Theoretical Calculations For Sputtering Yield of Beryllium Surface Bombard By Deuterium Plasma Ions

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Abstract:

Extended calculations for sputtering yield through bombed Beryllium – target by Deuterium ions plasma are accomplished . Accounts include changing the input parameters: the energy of Deuterium ions plasma, the hit target angle of Beryllium target, thickness of the Beryllium target layer, The program TRIM is used to accomplish these calculations. Results show that sputtering yield is directly dependent on these parameters. It can change the incident angle of Deuterium ions and energy lead to a significant change in Sputtering yield . On the other hand, the sputtering yields are highly affected by changing target width at fixed ion parameters.

Keywords- sputtering process, TRIM program, plasma Deuterium ions, Beryllium

Introduction:

Several possible processes may occur in a solid target material whose surface is bombarded by energetic particles . The colliding energetic particles may be single atoms , ions , or molecules , but the outcome of the collision is determined mostly by the kinetic energy of the incident particle [1]. Sputtering is a process whereby atoms are ejected from a solid target material due to bombardment of the target by energetic particles [2] . Important applications in plasma physics, is the process of sputtering material surfaces when the ion reacts with the surface of the target. When the package plasma ions collide the target surface, they Lose energy through two mechanisms :

1. Elastic Nuclear collision.
2. Inelastic electronic collision.

Depending on the energy , these ions can, recoil directly or they can be reflected from the surface after a series of Cascaded collisions . Or they could be in a rest state in the last of the eventually , where
implantation in target at a certain depth within the target. As the collision is an inelastic collision, therefore will lose ions a large amount of energy become in the end electrically neutral, as can that eject Secondary electrons. As a result, the collision occur Inelastic scattering lead produce Phonons [3].

Physical referred to the sputtering process, as the process of collision taken into account transmission of kinetic energy and momentum of bombarding ions to target atoms, if kinetic energy sufficient to overcome the surface binding energy Sputtering occurs from the surface atoms Target [4].

Of the simulation program which employs Sputtering process is a TRIM (The Transport of Ions in Matter) is part of the SRIM (Stopping and Range of Ions in Matter) software package created by J.F. Ziegler and J.P. Biersack [5]. SRIM is group of programs that calculate the stopping range of ions in matter through quantum mechanical treatment of ion - atom collisions [5].

TRIM uses Monte-Carlo calculations to make detailed calculations of the energy transferred to every target atom collision [6]. In this research we use TRIM program to calculate the sputtering yield of Beryllium by Deuterium ion, when changing the most important input parameters in the sputtering process, such as kinetic energy of bombarding ions and incidence angle, also changing the atomic mass of target.

Theory:

A bombarding particle must have a kinetic energy above the sputtering threshold, $E_{th}$, is defined as the minimum kinetic energy of the bombarding particle for sputtering to occur [3].

Sputtering is quantified by the sputtering yield, $Y$, the mean number of atoms removed per incident particle, as stated in Eq. (1).

$$Y = \frac{\text{atoms removed}}{\text{incident particle}}$$

When the bombarding beam of Deuterium ions to the surface of Beryllium, happen collision between incident ions surface of target materials. Which leads to sputtering phenomenon. The sputtering yield is dependens on properties of both the incident particle and the target as follows[7]:
• Incident Particle Properties
  - Energy.
  - Mass.
  - Incidence angle.

• Target Properties
  - Atomic mass.
  - Surface binding energy
  - Surface texture.
  - Crystal orientation.

If the bombarding particle transfers kinetic energy greater than the lattice displacement energy, $U_d$, of the target atoms, surface damage takes place. The lattice displacement energy is the energy a target atom needs to move more than one atomic spacing away from its original lattice position [5].

The definition sputtering yield is assumed that the number of atoms removed proportional with the number of incident particles while all the other factors remains constant, and where the target is a solid material, and that the package ions bombard energy $E_0$ and incident angle $\theta_0$, it leads to a series of elastic collisions when neglecting electronic excitation of the target[7]. The atom of target atoms will move recoil, after gaining energy of the collision process and can cause recoil movement of other atoms.

