ and $z$) directions in this relaxation, in addition to the pressure and temperature control over the entire cell. Next, for opening the surface of the cell and prepare it for irradiation, the pbc are applied only in the $x$ and $y$ directions while the pressure control is off.

In the present work, the (0001) surface in the hcp lattice was opened. As studied by Björkas et al. [55], the effect of the surface roughness -at the atomic scale- is negligible at the impact energy modeled here. Thus, per simplicity, a perfectly flat surface was opened and used initially for the irradiation.

Figure 3.3 shows the simulation setup. The starting point for the bombarding ion D was set to 5 Å, above the surface of the simulation cell. During the irradiation the pressure control was off. The temperature at the borders and the bottom was controlled to the desired temperature during the first 2 ps, for 3 ps impacts and the first 5 ps for 10 and 30 ps impacts. The two bottom layers were fixed in order to mimic an infinite lattice. The temperature of the whole cell was controlled during the rest of the simulation time. Periodic boundary conditions were applied in the both $x$ and $y$ directions.

The Be exposure to D plasma was modeled by simulating 2000 cumulative D bombardments of the perfectly flat Be surface. Both the substrate temperature and irradiation flux were varied. Cumulative bombardment refers to using the final cell after one impact as input for the next impact. Between two runs, the cell was shifted randomly in $x$ and $y$ directions. As shown in Fig 3.3, the Be surface was uniformly irradiated by the ions, while the ion was always positioned in the middle of the cell. All the impacts were normal to the surface.

The substrate temperatures chosen for this study are 320, 800, 1000, 1600 and
Figure 3.3: The setup in the cumulative sputtering simulations. The two bottom-most atom layers are fixed. To assure an even bombardment of the surface of the cell, the atoms are shifted randomly in \( x \) and \( y \) directions (arrow 1) after which periodic boundaries are applied (arrow 2). This is done after each bombardment [23].

2400 K. As the experimental melting temperature for Be (1600 K) and that given by the potential (2600 K) are very different from each other, the temperatures in this work must be scaled considering the experimental to potential melting temperatures ratio, for better interpretation of the results. Consequently, the scaled temperatures are about 200, 480, 600, 960 and 1440 K, respectively.

Different irradiation fluxes have also been used: \( 6.73 \cdot 10^{28} \ m^{-2}s^{-1} \), \( 2.02 \cdot 10^{28} \ m^{-2}s^{-1} \) and \( 0.67 \cdot 10^{28} \ m^{-2}s^{-1} \) which are equivalent to 3, 10 and 30 ps per impact, respectively, seen in the results.

The current study is done for two more temperatures (480 and 1440 K) under \( 2.02\cdot10^{28} \ m^{-2}s^{-1} \) particle flux.
4 Analysis and Results

4.1 Overview of previous studies on BeD

4.1.1 Experiments and simulations

In the PISCES-B facility at UCSD, the plasma-surface interactions are studied by exposing Be targets to D plasma. These experiments were done at a surface temperature of approximately 373 K and ion fluxes of $3 \cdot 10^{22} \text{ m}^{-2} \text{s}^{-1}$ [55].

D impacts on Be surfaces have already been modeled with the MD code PARCAS in Ref. [56]. In that work, Be (0001) and (1120) both for perfect and rough surfaces were bombarded for different energy ranges 3-100 eV. The impacts were at normal incidence. For each energy, 1000 cumulative bombardments were modeled, at a flux of about $2 \cdot 10^{28} \text{ m}^{-2} \text{s}^{-1}$ (an impact/10 ps) and a surface temperature of 320 K [55].

4.1.2 Sputtering yield

By bombarding the Be surface with D, the projectiles can lose a large fraction of their energy during the collisions with Be atoms. This results in a gain of Be atoms potential and kinetic energy, and could even lead to Be-Be bond breaking. In few cases, the D ions collide with a D atom which was implanted during the previous impacts. In these cases, the D atom is also able to break Be-Be bonds or re-implanted in lower lattice layers. This sputtering mechanism is known as swift chemical sputtering SCS.

As shown in Fig 2.5, SCS was observed in previous simulation studies of D impacts on Be surfaces. The study showed that SCS can be important both in covalently bonded materials and metals if the surface atoms are weakly bonded to the surface, for example, in the Be-D system due to the D pile-up at the surface. This is in contrast to an earlier study [57] where it is stated that SCS mechanism cannot happen in most metals, since it requires weak atomic bonds at the surface and atoms or molecules should only bound to the substrate by one or a few chemical bonds.

SCS generates a large molecule sputtering, in comparison to physical sputtering, where mostly single Be atoms are eroded.

Figure 4.1 shows both experimental and simulated data for the sputtering yield of Be as a function of the projectile’s energy. At intermediate energies (20-50 eV), the simulated yields agree with both II and III experimental sets.
4.1.3 Molecule fraction

The fraction of Be atoms that are sputtered as BeD molecules in both simulation and experiments is presented in Fig. 4.2. At low energies, almost all the reflected Be is sputtered as BeD. During the simulation, other species of Be molecules than BeD were observed, such as BeD$_2$. Due to experiment limitations, those other species than Be or BeD could not be identified.

