Theoretical Calculations For Sputtering Yield of Iron Bombarding by (H, D, T, He) Ions

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Abstract

Extended calculations for sputtering yield through bombed Iron – target by (H,D ,T ,He) ions plasma are accomplished .The calculations include changing the input parameters : the energy of (H,D ,T ,He) ions plasma, the hit target angle of Iron, change atomic mass of incident ion. The program TRIM is used to accomplish these calculations. The results show that sputtering yield is directly dependent on these parameters. It can change the incident angle of (H,D ,T ,He) ions and energy lead to a significant change in sputtering yield on the other hand. The sputtering yields are highly affected by changing of incident ion mass at fixed other target parameters. It can be shown from calculation that whenever increased incident ion mass increase sputtering yield, increases with incident ions energy and then begins to decline, sputtering will not occur , at incident ion energies below the threshold energy . In this study we found that the sputtering yield depends on incidence angle, incident ions energy and atomic mass of target.

Key words: sputtering process, TRIM program, Hydrogen ions, Deuterium ions, Tritium ions, Helium ions, iron

Introduction

Sputtering is a process whereby atoms are ejected from a solid target material due to bombardment of the target by energetic particles .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 [1,2].

Sputtering begins when an energetic particle strikes a target surface atom. This particle is predominantly called the incident, primary, or projectile particle. The energetic incident particle loses energy to the target through two mechanisms[3] : elastic nuclear collisions (kinetic energy conserved , atom-on-atom " billiard " ball collisions), and inelastic electronic loses (electronic excitation , ionization and electron-electron collisions) .

Sputtering processes are classified into three qualitative regimes. These regimes are distinguished by the behavior of the displaced atoms, which is a function of the energy transferred to them. Lattice atoms that are displaced by the ion are called primary knock-on atoms or PKAs [4].The PKAs can displace other atoms from the lattice creating secondary Knock - on atoms , tertiary knock - on atoms , and higher order knock-on atoms .

Sigmund has identified three sputtering regimes that can be classified by the incident ion energy .

1.The single knock-on regime
2. The linear cascade regime
3. The spike regime

in the single knock-on regime, collision cascades are not created. They are created by undergoing a collision with the primary particle and having a very small number of collisions which direct it toward the surface[5]. Sputtering occurs as the result of a series of elastic collisions within a collision cascade region.

Of the simulation program which employs Sputtering process is a **TRIM** program. The name comes TRIM Program from the first letters of the phrase "Transport of **I**on in **M**atter ", it is the most comprehensive, and included in the general program labeled SRIM. TRIM program is a Monte Carlo simulation method [6]. TRIM uses Monte - Carlo calculations to make detailed calculations of the energy transferred to every target atom collision . Incident ions and recoils are tracked through their slowing down process until their energy falls below a predetermined energy or they are so far from the surface that they are no longer candidates for sputtering [7,8].

In this research we use TRIM program to calculate the sputtering yield of Fe by (H, D ,T , He) ions ,when we change the most important input parameters in the sputtering process , such as kinetic energy of bombarding ions and incidence angle, also change the incident ion parameters such as mass.

Theory

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

$$Y = \frac{\text{atoms removed}}{\text{incident particle}} \qquad (1)$$

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].

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 [7].

The sputtering yield is dependent on properties of both the incident particle and the target as follows [9]:

• Incident Particle Properties

- energy.
- mass.
- incidence angle.

• Target Properties

- atomic mass.
- surface binding energy.
- surface texture .
- crystal orientation.

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 a solid material, the package ions bombard energy E_0 and incident angle θ_0 , it leads to a series of elastic collisions when neglecting electronic excitation of the target [10]. the atom of target atoms will make movement recoil , after gaining energy of the collision process and can cause recoil movement of other atoms , which can be expressed as a sputtering yield [10].

$$Y(E_0, \theta_0) = \Lambda F_D(0, E_0, \theta_0) \qquad (2)$$

As that Λ is factor associated with target material, associated only with advantages target, such as the surface binding energy. Expression of equation $F_D(0,E_0,\theta_0)$is in numerical calculations [10].

$$F_D(0, E_0, \theta_0) = \alpha N S_n(E_0) \qquad (3)$$

where α 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 N is atomic volume (atoms / volume), and θ_0 is initial angle of incidence, and $S_n(E_0)$ is a nuclear stopping power, so it can be described sputtering yield [10].

$$Y(E, \eta) = \Lambda \alpha N S_n(E_0) \qquad (4)$$

As η is a generic parameter of energy. In order to accurately calculate the sputtering yield, it can be used for nuclear stopping cross-section, a given $S_n(E_0)$ equation [10].

$$S_n(E) = \frac{8.462\, Z_1 Z_2}{(1+M_2/M_1)(Z_1^{0.23}+Z_2^{0.23})} S_n(\varepsilon) \quad [10^{-15}\ \mathrm{eV} \cdot \mathrm{cm}^2] \qquad (5)$$

As the Z_1 , Z_2 their atomic numbers for each of the incident particle and material target is bombard respectively, and that ε its reduced energy , which is given by equation [10].

$$\varepsilon = \frac{32.53 M_2 E}{Z_1 Z_2 (1+M_2/M_1)(Z_1^{0.23}+Z_2^{0.23})} \qquad (6)$$

The energy unit of the ion incident E is keV, and $S_n(E_0)$ limit the decline in the nuclear cross section. Pack of ions energy $\varepsilon \leq 30$ it is described by equation [10].

$$S_n(\varepsilon) = \frac{0.5\ln(1+1383\varepsilon)}{\varepsilon + 0.132\varepsilon^{0.21226} + 0.19593\varepsilon^{0.5}} \qquad (7)$$

Results and Discussion

1. Sputtering yield dependence on incidence angle.

Figure (1) shows the relationship between sputtering yield and incidence angle for fixed width target 1000 A°, and number of ions 5000, from light incidence ions (H,D ,T ,He) to a target of iron, at energy of incident ions is 0. 5 keV. The sputtering yield depends on the angle of incidence, measured from the surface normal. The sputter yield increases with the increase of angle of incidence (as the collision cascade moves closer to the surface) , reaches a maximum (typically between 55° and 80°, depending on the projectile target system), and decreases for glancing angles of incidence due to the increase of the particle reflection coefficient and the fitting process are subject to the following relationship from (H,D ,T ,He) respectively:

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

As shown that p_1 , p_2,… … p_6 are constants vary from one curve to another, the table (1) gives the values of these constants according to the different incident ions (H,D ,T ,He) angle (0^0 - 89^0) .

