Calculating the Sputtering Yield of Lithium, Sodium and Krypton Bombarded by Same Target Ion Using TRIM Simulation Program

Enas Ahmed Jawad
Mustafa Kamel Jassim
Huda Majeed Tawfeek
Dept. of Physics / College of Education for Pure Science (Ibn Al-Haitham)
University of Baghdad

Received in :10/April/2016,Accepted in :19 /July/2016

Abstract

Calculations of sputtering yield for Lithium,Sodium and Krypton bombarded by the same own ions are achieved by using TRIM program.The relation of angular dependent of sputtering yield for each ion/target is studied. Also, the dependence of the sputtering yield of target on the energy of the same ion is discussed and plotted graphically. Many researchers applied polynomials function to fit the sputtering data from experimental and simulation programs, however, we suggest to use Ior function for fitting the angular distribution of the sputtering yield. A New data for fitting coefficients of the used ion/target are presented by applying used function for the dependence of the sputtering yield on the ion energy.

Keywords: sputtering, TRIM program, ion plasma, Lithium, Sodium, Krypton.

Introduction

Sputtering is a process whereby atoms are ejected from a solid target material due to bombardment of the target by energetic particles [1 – 4]. Sputtering begins when an energetic particle strikes a target surface atom. This particle is often called the incident, primary, or projectile particle.Sputtering occurs as the result of a series elastic collisions where the momentum is transferred from the incident ions to the target atoms through a series of binary collisions or a collision cascades region. A surface atom may be ejected as a sputtered particle if it receives a component of kinetic energy that is sufficient to overcome the surface binding energy (SBE) of the target material [5]. The minimum ion energy required for sputtering is called threshold energy which depends on the heat of sublimation of target material; it is relatively insensitive to the nature of the bombarding ions [6].

TRIM (**Tr**anspo**r**t of **I**ons in **M**atter) is a simulation program which employs Monte Carlo algorithm to simulate sputtering process. It is part of the SRIM(**S**topping and **R**ange of **I**ons in **M**atter),the software package which contains a set of programs that related to the stopping range of ions in matter calculations through quantum mechanical treatment of ion - atom collisions [7].

In this paper we use TRIM program to calculate thesputtering yield of light/heavy target bombard by its own ion. We choose Li,Na and Kr to study the sputtering yield parameters that affect the sputtering process, such as kinetic energy of bombarding ions and incidence angle. In this way, we can explore how the sputtering yield is when the target is bombarded by its own ions.

Theory

Sputtering yield SYcan be defined as the mean number of atoms removed per incident particle:

$$SY = \frac{\text{atom removed}}{\text{incident particale}} \quad \ldots\ldots(1)$$

The sputtering threshold E_{th} is defined as the minimum kinetic energy of the bombarding particle for sputtering to occur [8].Thus, the bombarding particle must have a kinetic energy above E_{th} .The sputtering yield depends on the properties of both the incident particle (energy, mass and incidence angle) and the target(atomic mass, surface binding energy, surface etexture and crystal orientation) [9].The sputtering yield can be expressed as in the following expression [10].

$$SY(E_0, \theta_0) = \alpha \beta_D (0, E_0, \theta_0) \quad \ldots\ldots(2)$$

where α is a factor associated with target material, and $\beta_D\,(0, E_0 \; and \; \theta_0)$ have expression used in numerical calculations given as [10].

$$\beta_D\,(0, E_0, \theta_0) = \gamma\, N\, S_n\,(E_0) \quad \ldots\ldots(3)$$

in which γ is a correction factor, which is a function of the mass ratio between bombarding target mass to the mass of the particle projectileM_2/M_1, N is atomic density of the target , θ_0 is initial angle of incidence , and $S_n\,(E_0)$ is a nuclear stopping cross – section.The latter is given by [11]:

$$S_n\,(E_0) = \frac{8.462\, Z_1\, Z_2}{\left(1+\frac{M_2}{M_1}\right)\left(Z_1^{0.23} + Z_2^{0.23}\right)} S_n(\varepsilon) \quad [10^{-15}\text{eV}\,.\,\text{cm}^2] \ldots\ldots(4)$$

whereZ_1 , Z_2 are the atomic numbers for each of the incident particle and material target bombard respectively, and $S_n(\varepsilon)$ is the limit of the decline in the nuclear cross section and it is expressed by [10].

