مقایسه نتایج تجربی با محاسبه شبیه‌سازی بازدهی کندوپاش، یون‌های طلا توسط یون نئون در زوایا و انرژیهای مختلف

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چکیده - امروزه کاربردهای گسترده لایه نازک در زمینه‌های مختلفی مانند موارد صنعتی و علمی، رو به افزون است. لایه نشانی طلا دارای اهمیت بسیاری در ساخت قطعات میکروالکترونیکی است. در این مقاله کندوپاش طلا در انرژی‌های مختلف و زوایای مختلف یونهای فرودی مورد مطالعه قرار گرفته است. نتایج نشان می‌دهد، بازدهی اندازه گیری کندوپاش بصورت تجربی با نتایج شبیه‌سازی شده نرم افزار *TRIM.SP* در تطابق است. در گستره مشخص، بازدهی کندوپاش با افزایش انرژی و افزایش زاویه فرودی ذرات یونی بمباران شده، افزایش می‌یابد.

کلید واژه- کندوپاش طلا، بازدهی کندوپاش، مدل دینامیک مولکولی، انرژی یون فرودی، زاویه یون‌های برخوردی کندوپاش.

Experimental and Computer Calculated Sputtering Yield of Sputtered Au by Ne Ions at Different Energies and Various Incidence Angles

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Abstract- Nowadays a plenty of applications of thin film in different subjects such as scientific and industrial items has been grown. Au deposition is very important in microelectronic device fabrication. In this research project we studied Au sputtering in different energies and different angles of incident ions. Results show that the measured sputtering yield confirms the results that reached by TRIM.SP software. In specific range, sputtering yield increases by increasing energy and incident angle of bombardment ion particles.

Keywords: Au sputtering, sputtering yield, molecular dynamics model, incident ion energy, angle of sputtering collision ions.

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1 Introduction

Due to the importance of the thin gold layers in semi-conductor instruments and the fact that sputtering and sputter deposition are widely used techniques for the deposition of Au thin films therefore [1]. The value of the sputtering yield is significant for two parts; the producers of coating devices and semi-conductor materials. This paper focuses on the later aspect. In this study, Neon ions were used in coating gold layer. Neon was shot towards the target (Au) with different energies and angles and the sputtering yield was measured. These were compared with the results of simulation upon on molecular dynamics model which confirmed at high correspondence with them.

2 Theoretical Background

Sputtering is a variety of physical vapor deposition with wide applications. The physics processes of causing sputtering, i.e. the removal of atoms from the surface of solids or liquids at bombardment with particles having energies from the eV to the MeV range is today mostly understood [1].Sputtered atoms differ from evaporated atoms in their kinetics, due to the dynamics of the emission process. This is called cathode sputtering if it is done with positive ions. The sputtering yields determined by the average number of exported atoms from the target in return for each bomber ion or the proportion of the removed particles to the incident ions. This increases with the energy and the mass of the bomber ions [2].

The efficiency of cathode sputtering is given by the cathodes sputtering coefficient, *S*:

$$S = \frac{N_a}{N_i} = 10^5 \frac{\Delta W}{i.t.A}(atoms/ion) \qquad (1)$$

Where N_a is the number of sputtered atoms, N_i the number of incident ions, ΔW the decrease in the target's mass, *i* ion flow, *t*, bombardment time, and *A* the atomic mass of the sputtered substance [3].According to computer calculations the number of sputtered atoms for the incident particles usually changes to a great extends. The sputtering yield (efficiency of sputtering) in the case of amorphous (shapeless) or crystal targets systematically and interestingly depends on a number of factors including [4]:

- The kinetic energy of bombarding ions
- The cohesive energy of the target surface
- The type of incidental ion
- The angle of incidental ion with the target.

2.1 Sputtering Yield Dependence on Projectiles Energy

The sputtering yield of *S* depends on the energy of incident ions to the target. By increasing their energy, the sputtering yield first increases and then decline. The fall in the sputtering yield in higher energies is a result of deeper penetration of ions, into the target. A more than expected efficiency has been observed in case of heavy incident particles such as molecular ions or atomic cluster with the energy of 10keV or higher. In this condition, spike effects can lead to a non-linear change in the efficiency proportional to the number of atoms per molecule units or atomic cluster [5].