Show in figure (1) a maximum sputtering yield for (H, D ,T , He) incident ions angle from a target of iron in 75° incident ion angle.

Sputtering yield dependence on mass of incident ion.

We notice from the figure (1) that the sputtering yield increases with the increase of mass incident ion. We observe that the sputtering yield (0.357 Atom/Ion in incident angle 75°)is the largest from Helium which has the biggest mass of incident ion, and less sputtering yield (0.012 Atom /Ion in incident angle 75°)from Hydrogen which is less than a mass of incident ion , the sputtering yield from Deuterium ions is 0.1 Atom / Ion in incident angle 75°, from Tritium ions is 0.175 Atom /Ion. between the four ions , we observe whenever increased incident ion mass increase sputtering yield.

Effect of incident ions energy in sputtering yield :

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 the increase of energy of the projectiles the sputter yield increases, reaches an maximum and decreases again. This decrease at higher energies is caused by the increasing depth of the collision cascade, moving away from the surface. Whereas the collision kinetics is governed by the mass ratio of target atom mass to projectile mass , each element has its specific surface binding energy.

Figure (2) shows the relationship between sputtering yield and hydrogen ion energy from iron target using the equation (7), figures (3 ,4 and 5) from (H, D ,He) ion respectively , 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[11] , illustrates the comparison from four light ion using the equation(7) , in figure (6).

Figures (7,8,9) show the relationship between sputtering yield and ion energy from (H, D, He) respectively using the calculator [12]. figures (10,11,12) show the relationship between sputtering yield and (H, T, He) ion energy respectively using the equation (9) [13].

$$f(E) = k * \exp(-\beta/(E - E_{th}) - \gamma * (\log(E/E_{max})^2)) \qquad (9)$$

As that k, β, E_{th}, γ, E_{max} are constants vary from one curve to another, the table (2) gives the values of these constants according to the different incident ions (H,T ,He) angle (0^0 - 89^0) . in all previous figure a maximum sputtering yield for (H,D ,T ,He) ions incident energy from a target of iron in 1000 eV.

Conclusions

The calculations are carried using simulation program TRIM , to study sputtering yield of iron target , when the bombarding ion (H,D ,T ,He) to change input parameters to pack incident ions as well as to see how the effect of outputs sputtering yield , in this study we found that the best angles for these incident ions when close to the angle 80^0 , sputtering yield increases with increase of mass incident ion , sputtering yield increases with incident ions energy and then begins to decline ,we found in this study that sputtering yield depends on incidence angle , incident ions energy, mass of incident ion .

A maximum sputtering yield for (H, D ,T , He) incident ions angle from a target of iron in 75^o incident ion angle. And for (H,D ,T ,He) ions incident energy from a target of iron in 1000 eV.

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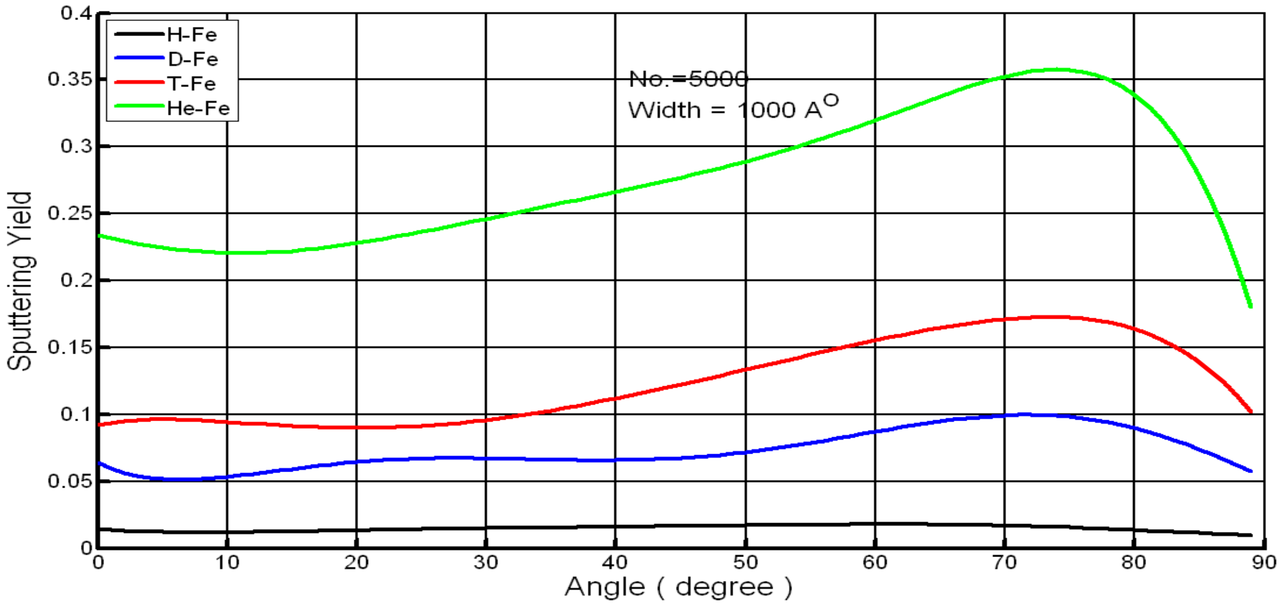
13. IGOR Pro, Copyright 2007 Wave Metrics, Inc.http://www.wavemetrics.com/.

ion	P_1	P_2	P_3	P_4	P_5	P_6	P_7
H	0.0013194	-0.00036	-0.003946	-0.001372	0.000194	0.003247	0.016444
D	0.012484	-0.00907	-0.052439	0.010669	0.051213	0.017962	0.067294
T	-0.007421	-0.00374	0.0048303	-0.021024	0.012207	0.065199	0.12223
He	-0.013084	-0.03480	0.0013172	0.034915	0.0245	0.067529	0.2769

Table No. (1): Constants fitting equation (8) Plotted in Figure (2) from Light incidence ions (H, D, T, He) from target of iron

ion	k	β	E_{th}	γ	E_{max}
H	0.059979	487.74	145.37	0.35826	75
T	0.18632	260.84	24.678	0.4394	160
He	0.42886	300.22	1.9516	0.59477	650