$$S_n\,(\varepsilon) = \frac{0.5 \ln(1+1383\varepsilon)}{\varepsilon + 0.0132\varepsilon^{0.21226} + 0.19593\, \varepsilon^{0.5}} \ldots\ldots(5)$$

where $\varepsilon$is the reduced energy which is given by equation [10]

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

Results and Discussion

1. Effect of increasing incident ion angle on the sputtering yield

Figures (1 – 3) show the sputtering yield as a function of ion incidence angle for Litarget bombarded by Li^{+}, Na target bombarded by Na^{+} and Kr target bombarded by Kr^{+} at fixed ion energy of1.5 KeV and with constant ion number of 5000.In all figures mentioned the sputtering yield has a slight increase from the incident angle of $(0^0 - 60^0)$, and then a significant increase between $(60^0 - 80^0)$ of incident angle until finally decreases rapidly at larger angles.The reason for the increase of the sputtering yield is that the deposited energy distribution is shifted closer to the surface. On the other hand, the drop – off of the sputtering yield at higher angles is thought to be caused by the increase of ion reflection from the target surface. This behavior is common and similar to most of elements and alloys target that are bombarded by various ions. The difference is in the sputtering yield values at different angles of incident as well as in the angle which provides the maximum of sputtering yield .For the sputtering yield of the elements used, it is clear that light Lithium has a higher sputtering yield than Krypton and sodium respectively. Obviously, from figures (1 – 3) the peak of sputtering yield of Krypton is located at lower angle than the other elements. Generally, the degree of effect of the bombarding angle on the sputtering yields depends on the target used.

Since the calculations are distinct and singular for each individual angle, the fitting process has to be working to provide equation that describes the behavior. of course, the suggested fitting would result in different coefficients for each element under consideration. We use two types of best – fit function to express the sputtering yield data for comparison provided by Igor Pro program. The first function is a six degree polynomial

$$y = k_0 + k_1 x + k_2 x^2 + k_3 x^3 + k_4 x^4 + k_5 x^5 \qquad (7)$$

and the second is called (Ior) function:

$$y = y_0 + \frac{A}{(X - X_0)^2 + B} \qquad (8)$$

where the coefficients of the best fit values of equation (7) which are given in table 1, and for equation (8) in table 2. Although, many researchers used polynomials function for fitting the sputtering yield vs. angle of incident ion , we suggest using and activating the other fitting given by Ior function due to the absence of fluctuations at small angles in compassion to the polynomial functions.

2. Effect of increasing ion energy on the sputtering yield

Figures (4 – 6) show the sputtering yield vs. ion energy for Li, Na, and Kr at direct incident of ions, respectively. The sputtering yield increases with the increase of incident ions energy until it reaches a maximum sputtering yield and then begins to decrease at higher ion energy. The width of the each target is 1000 A^0 , and the ion number used for these colocations is 5000. This huge of ion number will interact per second with the target atoms at a direct bombardment and will stop at certain range of the target. The maximum energy transferred by ions to the target occurs approximately at a half distance of the ion range in the target. Therefore, the collision cascades regions are extended from the surface to the distance of maximum energy deposited in to the target.

For the same reason mentioned above, we work the fitting process, but now we use a ready formula proposed earlier for a particular ion – target sputtering [11]:

$$f(E) = k \exp\left(\frac{-\beta}{E - E_{\rm th}}\right) - \gamma \log\left(\frac{E}{E_{\rm max}}\right)^2 \qquad (9)$$

For the presented work the coefficients of E_{th},E_{max}, k,β and γwhich give the best fitting of TRIM are tabulated in table (3).It is for a specific interaction between certain similarly ion/target using above equation and it is new and not mentioned before.

3. The effect of the mass of both incident ions and target

The calculations were carried out with 5000 ion number for each1.5 keVions incident on the same width element targets of 1000 A^{O}. The following table describes the properties of ion/target used in the calculations.

