A Computer Simulation Study of Sputtering Yield of GaAs Target Bombarded by Argon Ions

Huda M. Tawfeek, Mustafa K. Jassim, Firas M. Hady, Rafah I. Nori
Department of physics - College of Education For Pure Science (Ibn Al – Haitham) – University of Baghdad

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Abstract

Sputtering yield behaviour of GaAs target bombarded by Argon ions plasma is studied through the reduction of TRIM (Transport of Ions in Matter) simulation data . The angular dependence of normalized sputtering yield of GaAs is studied. Further the effect of increasing ion energy, the effect of increasing ion numbers , the influence of GaAs width, and the effect of changing the surface binding energy of elements composed GaAs target upon the sputter yield are studied. It was found that the entire parameters mentioned have very strong effects on the sputtering yield of GaAs.

Keywords: sputtering yield, TRIM (Transport of Ions in Matter) program, Argon ions, GaAs

محاكاة حاسوب لدراسة حاصل ترذيذ هدف من زرنيخ الغاليوم المقصوف بأيونات الاركون

هدى مجيد توفيق ، مصطفى كامل جاسم ، فراس محمود هادي، رفاه اسماعيل نوري
قسم الفيزياء – كلية التربية للعلوم الصرفة (ابن الهيثم) – جامعة بغداد

الملخص

دراسة سلوك حاصل الترذيذ لهدف من زرنيخ الغاليوم المقصوف ببلازما ايونات الاركون بواسطة بيانات برنامج التـــرم للمحاكاة. تم ايضا دراسة الاعتماد الزاوي لحاصل ترذيذ هدف من زرنيخ الغاليوم . بالاضافة الى ذلك تم دراسة تأثير زيادة طاقة الايونات ، و تأثير اعداد الايونات ، وتأثير عرض هدف زرنيخ الغاليوم و تأثير تغير طاقة الربط السطحية المكونة لزرنيخ الغاليوم على حاصل الترذيذ. لقد وجد بأن كل هذه المعلمات لها تأثيرات شديدة جدا على حاصل ترذيذ زرنيخ الغاليوم.

الكلمات المفتاحية: حاصل الترذيذ ، برنامج تـــرم ، أيونات الاركون ، زرنيخ الغاليوم.

Introduction

The sputtering can be stated as the physical removal of material from a surface by means of energetic particle bombardment. Physical sputtering is driven by momentum exchange between the ions and atoms in the material due to collisions [1]. Sputtering is quantified by the sputtering yield (the mean number of atoms removed per incident particle) . The sputtering depends on both the bombarded ion and target properties. The incident ions set off collision cascades in the target, when such cascades recoil and reach the target surface with an energy above the surface binding energy, an atom can be ejected. When a target is bombarded with fast heavy particles, erosion of the target material occurs: this is termed sputtering [2].

It is well known that GaAs is considered to be an important material for electronic and optical applications. However, there are only some studying efforts achieved to explore the effect of an ion – induced GaAs. The latter leads to modify the electronic and optical properties [3]. This works aim to explore the sputtering yield of GaAs bombarded by Ar^+ since the GaAs surface under ion bombardment becomes morphologically unstable. This instability under certain conditions leads to nanoscale and ripples or island and dot formation at an oblique incidence with respect to the surface normal [4]. The TRIM (Transport of Ions in Matter) Monte Carlo simulation code is adapted for calculations in this study due to its widely used to compute a number of parameters relevant to ion beam implantation and ion beam processing of materials [5]. Figure (1a) shows the tetrahedral geometry of Gallium arsenide under the study which has Zinc blende structure.

2. A brief description of TRIM Monte Carlo Simulation

Several possible processes may occur in a solid 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 [6]. There are several theoretical [7] and semi-empirical calculations [8-10] which provide valuable analytical expressions to describe the important physical mechanisms related to the sputtering and the corresponding dependencies of several variables.