Table No. (2): Constants fitting equation (9) Plotted in Figure (10,11,12) from Light incidence ions (H, T, He) from target of iron



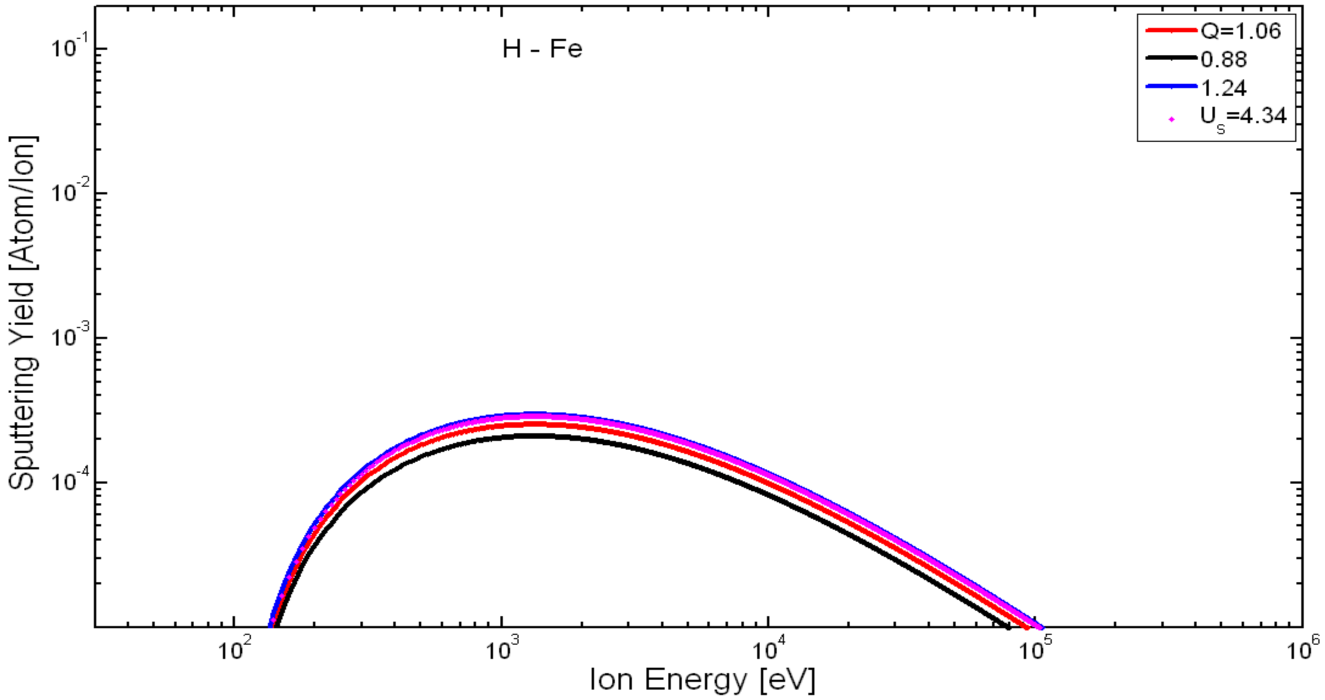


Figure No.(1): Relationship between sputtering yield and incidence angle from Light incidence ions (H, D, T, He) from target of iron

Figure No.(2): Relationship between sputtering yield and hydrogen ion energy from iron target .

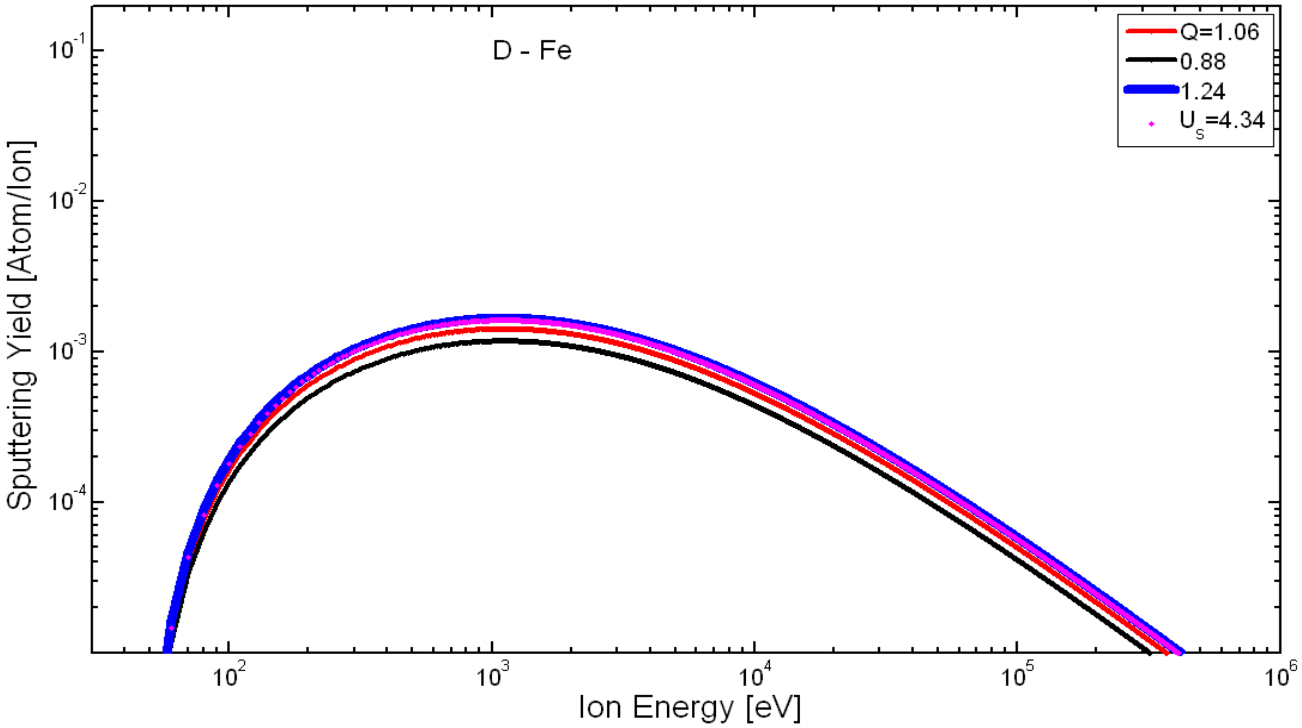


Figure No. (3): Relationship between sputtering yield and Deuterium ion energy from iron target