	Z	**Ion mass**	**Target mass**	**Target density**
Lithium	3	7.016 amu	6.941amu	$0.534\ \mathrm{g/cm^3}$
Sodium	11	22.99 amu	22.99 amu	$0.97\ \mathrm{g/cm^3}$
Krypton	36	83.912 amu	83.8 amu	$2.6021\ \mathrm{g/cm^3}$

Figure (7) shows the angular dependent of sputtering yield for mentioned ion/target.Clearly, the higher the sputtering yield takes place for Li, Na and Kr respectively. This is due to the lower mass and atomic number of the Li in comparison with the other used ions.On average the light atoms in the cascades carry far greater momentum towards the surface of the target than do the heavy atoms. Thus, this leads to a higher sputtering yield. In this paper the scheme is to use similar ion/target monoatomic element. This means the mass of incident ion is equal or less than the target atom mass. Thus there is probability that an elastic reflection of ion from the target surface to takes place. The reflected particle becomes neutral because the ions are neutralized shortly before it impact the surface and it is not unaffected by sheaths. These neutral particles believe to be a source of losing energy from incident ion energy. Therefore, this aspect leads to a significant effect of the sputtering process.

Conclusions

There are many mathematical models that illustrate the interaction of ions with metals, as well as several of the simulation programs describing these interactions. In this paper, the global TRIM program has been used to calculate the sputtering yield of Li, Na and Kr target bombarded by its own ion, respectively. We found that the sputtering yield depends on the mass of the target and the atomic number of both ion and target. The same lighter ion/target gives lower sputtering yield at lower angles of ion incident and a maximum point of sputtering yield at higher angles. Further, the same lighter ion/target has a shifted peak of sputtering towards higher angles. Moreover, the lower the sputtering yield of the same ion/target vs. ion energy is denoted by the lighter ion/target. Regard to the angular distribution of the sputtering yield we suggest to use (Ior) function instead of polynomial functions because it does not suffer from fluctuations and smother than the second functions.

Reference

1. Kirk, A. Z. (2007) “Differential Sputtering yield of refractory metals by ion bombardment at normal and oblique incidences” Colorado State University Fall
2. Lucille, A. G. , and . Fred. A . S, ,(2005) "Introduction to Focused Ion Beams: Instrumentation, Theory, Techniques, and practice". Springer.
3. Sigmund, P. ,(1969) " Theory of sputtering . I. Sputtering yield of amorphous and polycrystalline target", physical review, (148), (2), 383 – 416.
4. Behrisch,R. and Eckstein,W. (2007)"Sputtering by Particle Bombardment: Experiments and Computer Calculations from Threshold to MeV Energies", Springer, Berlin.
5. Orloff, J. ; Utlaut, M. and. Swanson, L. (2003). “High Resolution Focused Ion Beams: FIB and its Applications”, Kluwer Academic/Plenum Publishers, NY.
6. Shwartz, G.C.(2006) “Handbook of semiconductor interconnection technology”, CRC Press Book.
7. Ziegler ,J.F. and Biersack, J. P . (2003) SRIM. http://www.srim.org.
8. Lucille, A.G. and Fred, A.S. (2005) ,“Introduction to Focused Ion Beams: Instrumentation, Theory, Techniques, and practice”. Springer.
9. Behrisch, R.(1981).“Introduction and Overview ,Sputtering by Particle Bombardment I” , 1-8, Springer-Verlag, Berlin.
10. Guping ,D. Tingwen. X. and Yun. L. (2012). Preferential sputtering of Ar ion processing SiO_2 mirror, AOMATT, The 6th SPIE International symposium on advanced optical manufacturing and testing technologies.
11. Nakles ,M. R. (2004) ,“Experimental and Modeling Studies of Low-Energy Ion Sputtering for Ion Thrusters”, MSc Thesis, Virginia Polytechnic Institute and State University.
12. Bianchi,S.and Ferrara,A.(2005)."IGM metal enrichment through dust sputtering" Mon. Not. R. Astron. (22), 1–20.