2.1 Sputtering Yield Dependence on Projectiles Incident Angle

The sputtering yield depends on the incident angle of bombarding particles. Analogously to the energy dependence of the sputtering yield, the angular dependence of calculated values is fitted with an algebraic formula and subsequently compared to experimental data[5, 6].

$$\frac{Y(E_0,\theta_0)}{Y(E_{0,0})} = \left\{cos\left[\left(\frac{\theta_0}{\theta_0^*}\frac{\pi}{2}\right)^c\right]\right\}^{-f} exp\left(b\left\{1-1/cos\left[\left(\frac{\theta_0}{\theta_0^*}\frac{\pi}{2}\right)^c\right]\right\}\right) \qquad (2)$$

$$\theta_0^* = \pi - \arccos\sqrt{\frac{1}{1+E_0/E_{sp}}} \geq \frac{\pi}{2} \qquad (3)$$

Here E_0 is the incident energy and θ_0 the angle of incidence. Know that,*Y*stands for sputtering yeild. In this equation, by assuming θ_0^*, it is reminded that even if the projectile undergoes the binding energy of E_{sp} (it is even possible to have a chemical binding), the incident angle cannot reach 90 degrees. For the self-bombardment $E_{sp}=E_{sb}$ in which E_{sb} is the surface binding energy (sublimation heat); for Hydrogen and Nitrogen isotopes E_{sp}=1eV; for Nobel gases E_{sp} is assumed zero. This binding effect of the projectile is significant only in low energies especially self-bombardment. If E_{sp}=0 then the θ_0^* will be equal to $\pi/2$ and formula (2) besides parameter c approaches the Yamamura formula. If E_{sp}>0 the projectile is affected by the acceleration effect and undergoes refraction (a decrease in incident angle). The maximum yield is reached in θ_{0m} angle which is given by the following formula.

$$\theta_{0m} = \frac{2}{\pi}\theta_0^*[\arccos(b/f)]^{1/c} \qquad (4)$$

The quantities of parameters f, c, and b are gained by fitting the computed yield (using TRIM.SP software) by Bayesian statistics and are presented [table1] along with the amounts of θ_{0m}, θ_0^*, E_{sp} and $Y(E_{0,0})$.

Table1: fitting values f, b, c for the angular dependence of the sputtering yield

Ion	Target	E_0 (eV)	f	b	c
Ne	Au	6000	1.9240	0.6608	0.9121
Ne	Au	14000	1.6611	0.4130	0.9587

The overall behavior of angular dependence of computed efficiencies shows that the maximum angular dependence changes with increasing the energy of projectile to greater incident angles; also

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the proportion of maximum efficiency to the efficiency in a right incident angle increases with an increase in the incident energy. Close to the sputtering threshold the maximum incident moves in the direction of vertical incidence. This is different for the cases like self-sputtering in which the binding between target and projectile is important. The maximum close to the threshold sputtering energy occurs in large incident angles. Then it moves to smaller incident angles by an increase in the energy of projectile. In higher energies of rare gas ions in which the effect of the binding energy of projectile, E_{sp}, decreases, the same behavior is shown [7].

3 Computational Methods

There have been numerous efforts to compute the sputtering yield amorphous, multi-crystal and mono-crystal targets. Along with analytical approaches taken by Sigmund, a lot of efficiencies have been calculated using computer software with an estimate of a double incidence. A great part of the efficiencies have been largely provided by Yamamura using ACAT, and Eckstein using TRIM.SP software. They have used various incidence potentials including Nakagava-Yamamura and KrC(WHB) potential employed by Yamamura and Eckstein respectively. To determine the binding energy of the surface, sublimation heat was used [5]. In this research, yields have been calculated with TRIM.SP for different angles of incidence at various energies for several ion-target combinations.