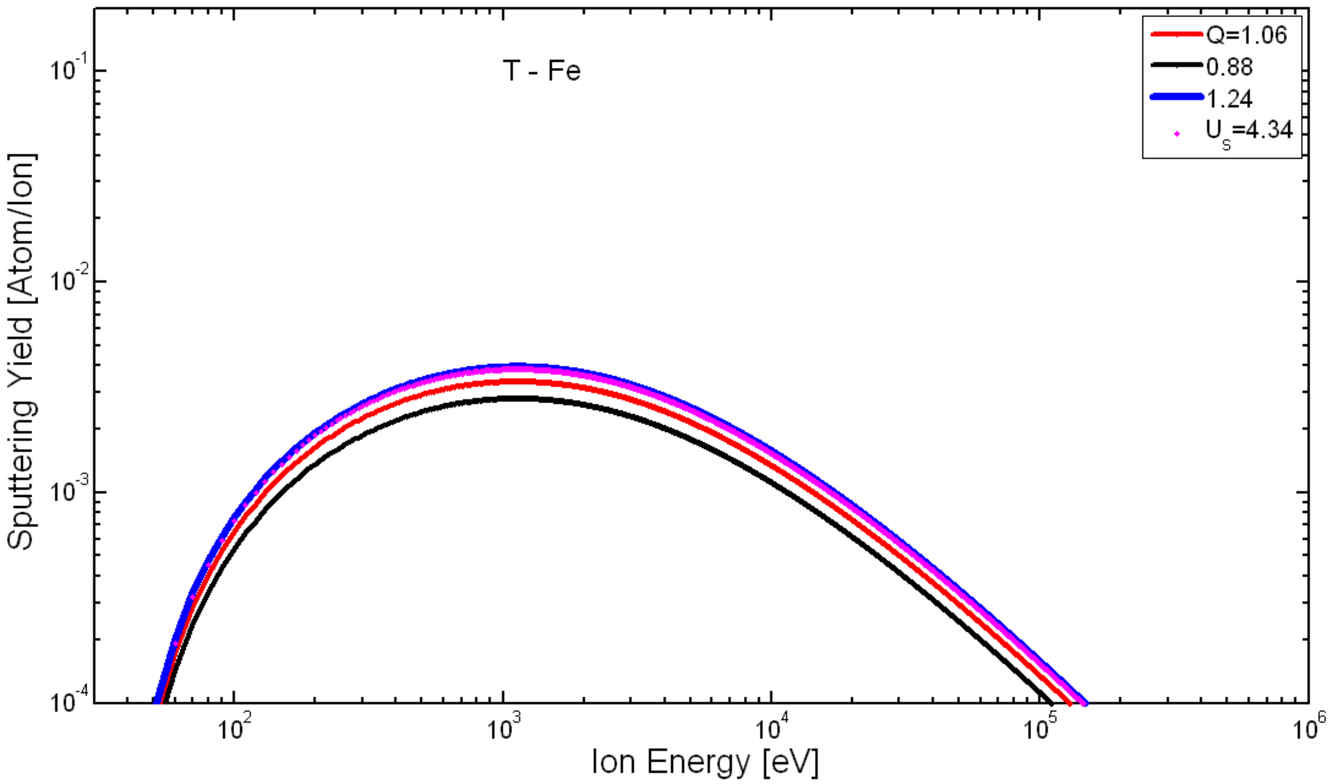


Figure No. (4) :Relationship between sputtering yield and Tritium ion energy from iron target

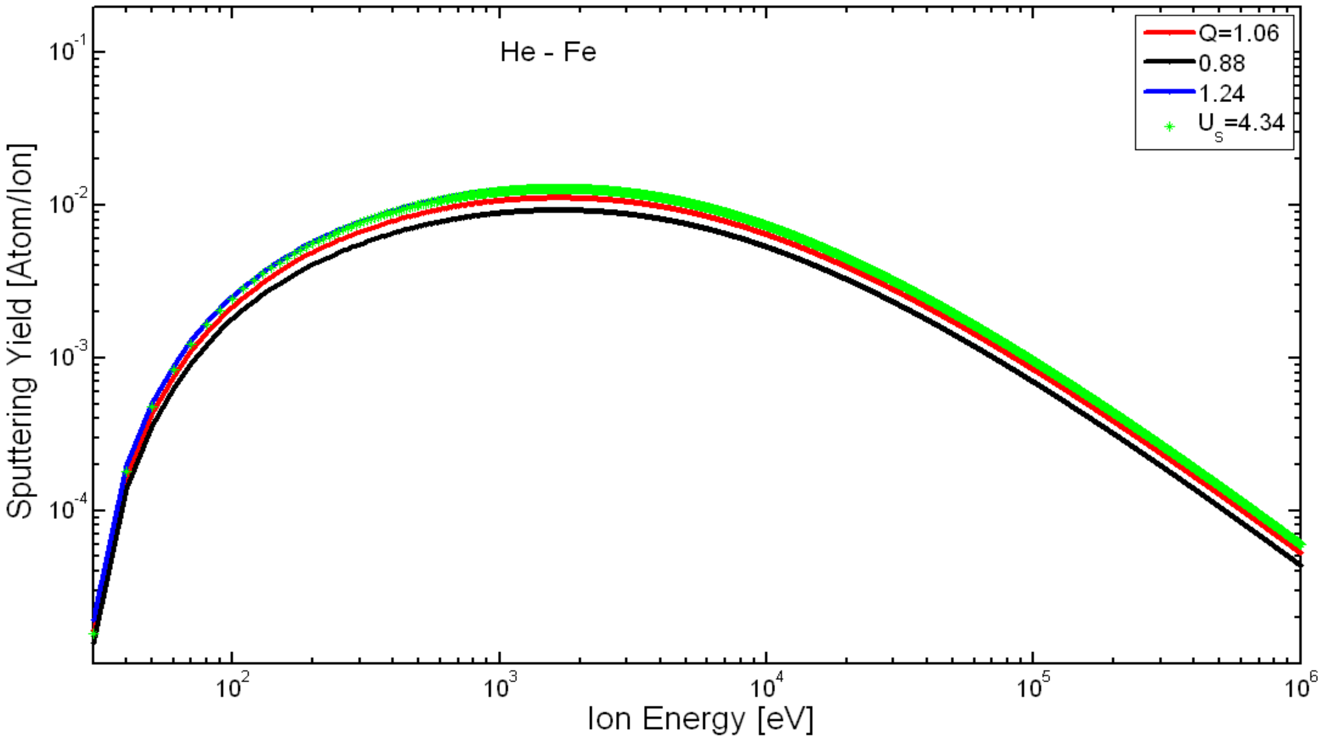


Figure No (5): Relationship between sputtering yield and Helium ion energy from iron target.