Table (1): The fitting coefficients of polynomial function for sputtering for(Li, Na and Kr), which is shown in figure (1,2,3).

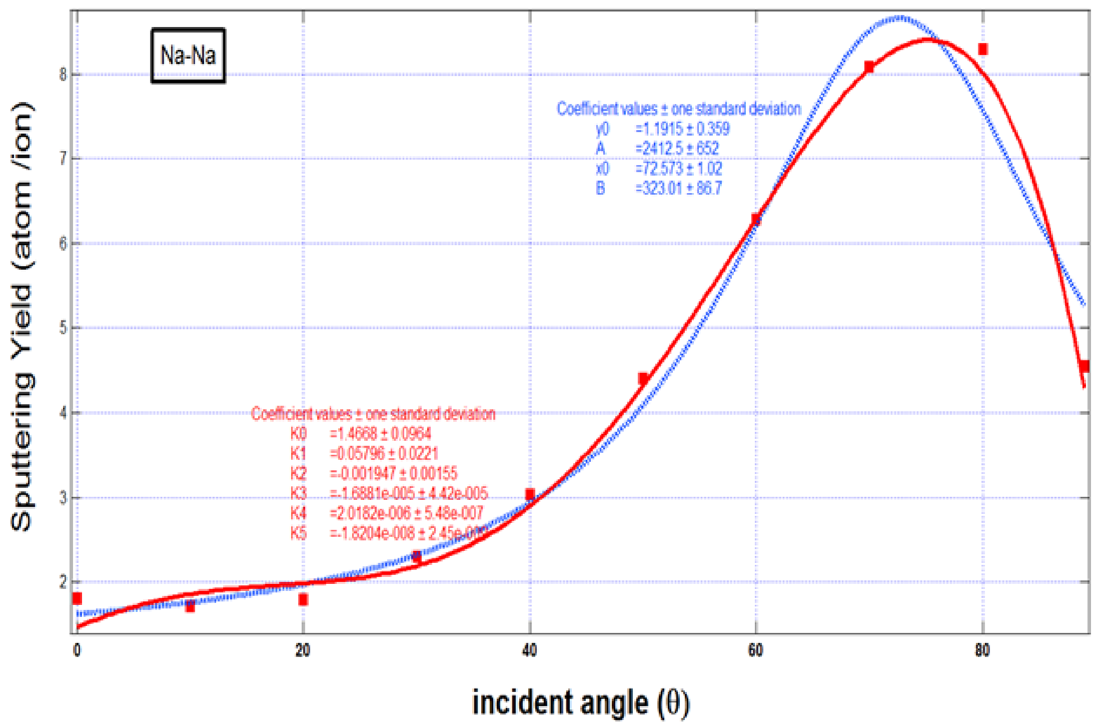
	K0	K1	K2	K3	K4	K5
Li-Li	1.4936	-0.39993	0.040218	-0.001451	2.1693e-3	-1.098e-7
Na-Na	1.4668	0.05796	-0.05796	-1.688e-5	2.0182e-7	-1.820e-8
Kr-Kr	2.0749	0.060443	-0.003202	0.007052	-8.694e-7	7.049e-10

Table(2): The fitting coefficients of Ior function for sputtering for (Li, Na and Kr), which is shown in figure (1,2, 3).

