Simulation Study of Sputtering Yield of Zn Target Bombarded By Xenon Ions

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Abstract

Using a reduction of TRIM simulation data, the sputtering yield behaviour of Zinc target bombard by heavy Xenon ions plasma is studied. The sputtering yield as a function of Zinc layer width, Xenon ion number, energy of ions, and the angle of ion incidence are calculated and illustrated graphically. The corresponding energy loss due to ionization, vacancies and phonons, are graphically shown and discussed. Further, we fit the calculations and expressions for fitted curves are presented with its coefficients.

Keywords: TRIM program, sputtering yield, Xenon ions, Zinc

Introduction

The sputtering, which is caused by the interaction of incident ions with target surface atoms, was first observed in middle of the nineteenth century [1]. The sputtering is defined as the physical removal of material from the surface by incident energetic particle bombardment. The physical sputtering is driven by mechanism of momentum exchange between the ions and atoms in the material due to collisions [2]. Quantitatively the sputtering is measured by the sputtering yield produced by the mean number of atoms removed per incident particle. Both the properties of target and the bombard ion are closed related to the sputtering process. Sputtering or sometimes called erosion of target surface material takes place as the fast particles bombard a surface material [3]. The incident ions establish cascades collision in the target. When the cascades recoil arrive the surface, an atom can be ejected. This takes place when the incident ions have energy above the surface binding energy of the target. The sputtering phenomenon is regarded as undesired side effect such as in the tokamak. On the other hand, sputtering now has been widely developed and used at large for surface cleaning and etching, surface and surface layer analysis, thin film deposition [4].

In this work we adapted TRIM (Transport of ions in matter) program for calculations. TRIM is based on Monte Carlo simulation method, specifically the binary collision approximation with random selection of the impact parameter of the next colliding ion [5]. It is used for simulation due to their widely considered to compute a number of parameters relevant to ion beam implantation and ion beam processing of materials [6].

It is known that the silvery – white metal Zinc is considered to be an important material for coating applications. Zinc and its compound are used to coat (galvanize) iron and steel to protect against corrosion and rust. Most of the pipe interior is coated by this rich paint. However, there are a little studying efforts achieved to explore the effect of an ion – induced Zinc. The latter leads to modify the surface properties and becomes morphologically rickety. This work aims to explore the sputtering yield of Zinc bombarded by one of heavy ions. We choose Xe^{+} ions beam to bombard Zinc to study various parameters that affect the sputtering process.

Description of TRIM Simulation Program

So many possible processes could be occurred at the surface and the core of solid which is bombarded by energetic particles. Colliding energetic particles may be single atoms, molecules, or ions; however, the yield of the collision is specified mostly by the kinetic energy of the incident particle [7]. There are many theoretical [8] and semi – empirical calculations [9-11] which supply worthy analytical expressions to represent the substantial of physical mechanisms related to the sputtering phenomena and to the other corresponding dependency of several variables. Thus, many of software simulation programs such as TRIM, ACAT, MARLOWE, and TRIDYN have been developed. These programs simulate the evolution of the collision cascade inside the target bombarded by a beam of ions. The program TRIM is a binary collision Monte Carlo code that simulates the sputter process and calculates the sputtering yield and other parameters corresponding to it. The program approximates the binary collision by treating the transport of atoms in a solid as it is a series of consecutive collisions between which that the particle follows a straight trajectory (Figure 1) [12].

The motion of particle that have E_i energy after making ith collision is expressed by the polar and azimuthal angles α_i and β_i. It is allowed for the recoil atom (ion) to move over the mean free path length of λ . Thus, the mean free path length is defined as the average atomic distance of the target material

$$\lambda = \frac{1}{\sqrt[3]{N}} \qquad (1)$$

such that N is the atomic density of the material. The particles after travelling λ distance it obey colliding again and scattered over the angles θ and ϕ with respect to the mass system. The angle ϕ in cylindrical symmetry can be randomly selected in the interval $(0, 2\pi)$, whilst the polar scattering angle θ can be numerically calculated using the classical path integral [13]

$$\theta = \pi - 2p\int_{r_{\min}}^{\infty} \frac{dr}{\sqrt{1-\frac{V(r)}{E_{\mathrm{cm}}}-\frac{p^2}{r^2}}} \qquad (2)$$