As the process of elastic collision between nucleus to the sputtering process, will be taking into consideration collisions on the target surface, this means that the recoil atoms must be overcome surface binding energy, can be expressed as sputtering yield [8].

$$Y(E_0, \theta_0) = \Lambda F_D(0, E_0, \theta_0)$$  \hspace{1cm} \text{(2)}

As that $\Lambda$ is factor associated with target material, associated only advantages target, such as the surface binding energy. expression of equation $F(x, E_0, \theta_0)$ in numerical calculations [8].

$$F_D(0, E_0, \theta_0) = \alpha N S_n(E_0)$$  \hspace{1cm} \text{(3)}

As that $S_n(E_0)$ is a nuclear stopping cross – section, and $\alpha$ is the correction factor, which is a function of the mass ratio between bombarding target mass to the mass of the particle projectile $M_2/M_1$. 
and \( \theta_0 \) is initial angle of incidence, and \( N \) is atomic density of the target, so it can be described sputtering yield [8].

\[
Y(E, \eta) = \Lambda \alpha N S_\eta(E_0)
\]  

(4)

As the \( \eta \) is a generic parameter of energy. In order to accurately calculate the sputtering yield, can be used for nuclear stopping cross-section, as given \( S_\eta(E_0) \) equation [9].

\[
S_\eta(E) = \frac{8.462 Z_1 Z_2}{(1+M_2/M_1)(Z_1^{0.23} + Z_2^{0.23})} S_\eta(\varepsilon) \quad [10^{-15} \text{ eV \cdot cm}^2] 
\]  

(5)

As the \( Z_1, Z_2 \) they atomic numbers for each of the incident particle and material target bombard respectively, and that \( \varepsilon \) its reduced energy, which is given by equation [8]

\[
\varepsilon = \frac{32.53 M_2 E}{Z_1 Z_2 (1+M_2/M_1)(Z_1^{0.23} + Z_2^{0.23})} 
\]  

(6)

\( S_\eta(\varepsilon) \) Limit the decline in the nuclear cross section. The energy unit of the ion incident \( E \) is keV, and pack of ions energy \( \varepsilon \leq 30 \) it is described by equation [8].

\[
S_\eta(\varepsilon) = \frac{0.5 \ln(1+1383\varepsilon)}{\varepsilon + 0.0132\varepsilon^{0.21226} + 0.19593\varepsilon^{0.5}} \quad \text{…………………}(7)
\]

**Results and Discussion:**

1. **Target width effect:**

Effect of the width of target beryllium in sputtering yield when Deuterium ions energy install, and different incident ions angle were studied. The increase width target leads to a nonlinear increase to sputtering yield. It is clear from the Figure (1) the effect of increasing the incident angle on sputtering yield, increases sputtering yield by increasing of incident angle for each width was used. The fitting process are subject to the following relationship:

\[
y = p_1 Z^6 + p_2 Z^5 + p_3 Z^4 + p_4 Z^3 + p_5 Z^2 + p_6 Z + p_7 \quad \text{…………………}(8)
\]

As that \( p_1, p_2, \ldots, p_6 \) are constants vary from one curve to another, table (1) gives the values of these constants according to
incident Deuterium ions angle (0$^0$ - 89$^0$), and Z represents the independent variable data of a width beryllium target, install a number of ions 1000 from Deuterium ion bombarding beryllium target in figure (1), and Energy of incident Hydrogen ion is 0.5 keV. Figure (2) shows the relationship between the sputtering yield and the width of the interaction of D-Be the number of ions 5000, width (30, 100, 200, 300, and 400)$A^0$, and angles (0$^o$, 10$^o$, 20$^o$, 30$^o$, 40$^o$, 50$^o$, 60$^o$, 70$^o$, 80$^o$, and 89$^o$). Sputtering yield the largest at angles 80$^0$ and less than incident angle 0$^0$, Namely that the sputtering yield increases with the corner when constant number of ions and sputtering yield for each fluctuate upwards and downward with increasing until becomes constant. Thus, the same number of ions increases width which constant the sputtering yield, the lower incident angle, angle 0$^0$ width greater need to constant sputtering yield, while angle 89$^0$ need to width less to decide for the same number of ions, figure (2).