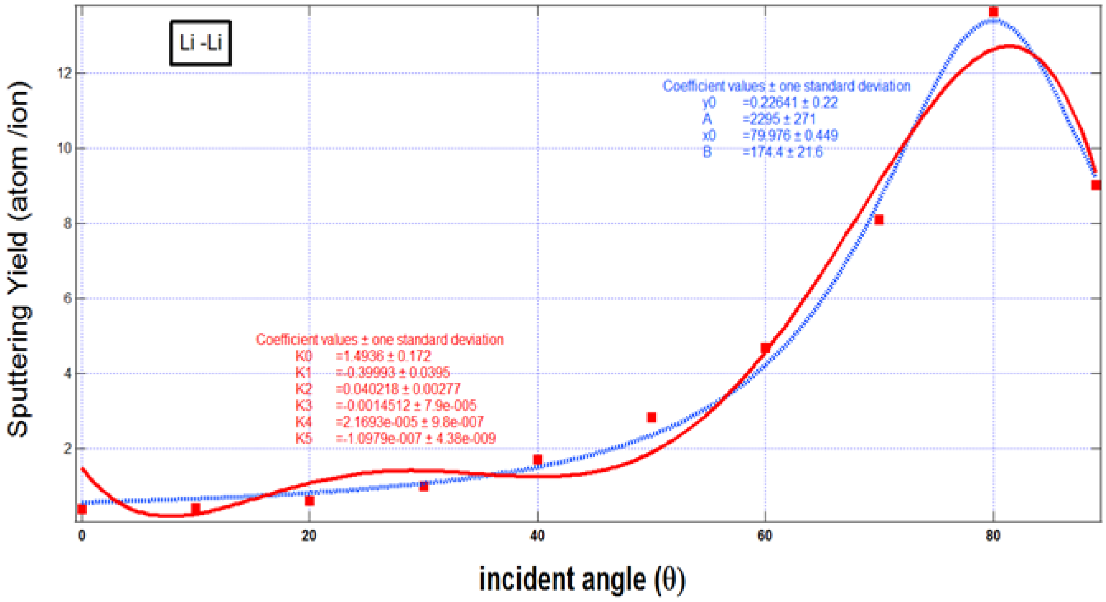
	Y0	A	X0	B
Li-Li	0.22641	2295	79.976	174.4
Na-Na	1.1915	2412.5	72.573	323.01
Kr-Kr	1.3784	4958.4	73.026	863.88

Table(3): The fitting coefficients of equation (10) for the curves are shown in figure (4 – 6).

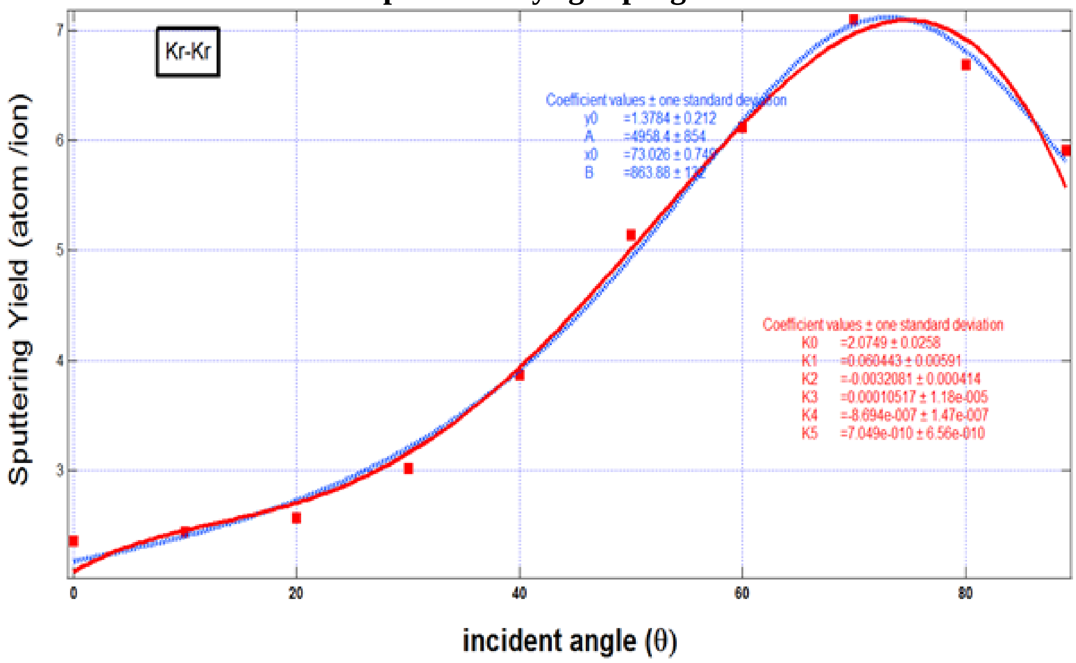
	k	β	E_{th}	γ	E_{max}
Li-Li	0.238	0.0004	3.000	0.688	2.000
Na-Na	2.2638	0.0004	6.000	0.4398	9.000
Kr-Kr	6.787	0.001	10.000	0.4154	62.000