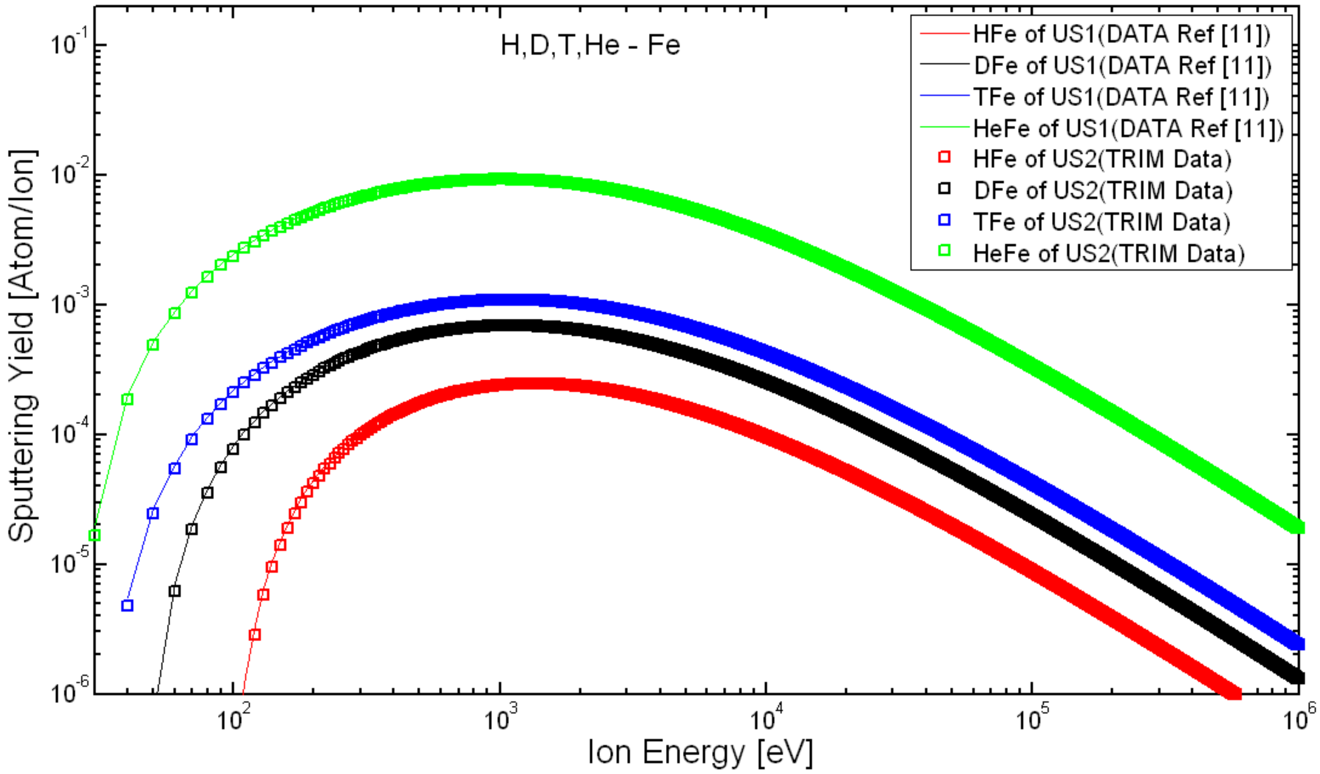


Figure No. (6): Illustrates the comparison from four light ion .