Since then several software packages such as TRIM (Transport of Ions in Matter) and ACAT (Atomic Collision in Amorphous Targets) and others that simulate the evolution of the collision cascade inside the target have been developed. TRIM(Transport of Ions in Matter) is binary collision Monte Carlo codes, available to simulate the sputter process and calculate the sputter yield. The TRIM (Transport of Ions in Matter) is a simulation of a binary collision approximation which treats the transport of atoms in a solid as a series of consecutive collisions between that the particle follows a straight trajectory (Figure 1b) [11].

The movement of the particle that has an energy E_i after ith collision is denoted by the polar and azimuthal angles α_i and β_i. The recoil atom (ion) is then allowed to move over the mean free path length λ that is mean atomic distance of the target material

$$\alpha = 1/\sqrt[3]{N} \tag{1}$$

where N is the atomic density of the material. The particle collides again, after travelling the distance λ, and scattered over the angles θ and ϕ, with respect to the center of mass system. Although the angle ϕ can be chosen randomly in the interval $[0, 2\pi]$ in the cylindrical symmetry, the polar scattering angle θ can be numerically calculated using the classical trajectory integral [12]

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

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

$$P = P_{max}\sqrt{r} \tag{3}$$

where the maximum impact parameter P_{max} given by

$$\pi p_{mx}^2 \lambda = 1/N \tag{4}$$

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

$$E_{i+1} = E_i - T - \Delta E \tag{5}$$

where T is the transferred kinetic energy and ΔE the electronic energy loss. Recoil is generated with initial energy $E_i = T - E_b$ if the transferred kinetic energy is larger than the displacement energy. Due to lack of knowledge the value of the bulk binding energy of the target material E_b is often set to zero. The incident ion and the generated recoils are tracked until their kinetic energy drops below a certain cut off energy. This cutoff energy can be chosen to be the surface binding energy since it represents the minimum energy an atom must have to escape the surface.

3. Results and Discussion

When a beam of ions with an energy of some keV interacts with a solid target, sputtering takes place which gives rise to the ejection of different particles such as the reflection of projectiles, electron emission and the sputtering of atomic and molecular species [13]. it should be noted that the sputtering yield vs. angle is important in determing how surface topography changes during the sputtering by ion bombardment. Simulations were run at various combinations of Ar^+ ion energy (Its mass is 39.962 amu), ion incidence angle, and some different ion number. It is noted that the calculations of TRIM (Transport of Ions in Matter) simulation provides data of sputtering yield of both Ga and As separately rather than the total sputtering of GaAs. A density $5.32\ \mathrm{g/cm^3}$ of GaAs is used in the calculations whereas the mass is 69.72 amu and 74.92 amu for Ga and Ar, respectively . The calculations run with a surface binding energy of 2.82 eV and 1.26 eV for Ga and As, repectively unless it noted other values. The lattice binding energy is the energy that every recolling target atom loses when its leaves its lattice and recoils in the target [14] is fixed during the simulation at 3 eV.

Further the displacement energy is the energy that a recoil needs to overcome the lattice forces and to move more atomic spacing away from its orginal site [14] is also fixed at $25\ \mathrm{eV}$. Figure (2) shows the normalized sputtering yield as a function of ion incident angle at different values of incident ions energy. The figure shows only the fitted data of the simulation to get rid of the slightly decreasing and increasing of sputtering data due to statistical nature of Monte Carlo algorithm used in the TRIM (Transport of Ions in Matter) program. Obviously as the angle of incidence slightly increases the normalized sputter yield increased reaching to a maximum and then the quickly drops toward lower values as it approaches an angle of 89^0. The normalized sputtering yield increases as the Ar^+ ion energy increased for both atoms of GaAs . However, the sputtering yield of Ga atom in the GaAs layer is higher than the corresponding As atom for the most of the energies used. The calculations and the plot of sputtering yield versus ion incidence angle show that the maximum yield of both Ga and As occur at about an angle of 70^0 incidence for all Ar^+ ion energies used. The curves show the same general shape, but the magnitude of the slope decreases as the ion energy decreases. The calculations denote one of the interest that is the fact that the sputtering yields for ions at an angle of 10^0 incidence are less than the yields for normal incidence 0^0 ions for ion energy range $1000-1500\ \mathrm{eV}$ for both Ga and As atoms. The width of the GaAs layer is $1000\ \mathrm{A}^0$ is used for these calculations.