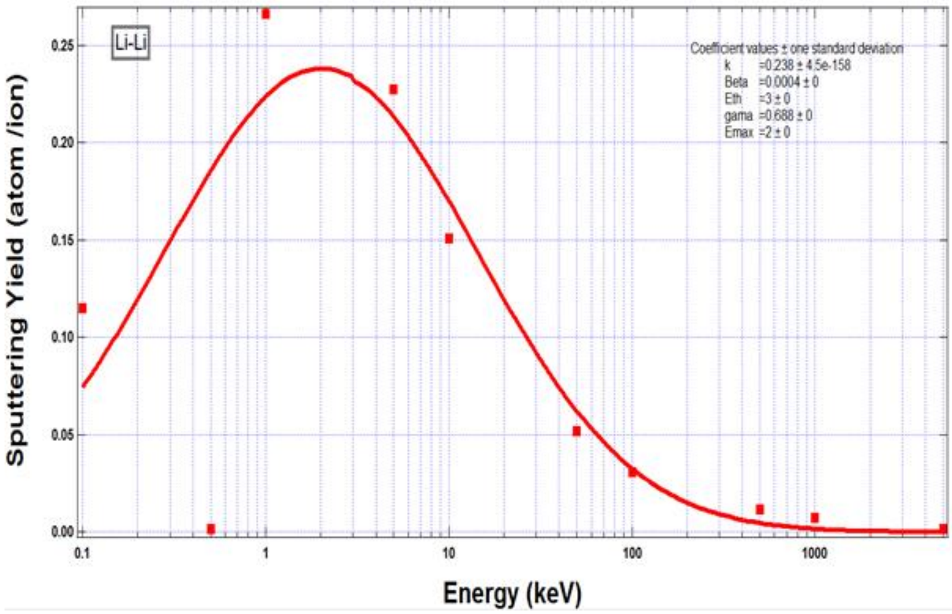
Figure(1): The sputtering yield as a function of ion incident angle for Na target bombarded by Na ion. The TRIM data are fitted using double functions; polynomial and Ior provided by Igor program.



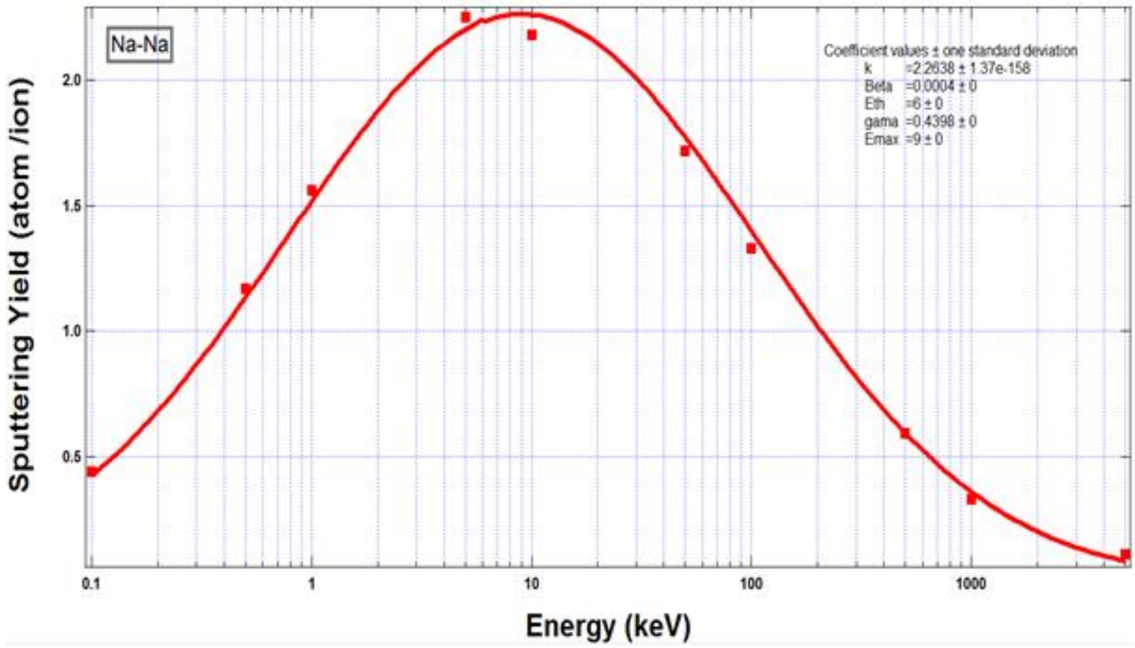
Figure(2): The sputtering yield as a function of ion incident angle for Li target bombarded by Li ion. The TRIM data are fitted using double functions; polynomial and Ior provided by Igor program.