where $r_{\min}$ is the minimum distance of approach, $V(r)$ is the inter atomic potential, E_{cm} is the energy of the particle in the center of mass system, and P is the impact parameter. The impact parameter value is calculated from a random number r, equally distributed in $(0, 1)$

$$P = P_{\max}\ r^{\frac{1}{2}} \qquad (3)$$

where the maximum impact parameter $P_{\max}$ is given by

$$\pi p_{\max}^2 \lambda = \frac{1}{N} \qquad (4)$$

This means that there is one target atom contained in a cylindrical volume with length λ and radius $P_{\max}$ and this atom corresponds with one collision per atomic volume $1/N$. After correctly rotating of the angles θ and ϕ to the laboratory system the new directional angles $\alpha_i + 1$ and $\beta_i + 1$ can be calculated from scattering angles Θ and Φ. Therefore, after the collision the particle energy is given by

$$E_{i+1} = E_i - T - \Delta E \qquad (5)$$

where ΔE is the electronic energy loss and T is the transferred kinetic energy. It is almost often, due to lack of knowledge, that the bulk binding energy of the target material E_b is set to zero. If the displacement energy is less than the transferred kinetic energy a recoil is generated with initial energy $E_i = T - E_b$. The incident ion and the generated recoils are tracked until their kinetic energy falls below a particular cut off energy. This cutoff energy can be selected to be the surface binding energy which represents the minimum energy an atom must have to escape the surface [14].

Result and Discussions

Figure (2a) shows the dependence of the sputtering yield on width of the Zn bombarded by Xenon at normal incident with 5000 ion number and ion energy of 50 keV. The sputtering yield profile as a function width behaves as in significantly increased manner then obeys to slowly fluctuation until it remains stable at critical width ≤ 400 A^0. This means that anymore further increase in the width would not affect the sputtering yields. Therefore, to get a rid of the fluctuation at lower width of Zn one refers to use this critical value or higher to study other parameters. Figure (2b) shows the corresponding energy loss due to ionization. This loss is electronic energy loss due to energy loss of incident ions to the electrons of the target whenever the ions penetrate into the target. The ions soon interact with the electrons of the target collectively or singly [15]. The way of interaction seems to be quite complicated and it is divided to two categories; ions and recoils. The recoils loss is due to very much less interaction of relatively slowly movement of recoiling target atoms with very fast moving electrons of the target. It is evidence that the ions loss decreases as the target width increases to a limit and remains stable then while the recoils loss increases to a peak and then steadily stabilizes as the width increases. The ion losses by ionization will result in target damage. Firstly, the target damage happens in the insulators whereas the change is building and then the cracking takes place. Figure (2c) shows the correspondent energy loss due to vacancies that is the energy loss to the target producing vacancies. The vacancy losses due to ions behave similarly as in the ionization, however, the recoils increase to a peak at a certain width, decrease and then remain constant as the width increases. The number of vacancies depends on the displacement energy assigned to each target atom. If the displacement energy is larger than the transferred energy, the atom stays in its lattice site. Thus the energy is moved into target phonons. If the displacement energy is lower than the transferred energy, the new recoil has this movement of energy subtracted the binding energy of the atom to its lattice position. Figure (2d) illustrates the correspondent energy loss due to phonons. Although, the phonon losses due to ions have similar behavior as in the ionization and vacancies, the recoils are higher than the former. The energy loss due to phonons by recoils rises as the width increases until it stays at the same level whatever the value of width would be. The ion's energy loss to the target phonon can be understood from the following physical picture; whenever, the colliding takes place between ion and target nucleus, it imparts some recoil energy to this atom. When the transferred energy is less than the displacement energy then it is assumed that the atom returns to its lattice site and its recoil energy is transferred into target phonons. To understand the vacancy occurrence, let the incident ion energy is E_1 and that for struck atom is E_2 and the target has energy E_d. The vacancy occurs when both, the incident ion and the struck atom have enough energy to leave the site, i.e. $E_1 > E_d$ and $E_2 > E_d$, then both of them become moving atoms of the cascade. The energy of struck atom is reduced the displacement energy before it has next collision. Now releasing a phonon takes place if $E_2 < E_d$ since the struck atom does not have enough energy yielding it to vibrate towards back direction to its original position releasing energy a phonon as E_2.