4.2 This work’s contribution

4.2.1 Sputtering

In the MD simulations, a particle can be considered to be sputtered if that single atom, or any other atoms it is bonded to, are not bonded to the surface atoms. Two atoms are considered to be bonded when the distance between them (r) is smaller than a certain cut-off radius. The cut-off radius depends on the interatomic potential. The same principle applies to the molecule sputtering.

In the cumulative simulations, to save computational time and to avoid sputtered particles interference with the new projectile, the reflected projectiles and the sputtered particles are removed after each bombardment. Analysis codes can also distinguish between back-scattered or eroded atoms and between single or molecule erosion.
Figure 4.2: Both simulated and experimental data of the fraction of Be atoms sputtered as BeD molecules after D impacts on Be [55].

Sputtering yield of Be and Be molecules

Figure 4.3 represents the simulated data for the sputtering yield of the Be and Be molecules due to D impacts as a function of temperature. The yields agree with the experimental values and previous simulations (see section 4.4.1).

As shown in Fig 4.3, with rising the temperature, both Be and Be molecules sputtering yields increased. For temperatures above 600 K there is a sharp increase of the yields as a result of desorption of atoms from the Be surface.

Figure 4.4 shows the same data as in Fig 4.3, plotted as a function of plasma flux. For a fixed temperature, the sputtering yield of both total Be atoms and Be molecules stay almost constant with increasing the particle flux. It can be seen from Fig 4.4.(b) that for 960 K, the sputtering yield of Be molecules slightly increases with the flux at high temperatures.
Reflection of single D and D$_2$ molecules from Be surfaces

During the D irradiation of the Be surfaces, the D can be implanted under or deposited on the surface. Further, some of these D atoms will be sputtered from the Be surface due to the upcoming impacts. They could sputter as a single D atom or be bound with other atoms at the surface, sputtering for example as D$_2$ molecules.

Figure 4.5 shows the fraction of D atoms that are not implanted in the Be cell but backscattered from the surface and those reflected as D$_2$ molecules as a function of the substrate temperature. The D reflecting yield depended considerably on the temperature. At a particle flux of 10 ps/impact, this value rises sharply in the range of 200-480 K. Then it increases moderately to reach its highest value at 1440 K. Regarding to the reflection of D$_2$ molecules, it reaches a peak in 480-600 K range and gradually decreasing at higher temperatures.

The comparison of these two plots (Fig 4.5.a and b) shows that also the fraction of D reflected as D$_2$ molecules varies strongly with the temperature.

At low temperatures (< 480 K), D is implanted deep in the cell. If D$_2$ molecules form, they will not easily desorb. At the 480-600 K temperature range, the D pro-
jectiles pile around the surface (instead of being implanted, they return toward the surface). Thus, the fraction of D at the surface increases in comparison to lower temperatures. Therefore the D atoms can desorb easily as they form D$_2$ molecules, increasing the fraction of D desorbed as D$_2$. At higher temperatures, the D desorbs from the Be surface even before forming any D$_2$ molecule. It should be noted that at any temperatures D can be bound to the surface atoms and forms Be-D molecules, but D$_2$ cannot be bound to the surface as it is a gas and desorbs from the surface as soon as it is formed.

**Molecule fraction**

The fraction of Be atoms that are sputtered as Be molecules in this work is shown in figure 4.6. At the lowest temperature, about 50% of the Be is sputtered as molecules. In contrast, at 480 K, this fraction is almost 100%, meaning hardly any Be is sputtered as atomic Be. With increasing temperature, the fraction decreases, reaching about 55% at 1440 K. This drop occurs as, when approaching the Be melting temperature, the Be-Be bonds break more easily without involving a large number of D impacts. In the latter case the sputtering mechanism tends to be physical sputtering rather than
Figure 4.5: (a). The amount of single D atoms that are not implanted in the Be cell, but reflected back from the surface as a function of surface temperature. (b). The amount of D$_2$ molecules that are reflected back from the surface over different temperatures.

A more accurate look at the Be molecules sputtering events showed that it is not the incident ion that formed the sputtered Be molecules, but rather D atoms that are initially bound to the Be surface atoms.

Figure 4.7 shows different types of Be molecules that sputtered from the Be surfaces due to SCS. Among the sputtered species we observed for example BeD$_3$, BeD$_4$, Be$_2$D$_2$, Be$_2$D$_4$, Be$_3$D$_5$ and Be$_5$D$_7$, but mostly BeD and BeD$_2$ molecules eroded from the surface.

Unfortunately, the experiments could only observe BeD molecules, since the emission from the larger molecules occurs in the infrared spectrum, out of scope of the spectrometer used in these measurements [55,58].