4 Experiment

Two experiment set up was prepared in this research, first one for energy dependence of sputtering yield, second one for projectiles angle dependency. For energy dependency survey, two ranges were selected; these ranges were 0-100eV and 100-1000eV.

For the angle dependency the angles were selected which can be selected in equipment ranges. The Bombardment angles: 0, 35, 45 and 63 Deg was selected.

5 Results and Comparison between Experimental and Simulation

5.1 The Dependence of Sputtering Yield on the Energy

-Experimental target: Au

-Bombardment ions: Ne

-The energy of Bombardment ions: 20eV, 50eV, 250eV and 900eV

- Number in each experiment: 4 samples

The dependence of sputtering yield on the energy of computed efficiency fittings is illustrated in figures 1. The correlation between experimentally determined efficiencies in the vertical incident angle with the computationally fitted quantities is generally acceptable. This acceptance guarantees the assurance of the computed quantities upon on molecular dynamics model.

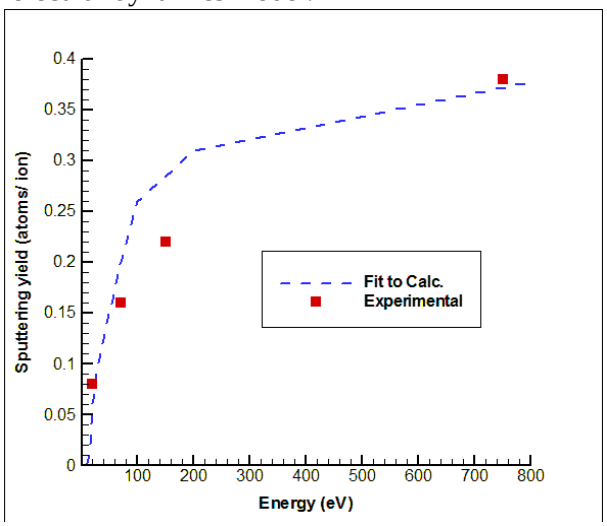


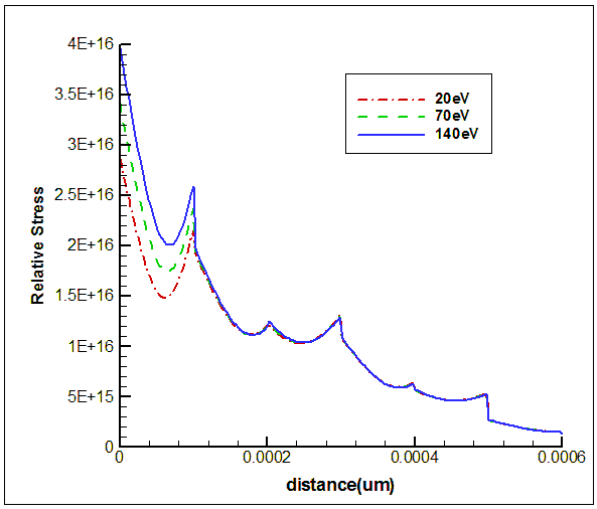
Figure 1– Au sputtering yield dependence to Ne bombardment energy under vertical incident angle

In bombardments, especially in low energies, the measured efficiencies are clearly smaller than the yield calculated from the curves. This indicates a different mechanism in sputtering, which is called chemical sputtering and in higher energy its fall. The fall in the yield in higher energies is a result of ions' deeper penetration into the target and can't help to separated surface atom from bulk surface [5, 8].

Busse et al. investigated ad atom production on the Al (111) surface and compared to experimental measurements [8].

For study of interaction of targets atom and bombardment ions the stress of surface was inspected. Here used the COMSOL multi-physics software for calculate the stress in deep of the sample. In molecular-dynamics computer simulation, as a rule, sputtering onto a flat surface is considered.

Figure 2 shows that in different energy forced different stress on the surface atoms but in deeper there aren't any difference, so the increasing of sputtered yield means growth of sputtered atom on the surface not in deeper ones.