If we consider the explicit values of the sputtering yield that depend on the Ar^+ ion energy, one find out a nonlinearly increase of the sputtering yield vs. increasing of ion energy for constant incident angle of ions. Figure (3) exhibits this dependence for both atoms of GaAs. As mentioned before the figure show the maximum of the sputtering yield occurs at incident angle of 70^0 for both atoms in the GaAs layer. The curves arise as the angle increased from 0^0 until angle 70^0 and start to be lower. The figure expresses that the sputtering yield for As is larger than Ga. For both atoms the lowest the sputtering yield takes place at incident angle of 89^0 at energy $\geq 1500\ \mathrm{eV}$ for Ga and $\geq 2700\ \mathrm{eV}$ for As. In these calculations a width of $1000\ \mathrm{A}^0$ is used.

Figure (4) illustrates the changing the number of incident ions the values of sputtering yield will change. In case as Ga atom of the curves separate for ion energy $\geq 1.5\ \mathrm{keV}$, slightly variable in the range of $1.5-3.2\ \mathrm{keV}$ and a gain separate at higher energy. Clearly the higher ion number leads to a lower sputtering yield at lower and higher ion energy. On the other hand the separable of sputtering yield vs. energy is obvious for the As. However, the higher number of ion gives higher sputtering yield until the ion energy increased to about $4.5\ \mathrm{keV}$ whereas gives lower sputtering yield as the energy increased. One prefers to work the simulation using 5000 ion number to save the time of calculations and seemly appears that the sputtering yield values is inconsiderable change using higher ion number. The GaAs layer width of these calculations is chosen to be $1000\ \mathrm{A}^0$ .The dependence of the sputtering yield on width of the GaAs bombarded by Ar^+ at normal incident for 5000 ion numbers and ion energy of $5\ \mathrm{keV}$ as shown in Figure (5).

The sputtering yield profiles as a function of width for both atoms behave in similar manner. At low widths lower than a critical width that is $240\ A^0$ the sputtering yields are fluctuated. After the critical width the sputtering yields are saturated, i.e. anymore increased in the width would not affect the sputtering yields. This is the reason that we used a width of $1000\ A^0$ in the previous calculations for the sake of avoiding the fluctuations in the sputtering yield. Figure (6) illustrates the effect of small change in the surface binding energy of the elements that composed the structure of GaAs. The surface binding energy is the energy that the target atoms must overcome to leave the surface of the target [14]. Typically the heat of sublimation is a good estimate of this energy. The left hand side of the figure expresses the small variation of Ga surface binding energy on the sputtering yield of GaAs layer where the typical value of the surface binding energy for As is fixed. Clearly the sputtering yield values decrease linearly as the surface binding energy increased. In spite of there is no noticeably variations in the sputtering yield of As in the figure a very small change takes place in the calculations. On the other hand, for a fixed typical value of the surface binding energy of Ga and allowing a small change in it for As shown in the right hand side of the figure, the sputtering yield vs. surface binding energy slope line increased. One can notice a very bit variations in the figure of the line for the Ga. As a result any change in this energy would produce a variation in the sputtering yield of the GaAs, and any slightly change in the surface energy of the one element would introduce change of the sputtering yield in other element of GaAs.