Previous computational studies also observed some BeD$_2$ molecules (about 10% of all Be-containing molecules [55]) but no further species were reported likely as the modeled temperature was low (320 K).
4.2.2 Depth profile

Depth profiling determines the D distribution in the Be cell as a function of the depth [4]. During the D impacts on Be, the D looses its energy through a series of collisions with the target atoms (the so called collision cascades) and finally comes to rest in the Be cell. This is called an implanted or dopant atom. In the present work, the implantation depth has shown a strong dependence on the substrate’s temperature.

Figure 4.8 shows the depth profiles of Be for different plasma fluxes and at different temperatures. Here, the number of Be atoms over a constant depth range in unit cell is normalized to the number of Be atoms in bulk. Since D is smaller than
Be, its atomic density can reach higher values. This is specially observed near the surface. There are Be atoms above the original surface due to D implantation and surface growth.

Figure 4.8: Depth profiles of Be atoms for different particle fluxes (time between impacts). The number of Be atoms in different layers are normalized to the number of Be atoms in the bulk. The $Z = 0$ depth is represented by the original surf, $Z > 0$ depth go towards the surface and $Z < 0$ depth towards the bulk.

4.2.3 Surface structure

The Be surface morphology, as the main wall material, can experience significant changes such as surface melting and erosion. The erosion may not be homogeneous leading to surface roughening. Moreover, deposition of D on the Be surface can cause surface amorphization at higher temperatures. In the present work, after only few D impacts, the surface was damaged and the Be atoms often had D atoms bound to them.
Figure 4.9 shows the influence of D irradiation and substrate sputtering on the Be surface. The morphology of the Be cell after 2000 impacts at different temperatures, for a particle flux of \(2.02 \times 10^{28} \text{ m}^{-2}\text{s}^{-1}\) (one impact/10 ps) are shown. On the surface of the cells, Be-D chains can be seen. These loosely bounded atoms could sputtered easily through the next impacts. Also the D atoms at the surface can weaken the surface binding energy of Be atoms and make them easier targets for sputtering.

![Image of Be cell structures at different temperatures](image)

Figure 4.9: Surface structure of Be cell after 2000 impacts at different temperatures, for a particle flux of \(2.02 \times 10^{28} \text{ m}^{-2}\text{s}^{-1}\) (an impact/10 ps). The D atoms are represented by small light pink spheres and the Be atoms are the larger blue spheres.

A comparison of the structures highlights the increase in the Be erosion with the temperature.

On one hand, regarding the depth profile for Be atoms at 200 K, a D pile-up can be seen in the center of the cell, with a separate atomic layer containing mostly \(D_2\) molecules. The D concentration at these layers increases with increasing the D influence.

On the other hand, with increasing temperature, the atomic motion at the surface increases, results in weaker atomic bonds, and thus larger erosion. The 1440 K temperature is close to the melting temperature of Be, causing the Be bond to break easily.
and sputter or desorb. At this temperature, around half of the surface is eroded along the z direction as illustrated in Fig 4.9.

5 Summary

ITER is expected to be the first fusion reactor reaching ignition. Its performance is based on a deuterium (D)-tritium plasma. ITER’s success highly depends on understanding the interaction between plasma particles and the wall materials of the reactor. Because of the variable conditions in the reactor, such as temperature and particle fluxes, the requirements for the wall materials vary with their location in the reactor. Plasma particles cause the wall materials to erode due to their high particle flux and energy. This erosion of the wall materials is not desirable not only because the walls get thinner, but also because the eroded particles cause radiation losses when entering the plasma.

One of the best candidates for the main wall of the ITER is Beryllium (Be) due to its low atomic number. Therefore, it is essential to understand the behavior of Be under reactor-relevant conditions and to obtain insight on how Be behave in fusion reactor first walls, such as identifying the sputtered species under D bombardment and quantifying the Be erosion both from wall life-time point of view and to explain the impurity transport, re-deposition and re-erosion patterns.

A wide range of experiments have been performed on Be exposed to D plasma mainly in linear plasma devices, where the exposure conditions can be controlled. A broad database for the sputtering yields of Be is provided by these experiments. Unfortunately, experiments are not always able to describe the underlying mechanisms completely. Hence, modeling is necessary for a complete description of the system. Molecular dynamics (MD) simulations can be a powerful tool to study many-body effects, such as chemical erosion and molecule formation. This work presents a MD study on the Be erosion by D irradiation, under fusion relevant conditions, scanning over the plasma flux ($10^{27} - 10^{28} m^{-2}s^{-1}$) and surface temperature (200 - 1440 K) at low irradiation energy (50 eV).

Our results show the large fraction of Be erosion at high temperatures is due to
swift chemical sputtering mechanism. The sputtering yields show little dependence on the D flux range studied here, but strongly vary with the surface temperature. The Be sputtering yield increased rapidly at temperatures above 600 K, as does the Be molecule sputtering yield. A large fraction of sputtered Be is for different Be molecules, mainly BeD or BeD$_2$, but some larger ones are also observed.
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