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Figure 2– comparison of relative stress on the surface atoms vs. deeper ones (molecular dynamics model)

figure 3 shows that stress of second layer of atom increased by increase of energy but this increasing is slowly, aswhen energy increase from 20eV to 140eV, the stress from surface atom to other atom in deep only 23% increased from 1.3 to 1.54.

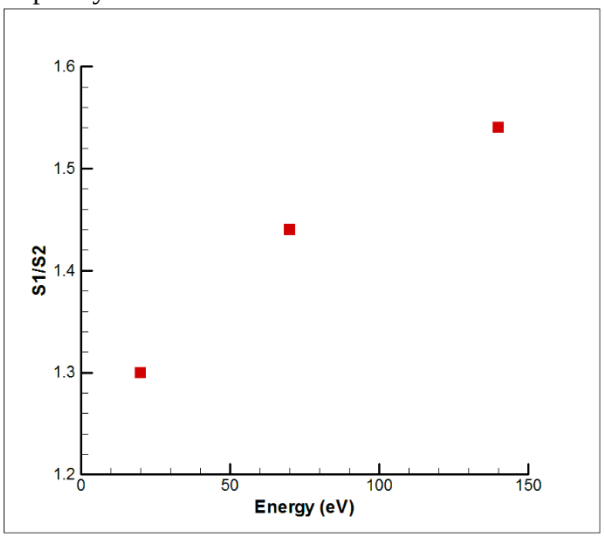


Figure 3– variations of stress from surface atom to other atom in deep (molecular dynamics model)

5.2 The Dependence of Sputtering Yield on the Incidence Angle of the Bombardment

- Experimental target: Au
- Bombardment ions: Ne
- The energy of bombardment ions: 1keV
- The bombardment angles: 0, 35, 45 and 63 Deg

Figure 4shows that experimental and calculated dependence of sputtering yield on the incidence angle for Ne energy in 140eV and calculated result for Ne energy in 80eV. The yield shape is uniform but value of sputtering yield is different.There you see the upper limit for angle is logical because of roughness domination. Total yields from off-normal sputtering (oblique) increase as the angle of incidence increases due to more energy becoming increasingly available in the near surface region until a maximum is reached and then the yield quickly drops to zero by as angle approaches 90°.

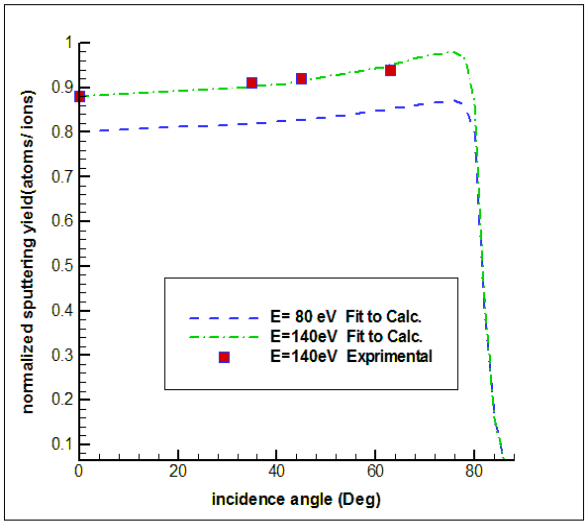


Figure 4– comparing the dependence of sputtering yields on the quantities of the measured and computed angles in various angles and sets of ion-target: Ne with an energy of 1keV on Au (molecular dynamics model)

6 Conclusion

The threshold energy depends also on the angle of incidence. It has been shown by simulations, that this dependence is stronger for heavy projectiles than light incident ions. In this research we use the light atom for bombardment, Ne. For the survey of the many experimental and calculated sputtering yields at normal incidence, the following procedure has been adopted. The calculated values have been fitted by an empirical formula and will be compared with experimental data, here 1keV Ne was used. This energy is in the region of the linear increasing of sputtering yield with respect to energy. In the second part of this study there are a good agreement between of simulation and experimental result for dependence of sputtering yields on the sputtering particle angles in various angles.

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