Conclusion

A TRIM (Transport of Ions in Matter) simulation code data is used to study the sputtering yield of GaAs target. The normalized sputter yield increased as the angle of incident ion increased leading to a maximum peak at 70^0 incidence for both elements composed the GaAs target, and for the entire ion energy used and then the quickly drops toward lowest values as it approaches 89^0. Depending on the ion incident angle the sputtering yield increases as the ion energy increased. Since the sputtering yields are not strongly affect by increasing the ion number but only in the lower and higher energy $\leq 5\ \text{keV}$ one chooses to use 5000 ion number when working in TRIM (Transport of Ions in Matter) to save the time of calculations. The width of GaAs target lower than $240\ A^0$ for certain energy and ion number indicates fluctuation in sputtering yield, however any larger value than the mentioned width the sputtering yield mostly unaffected. The slightly change in the surface binding energy of one element of the target leads to significant change in the sputtering yield. The effect consists slightly change in sputtering yield of the other corresponding element composed the target.

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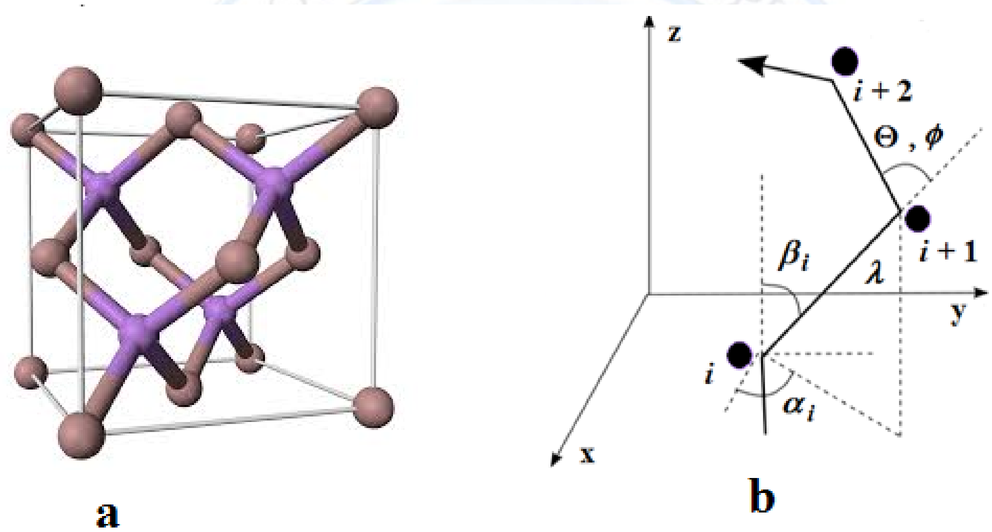

Figure 1a): Tetrahedral geometry of Gallium arsenide which has Zinc blende structure [11]. 1b): Section of an ion or recoil trajectory with consecutive collision with target atoms denoted by i, $i+1$ and $i+2$. The solid lines represent the ion trajectory [12].

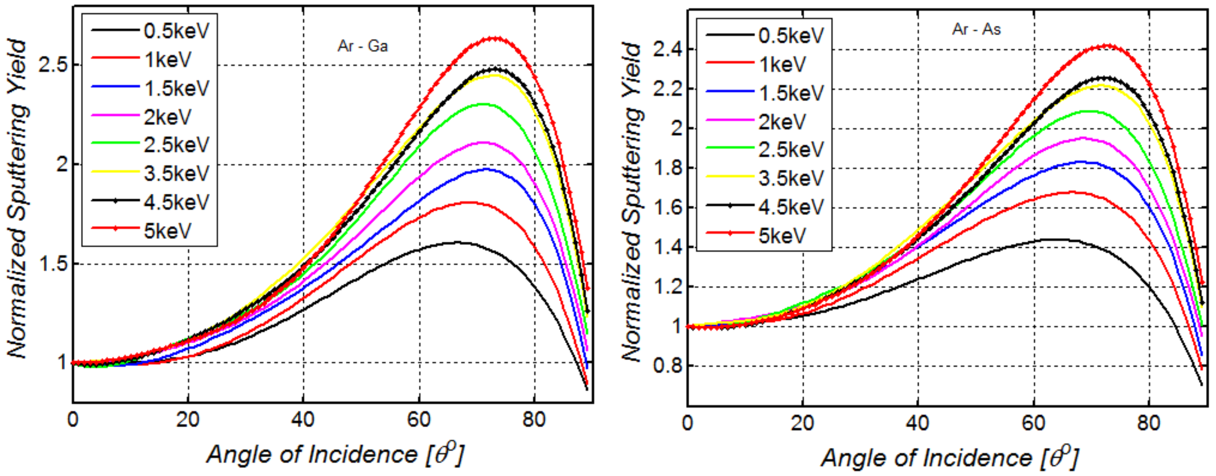

Figure 2: The angular dependence of the normalized sputtering yield of GaAs bombarded by Ar^+.