Figure (3) shows that there is a bit slightly changes at lower ion energy in the sputtering yield values of Zn as the number of incident Xenon ions increased for direct bombardment and constant layer of Zn. However, at higher ion energy ≤ 35 keV the fitted curves split up. The whole curves of sputtering yield increase monotonically with increased ion energy. The fitted curves are made in Igor Pro software and the profile of them obeys to lognormal equation given by

$$y = y_0 + \exp\left[-\left\{\frac{\ln\left(\frac{x}{x_0}\right)}{\text{width}}\right\}^2\right] \qquad (6)$$

where the coefficients of each curve are tableted in table 1. In spite of difference of sputtering yield with ion number at higher ion energies, we prefer to use 5000 ion number in this work to study other parameters that affect the sputtering yield to save the time of calculations and that the sputtering yield is considerably not changed in great manner.

Figure (4) shows the effect of increasing the ion number on the sputtering yield at fixed width of Zn target, normal bombardment, and constant Xenon ion energy. It is clear that there is a frequent change between in this graph. For lower value of ion number the sputtering yield exhibits higher fluctuations than that for higher ion number. As mentioned before to avoid higher fluctuations in sputtering yield at low ion number we prefer to work with 5000 ion number to study other parameters due to very less change in the values sputtering yield compared to the higher ion number.

It is often usually for the researchers in topic of sputtering to use normalized sputter yield rather than direct sputter yield as soon as they treat with ion angle of incidence dependence. For different values of incident ions energy, figure (5) illustrates the normalized sputtering yield as a function of ion incident angle. The data are fitted using Matlab software by 6th degree polynomials for four curves. It is noted that, a slightly increase of the angle of incidence yields to a gradual increases in the normalized sputter yield reaching to a highest point and then it drops rapidly towards low values as it approaches 89^0. Obviously, the normalized sputtering yield considerably increases as the Xenon ion energy increases. From the extended calculations and also the graph, it appears that that peak of sputtering yield shifted towards higher angle as the energy of incident ions increased even if the profiles are similar but the magnitude of the slope decreases as the ion energy decreases. We refer to one of interest in the calculations using TRIM that the sputtering yield in nearby angle to 0^0 gives lower value than that of the normal incidence whatever the ion energy used. In the calculation we use a Zn layer with $500\ A^0$ and 5000 ion number.

For fixed Xenon ion incident angle, width of the Zn target, and ion number mentioned the sputtering yield nonlinearly grows as the ion energy increases. Figure (6) shows this dependence using four angles of incidence. The curves are fitted using Igor Pro software Package by Hill-equation which is given by

$$y = \frac{\mathrm{base}-(\mathrm{max}-\mathrm{base})}{\left[1+\frac{\mathrm{xhalf}}{x}\right]^{\mathrm{rate}}} \qquad (7)$$

Table (2) gives the coefficients for each fit of curves. One notices from the graph that at higher angle, the higher energies result in the higher sputtering yield.

Conclusion

Using TRIM simulation program we studied some of the parameters that affect the sputtering yield of Zinc bombarded by Xenon ions. Regard to the increasing the width of Zinc and its effect on the sputtering yield, we found that the sputtering yield profile possesses fluctuations before a critical width $400\ A^0$ whereas any larger value of width more than the mentioned the sputtering yield mostly unaffected and stable. The energy loss due to ions by ionization, vacancies, and phonon has commonly the same behavior. Similarly, the energy loss due to the recoils has the same profile expect for the phonons where it is somehow different. For different Xenon ion number, the sputtering yields vs. ions energy curves have only separation at higher energy. For constant ions energy the sputtering yields as a function of ion numbers have larger fluctuations at lower number of ions. The normalized sputter yield increased as the angle of incident ion increases leading to a maximum peak and then to a quickly drops towards lowest values as it approaches 89^0. The normalized sputtering yield increases as the Xenon ion energy increases and it appears that that peak of sputtering yield shifted towards higher angle as the energy of incident ions increased. For different angle rather than the normal incidence, the sputtering yield as a function of ion energy grows in nonlinearly manner. Finally, we carried out new fitting for some calculations.