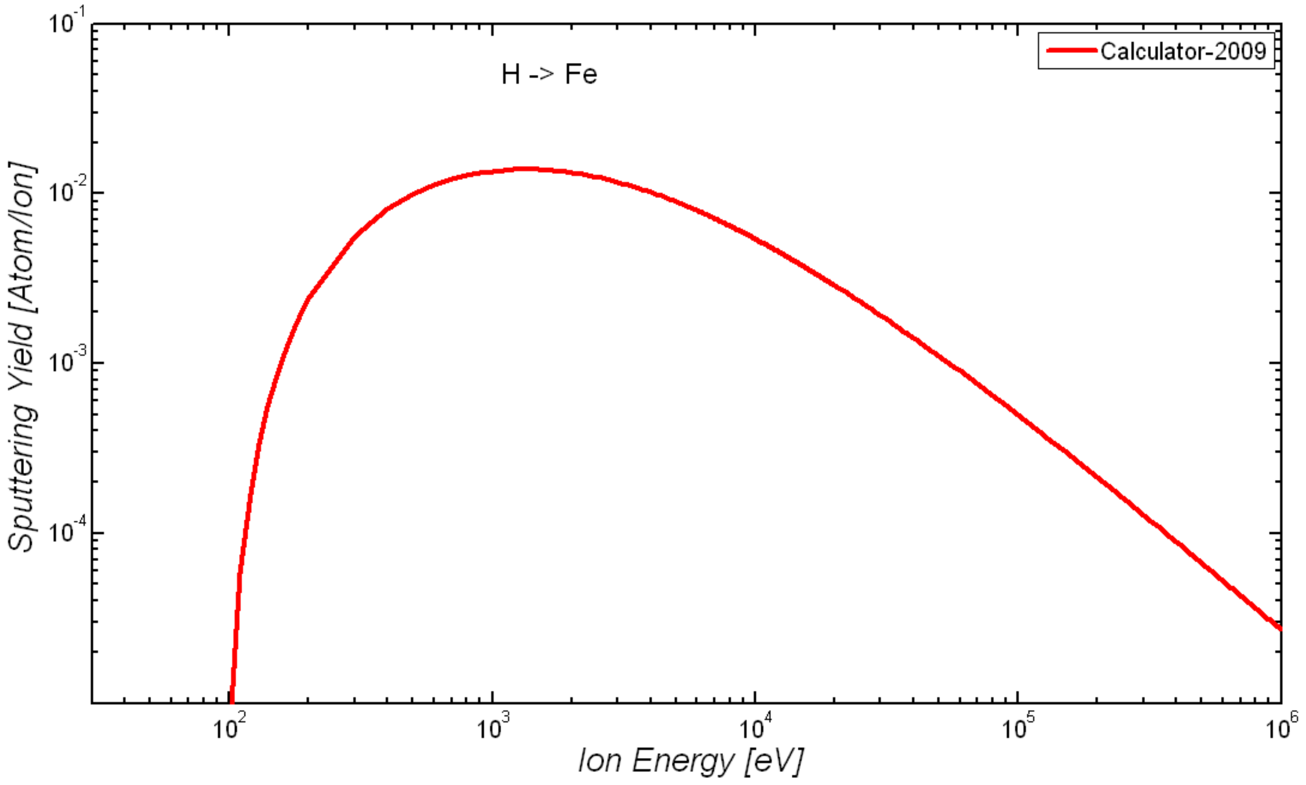


Figure No. (7): relationship between sputtering yield and hydrogen ion energy from iron target

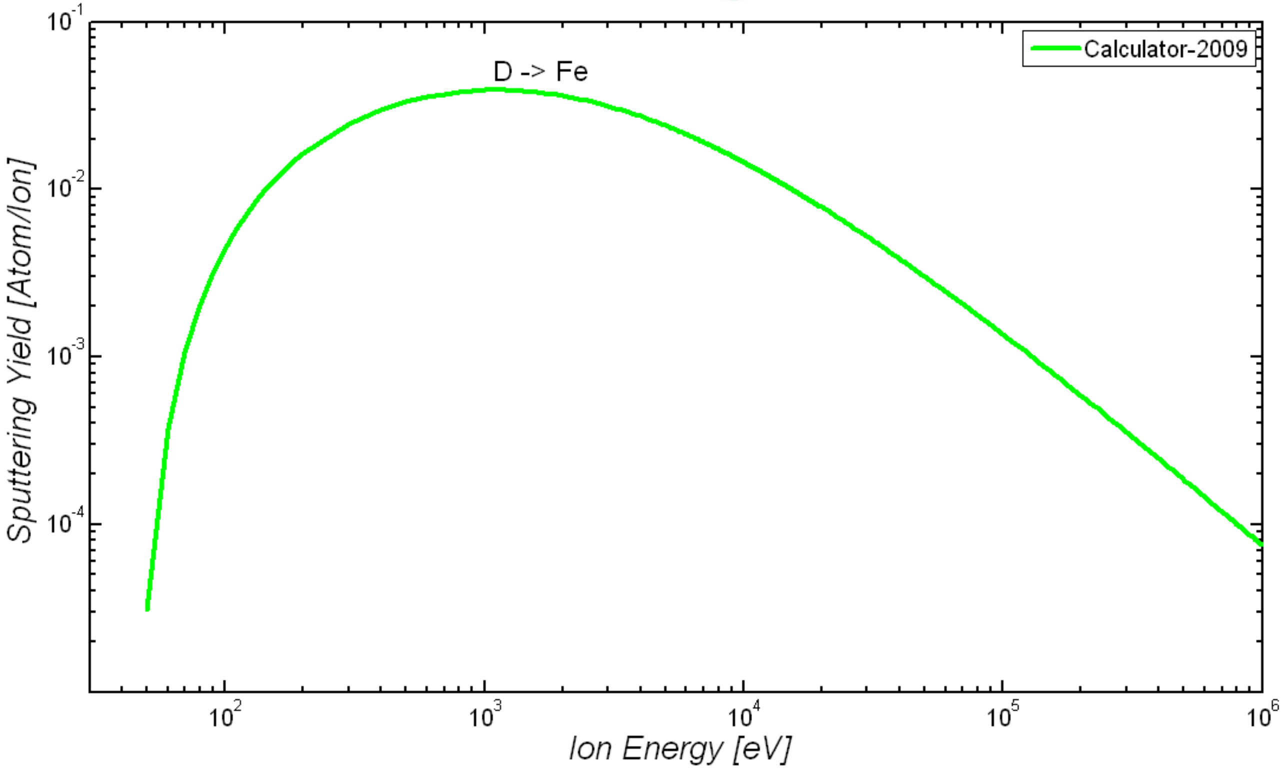


Figure No. (8): relationship between sputtering yield and Deuterium ion energy from iron target