2. Effect the number of incident ions:

Figure (3) shows the relationship between normalized sputtering yield and angle for width target 400 $A^0$, and (D - Be) reaction to a number of various ions (500, 1000, 2500, 5000, 10000), sputtering yield has a slight increase for the incident angle of (0$^0$ - 50$^0$), and increasing sputtering yield clearly and significant increase between (60$^0$ - 80$^0$) incident angle and then start to decline, sputtering yield became less at the number of ions (5000, 7500 and 10000) and larger when the number of ions 1000, followed by 500, followed by 2500. sputtering yield at least increase the number of ions at a constant width target and energy of incident Deuterium ion is 0.5 keV, and the fitting process are subject to the following relationship:

\[ y = p_1z^6 + p_2z^5 + p_3z^4 + p_4z^3 + p_5z^2 + p_6z + p_7 \] ................................................. (8)

As that p$_1$, p$_2$, ……p$_6$ are constants vary from one curve to another, the table (2) gives the values of these constants according to the different incident Deuterium ions angle (0$^0$ - 89$^0$), and Z represent the independent variable data of number of incident ion, install width target in 400 $A^0$. Figure (3) and (4) show the relationship of the width and the sputtering yield on the angle 40$^0$ and a different number of ions
(500, 1000, 2500, 5000, 7500 and 10000) note the fluctuation of ion sputtering yield for each increase of width to constant.

Figure (5) shows the constant sputtering yield for different ions to various width for one angle is $80^0$. The greater number of ions to the same angle width that is constant by the sputtering yield increase.

3. Effect of incident ions energy:

Sputtering yield increases with incident ions energy and then begins to decline, the reason for this is attributable to the incident ions of high-energy because it does not happen sputtering, but implemented ions from the target sputtering will not occur. At incident ion energies below the threshold energy, Figure (6) illustrate the sputter yield as a function of ion energy which is given by equation (9) for Beryllium target materials bombarded by Deuterium ions. The data points computed with TRIM were fitted with the following function [10]:

$$ f(E) = k \exp\left(\frac{-\beta}{E-E_{th}}\right) - \gamma \log\left(\frac{E}{E_{max}}\right)^2 $$

The best-fit values of $E_{th}$, $E_{max}$ and the parameters $k$, $\beta$ and $\gamma$ can be found in Table(3).

Figure (7) illustrate the sputter yield as a function of ion energy which is given by equation (10) for Beryllium bombarded by Deuterium ions at direct incidence. The empirical formula (Yamamura equation) which is used to describe the sputtering at normal incidence of particles which is [11]:

$$ Y(E) = 0.42 \frac{\alpha^*QKs_n(\epsilon)}{U_s[1+0.35U_s\epsilon]} [1 - (E_{th}/E)^{1/2}]^{2.8} $$

Conclusions:

Simulation program TRIM used in this search, to study sputtering yield of target beryllium material when the bombarding plasma Deuterium ions. To change input parameters to pack incident ions as well as to see how the effect of outputs sputtering yield. We found in this study that the best angles for these incident ions when close to the angle $80^0$, and that the more incident ions energy was larger sputtering yield, also studied the effect of target width in sputtering yield. Different widths of a target yields to different profile of sputter yield. The sputter yields fluctuate for a width less than the critical value and tends to be unaffected after the critical value. The critical width depends on certain interaction involved.
For Beryllium target we found that working with width of 400 A0 is the best to avoid such fluctuation when TRIM is used. Sputtering will not occur, at incident ion energies below the threshold energy. The sputter yield exhibits a threshold below which the amount of energy transferred to the target atoms is too small for them to overcome the surface barrier. With increasing energy of the projectiles the sputter yield increases, reaches a maximum and decreases again. This decrease at higher energies is caused by the increasing depth of the collision cascade, moving away from the surface.

Reference:

**Table 1:** Parameters fitting for 1000 deuterium ions number with angle (10°, 20°, 30°, 40°, ..., 89°) and width (40, 100, 200, 400, 1000)Å, as shown in figure (1).