References

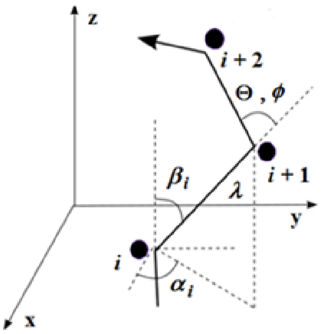
1. Wasa, K.; Kitabatake, M. and Adachi, H., (2004), “Thin Film Materials Technology - Sputtering of Compound Materials”, William Andrew Publishing/Noyes.
2. Behrisch, R. and Eckstein, W. , (2007), “Sputtering by Particle bombardment: Experiments and Computer Calculations from Threshold to MeV Energies”, Springer, Berlin (eds.).
3. Abdelrahman, M. M., (2010), “Study of Ion Beam Sputtering using a Glow Discharge Ion Source”, Brazilian Journal of Physics, (40), (1), (26 – 29) .
4. Wang ,Y. ; Yoon, S. F.; Ngo, C. Y.and Ahn, J., (2007), “Surface Morphology Evolution of GaAs by Low Energy Ion Sputtering” , Nanoscale Res Lett, (2).504–508.
5. Was, G. S., (2012) , “Fundamentals of Radiation Materials Science”, Springer.
6. Stoller, R. E.; Toloczko, M. B.; Was, G. S.;Certain, A. G.; Dwaraknath, S.and Garner ,F. A., (2013), “On the use of SRIM for computing radiation damage exposure”, Physics Research Section B: Beam Interactions with Materials and atoms, (310), (75 – 80).
7. Michael, R. Nakles, (2004) , “Experimental and Modeling Studies of Low-Energy Ion Sputtering for Ion Thrusters”, MSc thesis, Virginia Polytechnic Institute and State University, USA.
8. Sigmund, P., (1969) , “Theory of sputtering. 1. Sputtering yield of amorphous and polycrystalline targets” Physical Review, (184), (2), (383 – 416).
9. Yamamura, Y. , (1981) , “ Contribution of anisotropic velocity distribution of recoil to sputtering yields and angular distribution of sputtered atoms” Radiation Effects and Defects in Solids, (55), (1-2), (49–55).
10. Takeuchi, W. and Yamamura, Y., (1983) , “ Computer studies of the energy spectra and reflection coefficients of light ions”, Radiation Effects and Defects in Solids, (71), (1-2), (53–64).
11. Yamamura ,Y. and Tawara, H., (1996), “ Erratum, 62, 2 (1995) Energy dependence of ion – induce sputtering yield from monatomic solids at normal incidence”, Atomic Data and Nuclear Data Tables, (63), (2), (353–353).
12. Boydens, F., (2013) ,“Key aspects of sputtering illustrated by the use of multi-element powder mixtures” PhD thesis, Gent University, Belgium.
13. Dolique ,V.; Thomann, A.-L.,; Brault, P.;Tessier, Y. and Gillon, P., (2009) , “Complex structure/composition relationship in thin films of AlCoCrCuFeNi high entropy alloy” , Materials Chemistry and Physics, (117), (1), (142–147).
14. Egerton, R.F.; McLeod, R.; Wang, F.and Malac M., (2010) ,“Basic questions related to electron-induced sputtering in the TEM”, Ultramicroscopy, (110), (991–997).
15. Ziegler, J. F.; Biersck, J. P. and Ziegler, M. D. (2008) , “SRIM: The Stopping and Range of Ions in Matter”, Lulu Press Co.

Table (1): The coefficients of equation (6) that appears in figure 3.

Ion number	**2500**	**5000**	**7500**	**10000**	**15000**
y_0	−3.1383	29.94	−1.8699	−1.8699	29.554
A	30.571	−27.919	26.812	26.812	−27.388
x_0	318.24	0.26056	163.63	163.63	0.27565
Width	4.9255	4.4593	4.2811	4.2811	4.3591

Table (2): the values of coefficient in equation (7) for each angle

Angle	0^0	30^0	65^0	85^0
base	−1.8233	−1.5304	−3.9611	−2.8846
max	28.804	37.198	163.16	339.07
rate	0.70117	0.77313	0.71694	0.68002
xhalf	6.5833	5.6775	20.05	124.61



Figure(1) Section of an ion or recoil trajectory with consecutive collision with target atoms denoted by $i, i+1$ and $i+2$. The solid lines represent the ion trajectory [12].