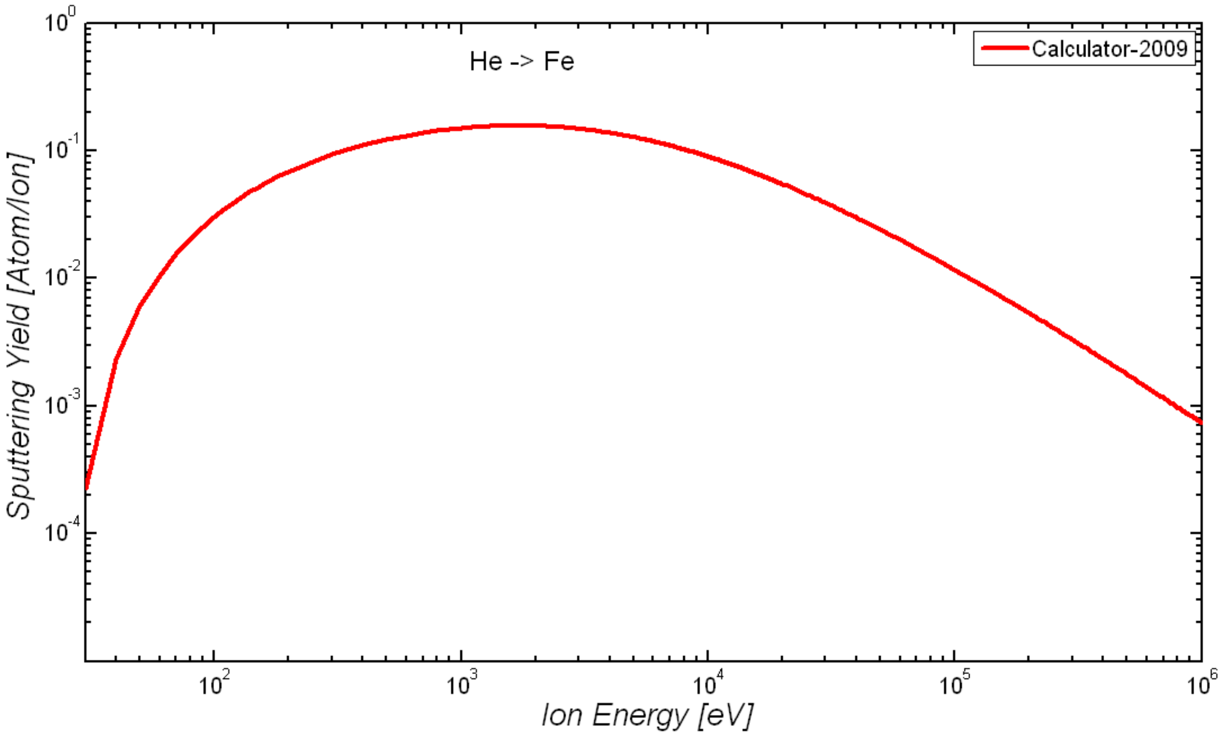


Figure No (9): Relationship between sputtering yield and Helium ion energy from iron target

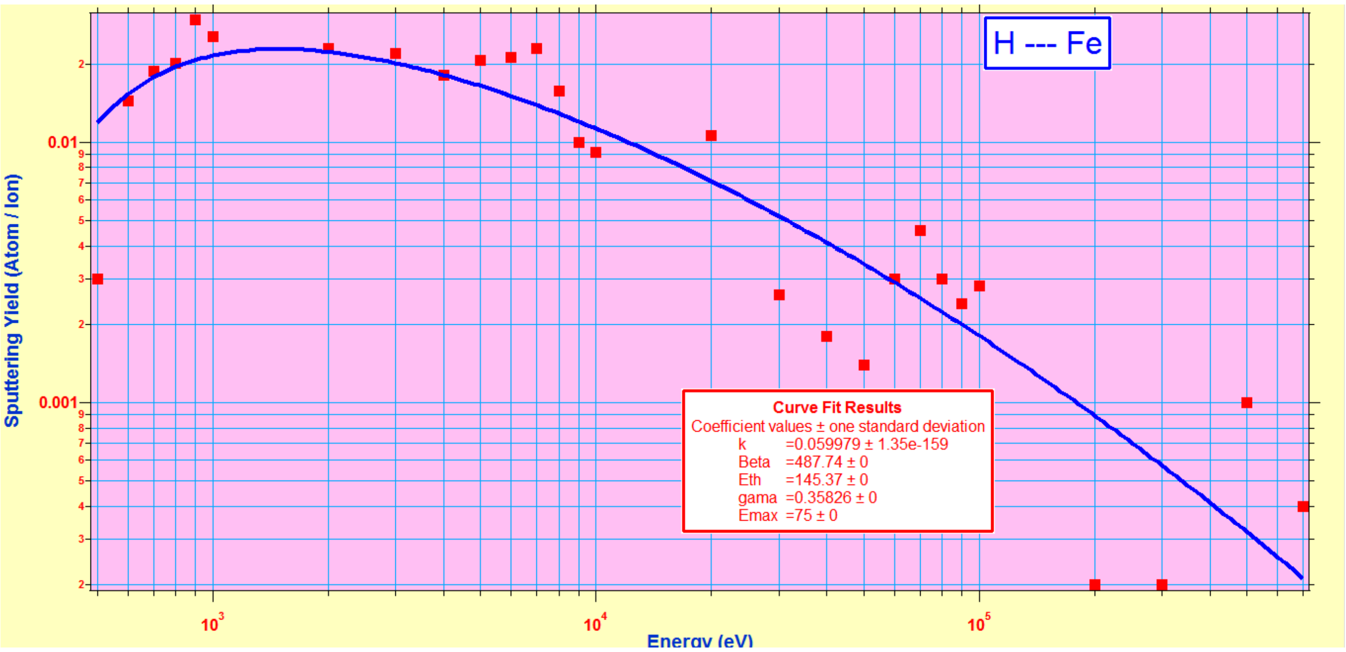


Figure No. (10): Relationship between sputtering yield and hydrogen ion energy from iron target