Figure(3): The sputtering yield as a function of ion incident angle for Kr target bombarded by Kr ion. The TRIM data are fitted using double functions; polynomial and Ior provided by Igor program.



Figure(4): Sputtering yield vs. ion energy for sputtering of Li with theoretical equation fitting.



Figure(5): Sputtering yield vs. ion energy for sputtering of Na with theoretical equation fitting.

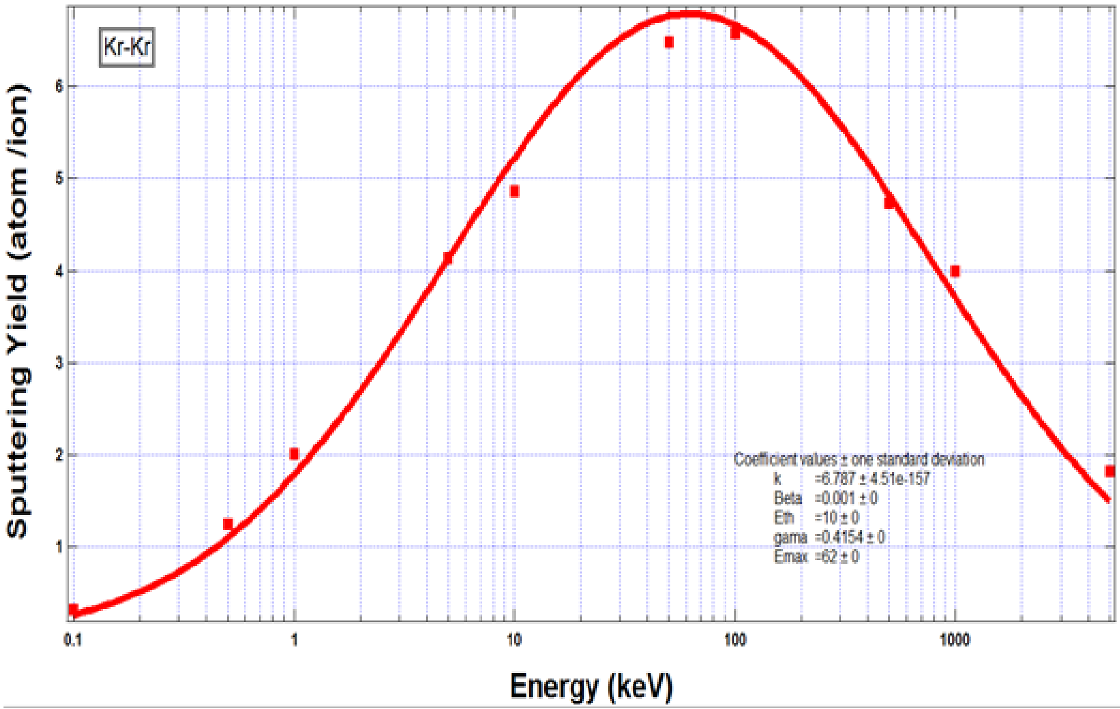
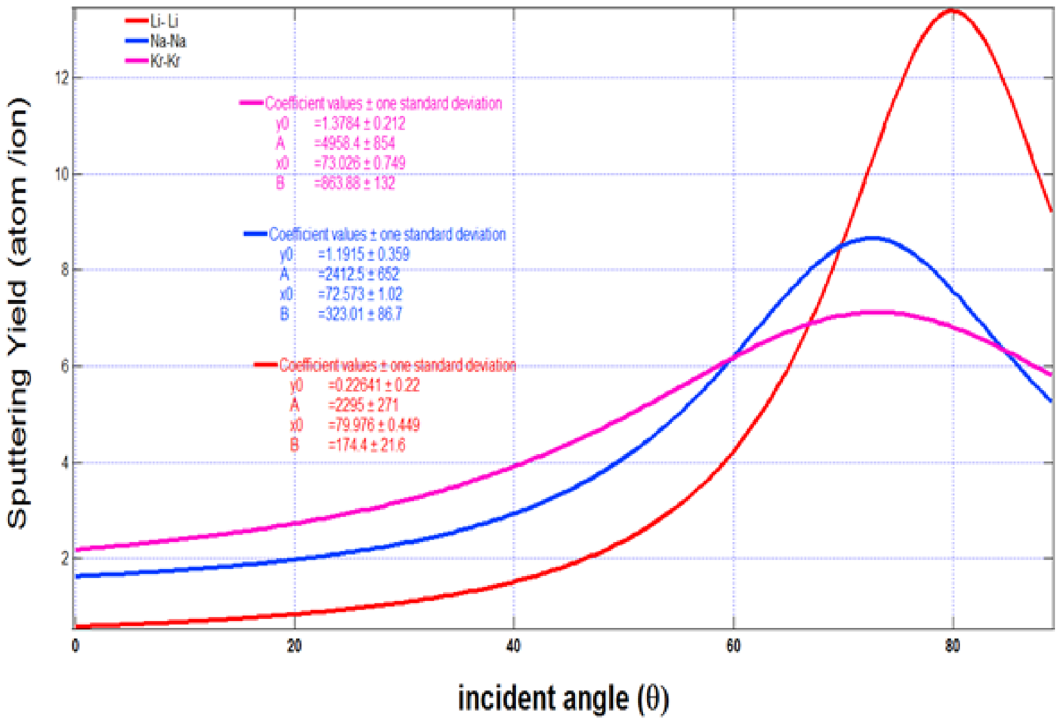