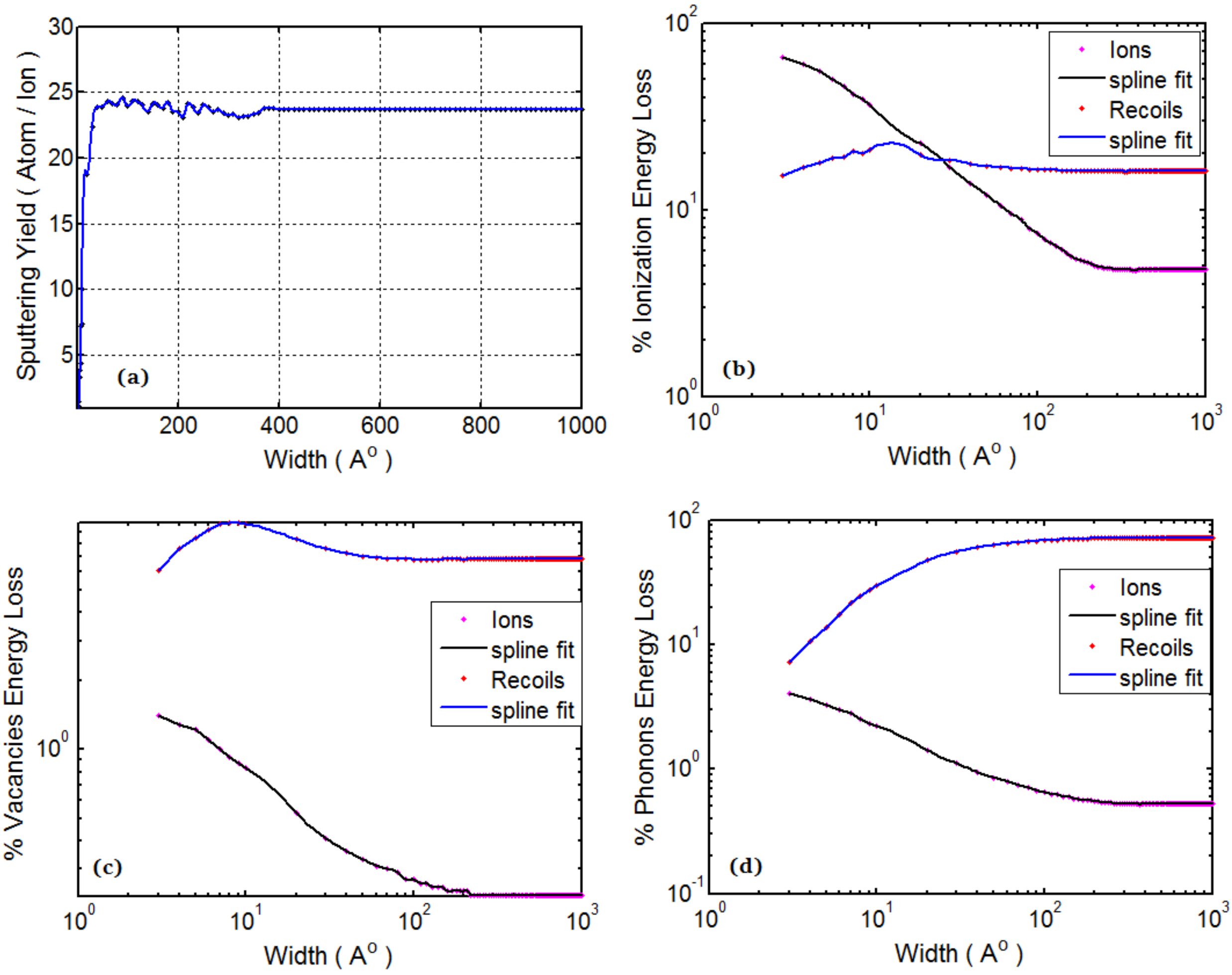
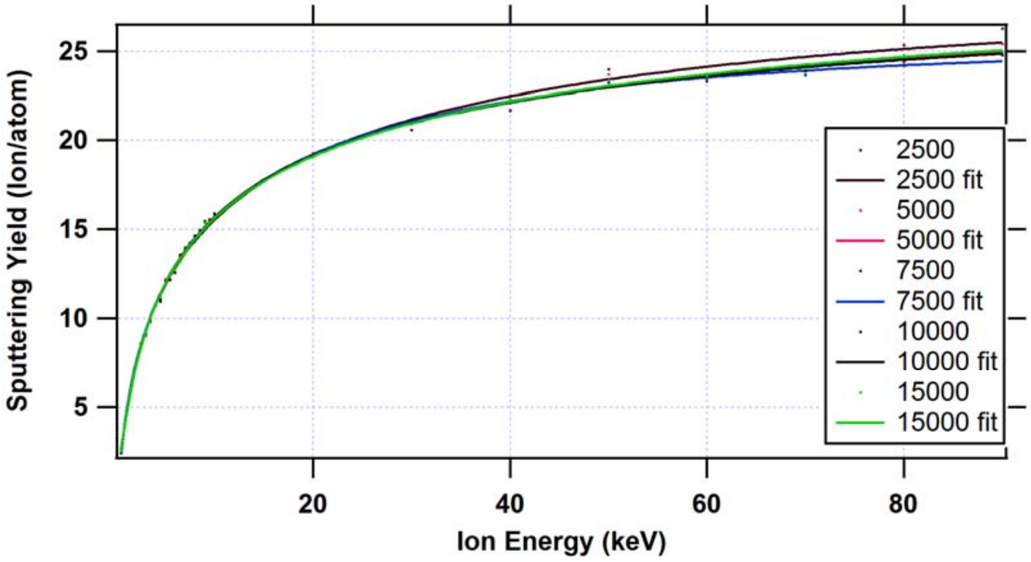