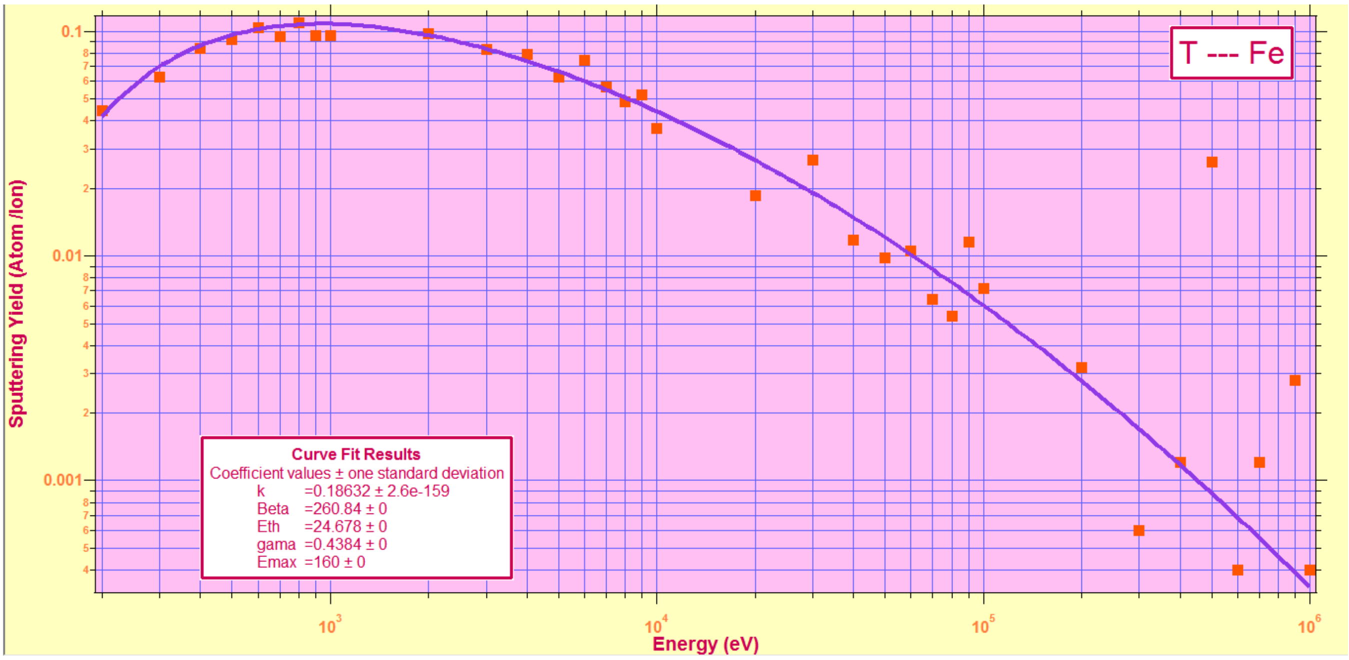


Figure No. (11): Relationship between sputtering yield and Tritium ion energy from iron target

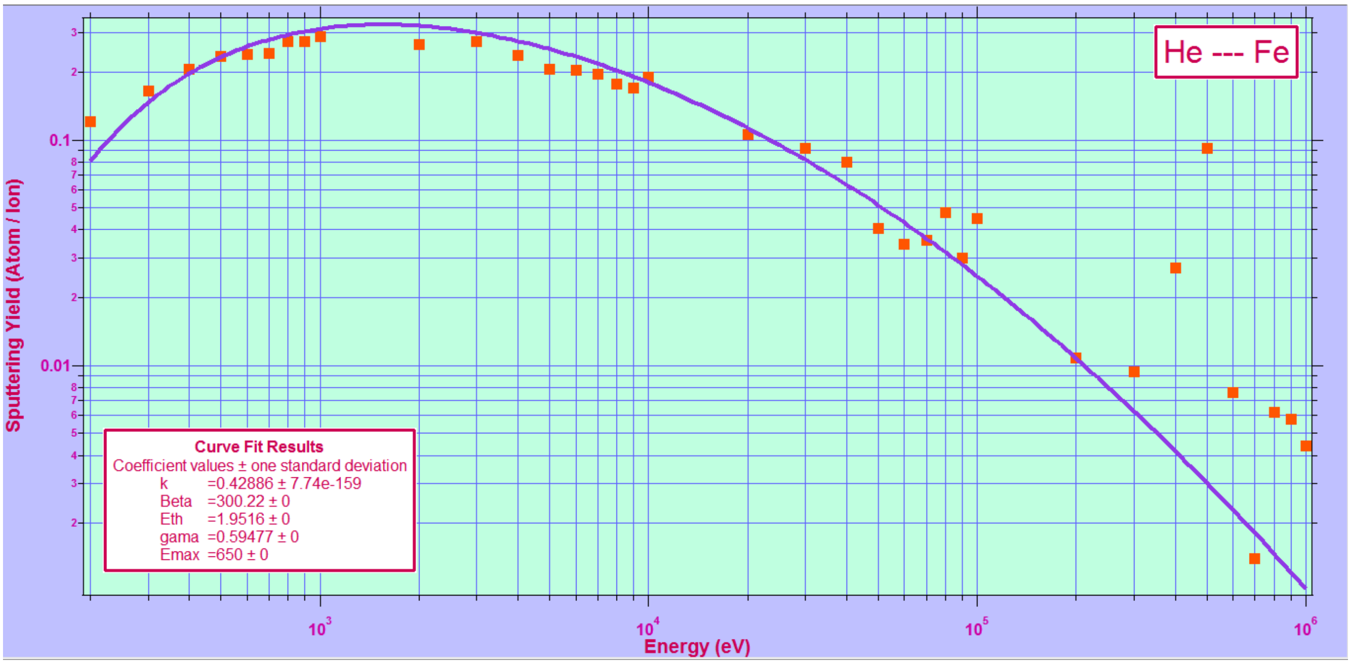


Figure No. (12): Relationship between sputtering yield and Helium ion energy from iron target

حسابات نظرية لحاصل ترذيذ (الرش) سطح من الحديد بواساطة حزمة من ايونات الهيدروجين و الديوتيريوم و التريتيوم والهليوم

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الخلاصة

لقد أنجزت حسابات لعملية الترذيذ(الرش) لهدف من الحديد بواساطة قصف بلازما ايونات الهيدروجين و الديوتيريوم و التريتيوم والهليوم . تشتمل الحسابات على تغيير معلمات الإدخال لكل من طاقة ايونات الهيدروجين و الديوتيريوم و التريتيوم والهليوم .وزاوية سقوطها على هدف من الحديد ، و كتلة الايونات وتأثيرها في حاصل الترذيذ . لقد وظّف برنامج TRIM لانجاز الحسابات. تبين النتائج إن حاصل الترذيذ يعتمد اعتماداً مباشراً على هذه المعلمات إذ إن تغير زاوية سقوط ايونات البلازما وطاقتها تؤدي إلى تغير محسوس في نتائج حاصل الترذيذ . وكتلة الايون له تأثير مباشر في حاصل الترذيذ.يتأثر حاصل الترذيذ بشدة عن طريق تغيير كتلة الايون الساقط بثبوت معلمات الهدف الاخرى . تظهر من الحسابات التي اجريناها انه كلما زادت كتلة الايون الساقط زاد حاصل الترذيذ . الزيادة في طاقة الايون الساقط تبدا بالانخفاض . الترذيذ لايحدث عندما تكون طاقة الايون الساقط اقل من طاقة العتبة. في هذه الدراسة وجدنا أن حاصل الترذيذ يعتمد على زاوية السقوط ، طاقة الايون الساقط و الكتلة الذرية لمادة الهدف.

الكلمات المفتاحية : حاصل الترذيذ ،برنامج TRIM ،ايونات الهيدروجين ، الديوتيريوم ، التريتيوم ، الهليوم ، الحديد .