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

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چکیده - امروزه گاروبره‌های گسترده‌ای لایه نازک در زمینه‌های مختلف مانند موارد صنعتی و علمی، رو به افزایش است. لایه نشانی طلا دارای اهمیت بسیاری در ساخت قطعات میکروالکترونیکی است. در این مطالعه کندوپاش طلا در انرژی‌های مختلف و زاویای مختلف یون‌های نئون فرود مورد مطالعه قرار گرفته است. نتایج نشان می‌دهد، بازدهی اندازه گیری کندوپاش با توجه به انرژی تجربی یقیناً شبیه‌سازی شده برحسب نرم افزار TRIM.SP در تطبیق است. در گستره مشخص، بازدهی کندوپاش با انرژی زاویه فرودی دراز یونی بسیاران شده، افزایش می‌یابد.

کلید واژه‌ها- کندوپاش طلا، بازدهی کندوپاش، مدل دینامیک مولکولی، انرژی یون فرودی، راهی یون، 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.
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:

\[ S = \frac{N_s}{N_i} = 10^5 \frac{\Delta W}{t \cdot f \cdot A} \text{(atoms/ion)} \]  

Where \( N_s \) is the number of sputtered atoms, \( N_i \) the number of incident ions, \( \Delta W \) 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].

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

\[ \theta_0^* = \pi - \arccos \left( \frac{1}{1 + E_0/E_p} \right) = \frac{\pi}{2} \]  

Here \( E_0 \) is the incident energy and \( \theta_0^* \) the angle of incidence. Know that, \( Y \) stands for sputtering yield. In this equation, by assuming \( \theta_0^* \), it is reminded that even if the projectile undergoes the binding energy of \( E_p \) (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 \( E_{sp} \) is the surface binding energy (sublimation heat); for Hydrogen and Nitrogen isotopes \( E_{sp}=1 \text{eV} \); 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 \( \theta_0^* \) 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 \( \theta_{om} \) angle which is given by the following formula:

\[ \theta_{om} = \frac{2}{n} \theta_0^* \arccos \left( \frac{b/f}{n} \right)^{1/c} \]  

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 \( \theta_{om}, \theta_0^*, E_{sp} \) and \( Y(E_{0, 0}) \).

<table>
<thead>
<tr>
<th>Ion</th>
<th>Target</th>
<th>( E_0 ) (eV)</th>
<th>( f )</th>
<th>( b )</th>
<th>( c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ne</td>
<td>Au</td>
<td>6000</td>
<td>1.9240</td>
<td>0.6608</td>
<td>0.9121</td>
</tr>
<tr>
<td>Ne</td>
<td>Au</td>
<td>14000</td>
<td>1.6611</td>
<td>0.4130</td>
<td>0.9587</td>
</tr>
</tbody>
</table>

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
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 Nakagawa-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.
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, as when 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.

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 4 shows 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°.

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.

References