Figure 2 (a) the sputtering yield vs. width of Zn bombarded by Xenon at normal incident with 5000 ion number and ion energy of 50 keV . (b) – (d) the correspondent energy loss due to ionization, vacancies and phonons, respectively.



Figure(3) The dependence of the sputtering yield of Zn on the Xenon ion energy for different ion number and 500^{0}A and direct incident.

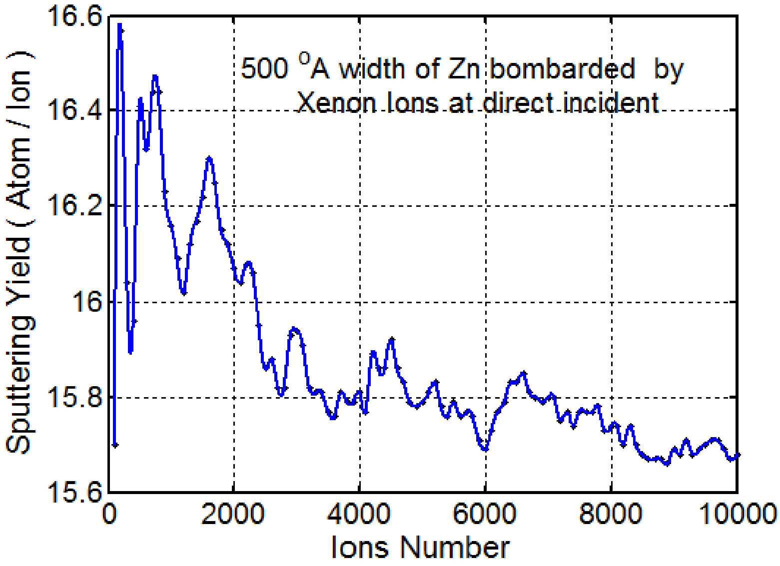
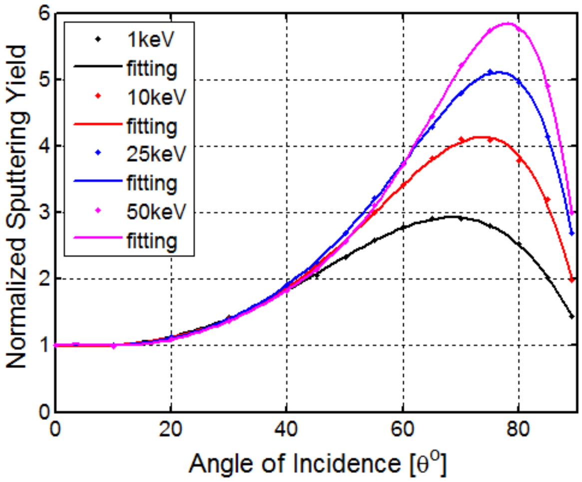
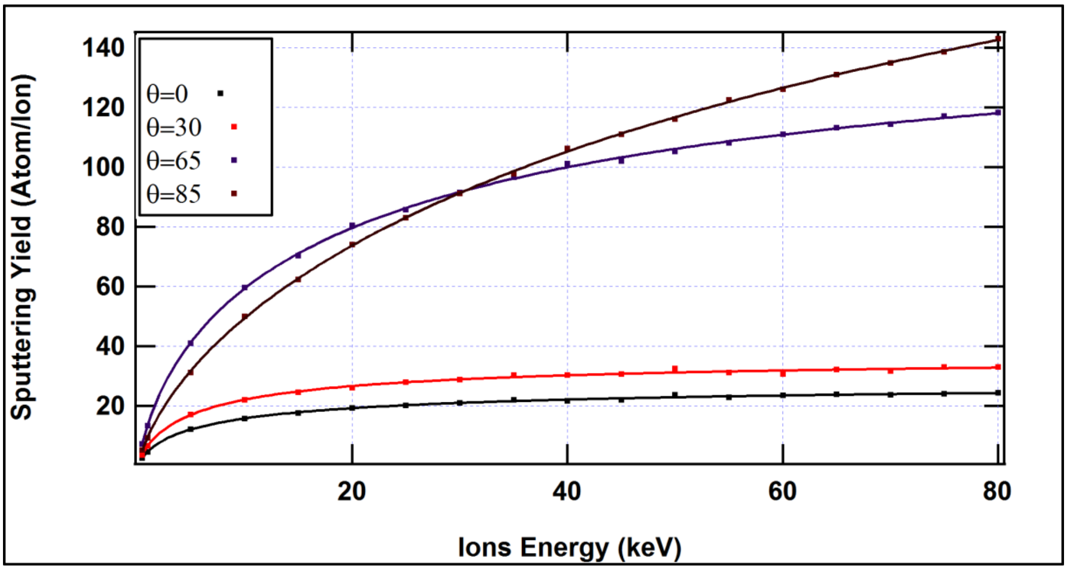


Figure 4: The dependence of the sputtering yield of Zn target bombarded directly by 10 keV Xenon ions on the ions number for fixed of target at 500⁰A



Figure(5): The angular dependence of the normalized sputtering yield of 500 ⁰A width target of Zn bombarded by 5000 ions number of Xenon.



Figure(6): The dependence of the sputtering yield on the ion energy for the Zn target bombarded by Xenon ion at different angles of incidence.

محاكاة لدراسة حاصل ترذيذ هدف من الزنك المقصوف بأيونات الزينون

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الخلاصة

باستخدام بيانات محاكاة برنامج التـرم TRIM، تم دراسة سلوك حاصل الترذيذ لهدف من الزنك المقصوف بوساطة ايونات بـلازما الزينون Xe الثقيلة. تمت اجراء حسابات حاصل الترذيذ كدالة لعرض طبقة من الزنك Zn، ولعدد ايونات الزينون ، وطاقتها ، وزاوية السقوط أيونات على الهدف وتم مناقشتها ورسمها. كذلك تم مناقشة ورسم خسائر الطاقة المترافقة مع الترذيذ بسبب التأين ، والشواغر والفونونات. وعلاوة على ذلك ، تم ملائمة الحسابات والتعبير عن منحنيات الحسابات بمعادلات ملائمة و وضعت معاملاتها.

الكلمات المفتاحية: برنامج التـرم TRIM، حاصل الترذيذ ، أيونات الزينون Xe، الزنك Zn