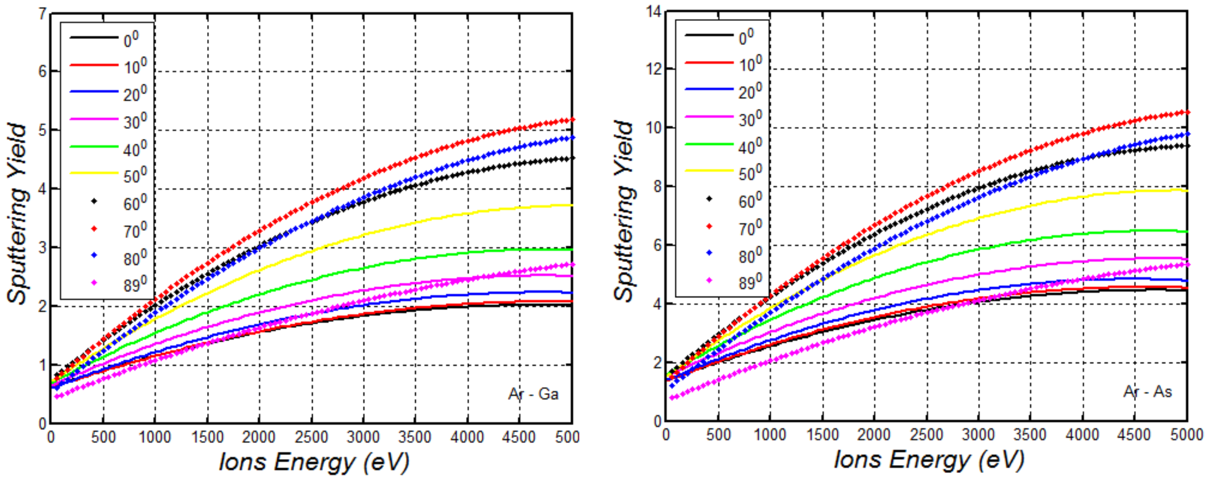

Figure 3: The dependence of the sputtering yield on the ion energy for the GaAs bombarded by Ar^+.