Figure (6): Sputtering yield vs. ion energy for sputtering of Kr with theoretical equation fitting.



Figure(7): The angular dependent of the sputtering yield of Li,Na and Kr with fixed ion number, the width of the target and ions energy.

حسابات حاصل الترذيذ لكل من اللثيوم و الصوديوم و الكريبتون عند قصفها بنفس ايون الهدف باستخدام برنامج محاكاة التـــرم

ايناس احمد جواد
مصطفى كامل جاسم
هدى مجيد توفيق
قسم الفيزياء / كلية التربية للعلوم الصرفة (ابن الهيثم) / جامعة بغداد

استلم في :10/نيسان/ 2016،قبل في19 /تموز/2016

الخلاصة

انجزت حسابات حاصل الترذيذ لكل من الليثيوم ، والصوديوم والكريبتون عند قصفها بنفس أيوناتها باستخدام برنامج التـــرم . تم دراسةعلاقة الاعتماد الزاوي لحاصل الترذيذ لكل أيون/الهدف قيد البحث. أيضا، وتم مناقشة اعتماد حاصل ترذيذ الهدف على طاقة نفس أيون الهدف ورسم بيانيا. ان العديد من الباحثين في هذا المجال عند اجراءهم ملائمة بيانات حاصل الترذيذ النتائج التجريبية وبرامج المحاكاة يستعملون متعددة الحدود، ومع ذلك، نقترح استخدام دالةIOR لملائمة التوزيع الزاوي لحاصل الترذيذ. في هذا البحث قدم تقيم معاملات جديدة لملائمةبيانات حاصل الترذيذ أيون /الهدف قيد البحث المعتمد على الطاقة الايونات الساقطة.

الكلمات المفتاحية :حاصل الترذيذ، برنامج تـــرم،البلازما، الليثيوم،الصوديوم، الكريبتون