<table>
<thead>
<tr>
<th>Width A°</th>
<th>P₁</th>
<th>P₂</th>
<th>P₃</th>
<th>P₄</th>
<th>P₅</th>
<th>P₆</th>
<th>P₇</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>-0.4927</td>
<td>-1.0211</td>
<td>0.5162</td>
<td>2.195</td>
<td>1.4871</td>
<td>0.51431</td>
<td>1.0587</td>
</tr>
<tr>
<td>100</td>
<td>-1.5593</td>
<td>-0.86488</td>
<td>3.4801</td>
<td>1.3109</td>
<td>-0.2286</td>
<td>2.1808</td>
<td>2.6823</td>
</tr>
<tr>
<td>200</td>
<td>-0.73092</td>
<td>-1.0025</td>
<td>1.292</td>
<td>1.9715</td>
<td>0.75704</td>
<td>0.86909</td>
<td>1.3972</td>
</tr>
<tr>
<td>300</td>
<td>-1.5438</td>
<td>-1.4105</td>
<td>3.3234</td>
<td>2.9352</td>
<td>0.13994</td>
<td>1.0774</td>
<td>2.1531</td>
</tr>
<tr>
<td>400</td>
<td>-0.94205</td>
<td>-1.8099</td>
<td>1.6182</td>
<td>4.0142</td>
<td>1.0057</td>
<td>0.67072</td>
<td>2.0537</td>
</tr>
<tr>
<td>1000</td>
<td>-0.94205</td>
<td>-1.8099</td>
<td>1.6182</td>
<td>4.0142</td>
<td>1.0057</td>
<td>0.67072</td>
<td>2.0537</td>
</tr>
</tbody>
</table>

**Table 2:** Parameters fitting of deuterium ions with angle (10°, 20°, 30°, 40°, ..., 89°) and number of ions (500, 1000, 2500, 5000, 7500 and 10000), as shown in figure (3).

<table>
<thead>
<tr>
<th>Ion No.</th>
<th>P₁</th>
<th>P₂</th>
<th>P₃</th>
<th>P₄</th>
<th>P₅</th>
<th>P₆</th>
<th>P₇</th>
</tr>
</thead>
<tbody>
<tr>
<td>500</td>
<td>-0.82262</td>
<td>-1.51</td>
<td>1.2679</td>
<td>3.0699</td>
<td>1.1375</td>
<td>1.051</td>
<td>1.8504</td>
</tr>
<tr>
<td>1000</td>
<td>-0.94205</td>
<td>-1.8099</td>
<td>1.6182</td>
<td>4.0142</td>
<td>1.0057</td>
<td>0.67072</td>
<td>2.0537</td>
</tr>
<tr>
<td>2500</td>
<td>-0.65324</td>
<td>-1.2065</td>
<td>0.79638</td>
<td>2.5799</td>
<td>1.6544</td>
<td>0.99039</td>
<td>1.6823</td>
</tr>
<tr>
<td>5000</td>
<td>-0.59986</td>
<td>-0.88272</td>
<td>0.87136</td>
<td>1.6945</td>
<td>1.2</td>
<td>1.3115</td>
<td>1.6697</td>
</tr>
<tr>
<td>7500</td>
<td>-0.54712</td>
<td>-0.81495</td>
<td>0.80451</td>
<td>1.5699</td>
<td>1.0701</td>
<td>1.0655</td>
<td>1.4317</td>
</tr>
<tr>
<td>10000</td>
<td>-0.5598</td>
<td>-0.82788</td>
<td>0.82702</td>
<td>1.5928</td>
<td>1.0853</td>
<td>1.0823</td>
<td>1.4327</td>
</tr>
</tbody>
</table>

**Table 3:** Parameters fitting for Deuterium incidence ion bombarding of Beryllium, target, as shown in figures (6).

<table>
<thead>
<tr>
<th>Target</th>
<th>K</th>
<th>B</th>
<th>Eₜh</th>
<th>γ</th>
<th>E_max</th>
</tr>
</thead>
<tbody>
<tr>
<td>Be</td>
<td>0.11863</td>
<td>20.988</td>
<td>30.185</td>
<td>0.9974</td>
<td>380</td>
</tr>
</tbody>
</table>
Figure 1: The angular distribution of the normalized sputtering yield when deuterium ions number are 1000.

Figure 2: Effect of beryllium target width on sputtering yield for various deuterium incident angle of ions number are 5000.
Figure 3: The angular distribution of normalized sputtering yield when beryllium target width is 400 Å.

Figure 4: Effect of beryllium target width on sputtering yield for various deuterium ions number at angle is 40°.
Figure 5: Relationship between beryllium target width and various deuterium ions number at angle is $80^\circ$.

Figure 6: Sputtering yield vs. ion energy for Be material bombarded by $D^+$ ions with Theoretical equation.
Figure 7: Sputtering yield as a function of $D^+$ energy for Be material, using Yamamura empirical equation.