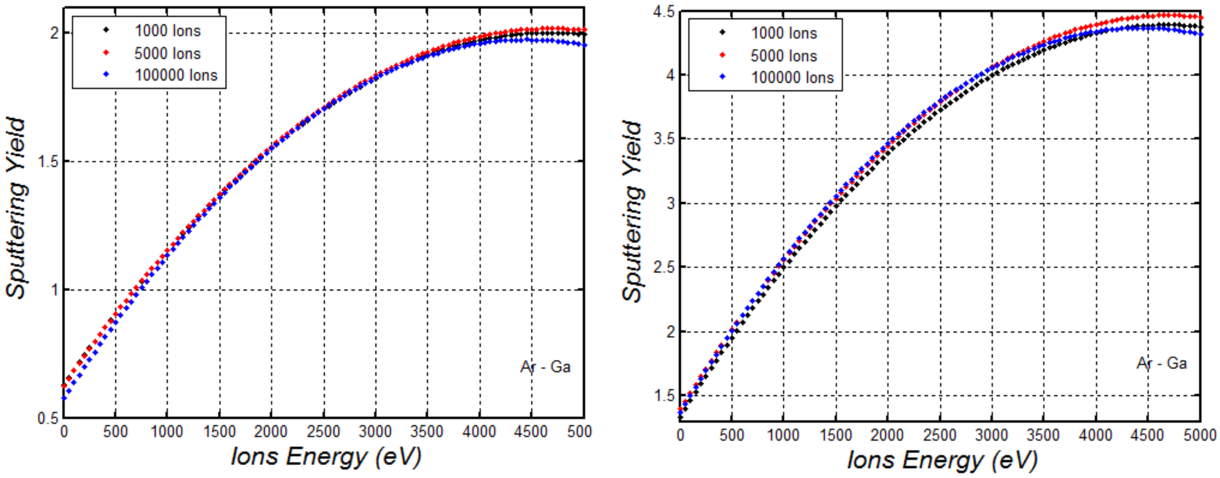

Figure 4: The dependence of the sputtering yield on the ion energy for the GaAs bombarded by Ar^+ at normal incident for different ion number.

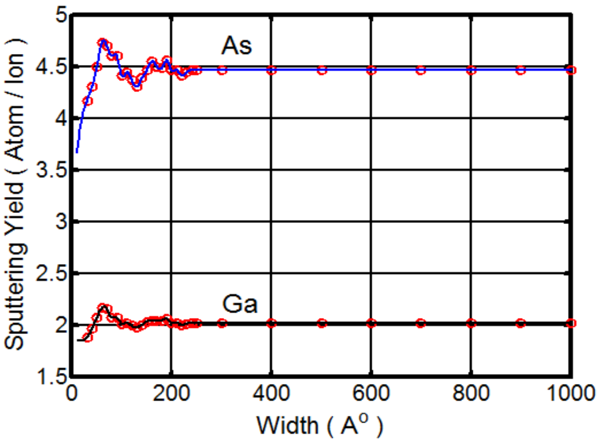

Figure 5: The sputtering yield vs. width for GaAs bombarded by Ar^+ at normal incident for 5000 ion numbers and ion energy of 5 keV .

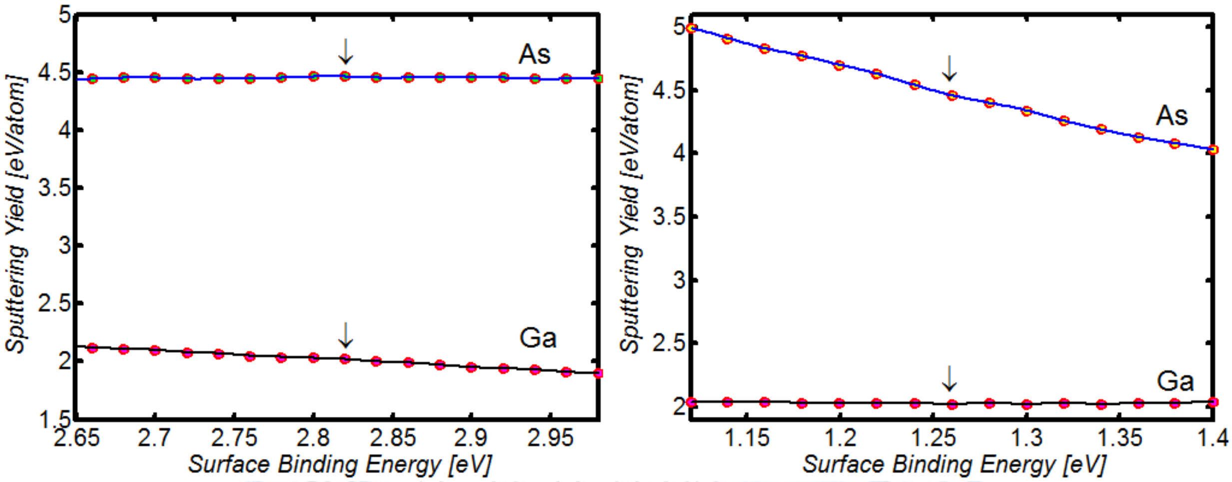

Figure 6: The sputtering yield vs. surface binding energy for GaAs bombarded by Ar^+ at normal incident for 5000 ion numbers , ion energy of 5 keV and 500 A^0 width layer.