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Characterizing the Relationship Between Sputtered Atom Flux Generated by Electrical Discharge in Plasma and Thin Film Deposition Quality

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Abstract: Thin film technology is still under development, to comply with industrial demands it is necessary to be able to produce a high quality thin film, to accomplish this we must know the several parameters which contribute to the disposition of the ejected particles, on this work we have presented the analysis of semiconductor atom deposition on magnetron sputtering in 3D curves, using SIMTRA software we created a vacuum chamber which has dimension of 25cm×25cm×40cm, the magnetron used has a circle shape target with a radius of 4cm which contains two different target (Si and Ge) and the substrate has a 10cmx10cm rectangle shape, after this adjustments with the use of Monte Carlo code we simulated the particle ejected away from target to find the number of collisions and the number of atoms arrived on the substrate with a variation of the distance that the atoms ejected had to cross, a very clear result was found which will show you that widening the distance negatively affects the coating and the deposition of the atoms.

Keywords: thin films, sputtering, vacuum chamber, Monte Carlo codes.

1 Introduction

The physical vapor deposition (PVD) process has been known for a long time; it's based on a thin-film deposition process in which the coating grows on the substrate atom by atom. The most common gaseous coating methods for the PVD process are: evaporation and sputtering [1-6]. These techniques allow the particles to be removed from the target at very low pressure and deposited on the substrate, the sputtering process appears to be an alternative for applications requiring improved surface morphological quality where roughness, particle size, stoichiometry and other requirements are greater than deposition rate. Due to the stresses generated by the cooling process with the drop in temperature or the melting temperature of the substrate (polymers), the deposition process has temperature limits for some applications [7-11]. Many sputtering methods have appeared such as the appearance of magnetron sputtering. Magnetron sputtering (MS) is one popular growth technique due to its low cost and low operating temperature[12,13], this technique is another way of deposition of thin films on a substrate, the procedure of this approach is based on the formation of a ring glow plasma (usually confined around the target by a magnet) beyond the surface of the cathode due to the collision of electrons with the available gas molecule, the resulting ions accelerated towards the cathode and bombarded its surface so that particles were released, the particles released from the target were deposited as a film on the substrate and some particles were disturbed along the path and deposited inside the working chamber[14,15].

To study this technique there are several software based on sputtering process such as SRIM and SIMTRA, both of this software are based on Monte Carlo simulations and these two programs are used to study the entire sputtering process and they allow to study all the steps that the ejected particles face in order to create the thin layer[16-18] , first SRIM (Stopping and Range of Ions in Matter) is used for the calculation of the sputtering yield, it gives the number of atom ejected of any material used, then the transport of this atoms ejected into the substrate is studied by the use of the second software SIMTRA (Simulation of Metal Transport)[19-21].

In this work we will first study the number of collisions created in the chamber during the transport of the ejected atoms into the substrate for the semiconductors (Si and Ge) with a variation of the distance between target and substrate, then we're going to build a three-dimensional graph to analyze the deposition of atoms ejecting on the substrate during each distance, to carry out this work we will utilize first SRIM to calculate the energy and the direction of the particles that are sputtered away from the targets, The transport of these species toward the substrate is then handled by the SIMTRA code with the application of a constant temperature and pressure value, the objective of this work is to deduce the best possible configuration inside the vacuum chamber to achieve the finest coating of the substrate and to offer the best possible deposition of atoms, all the results found will be represented in a curves by Origin software. Our goal is to participate on the technology development of thin film and to offer a result that will allow

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us to solve several problems on the formation of cells and thin films.

Sputtering equations

A. Target:

Three fractions are considered θm, θr and θc. The fractions θ_m and θ_r represent the fraction of non-reacted and of reacted target atoms in the surface layer of the target, while θ_c is the fraction of target atoms that has chemisorbed reactive gas molecules. The reacted fraction θ_r accounts for compound molecules formed in subsurface regions by implanted reactive ions, after which they are transported to the surface by sputtering. The sputter yield of the target will be defined as:

$$Y_s = Y_m\theta_m + Y_r\theta_r + Y_c\theta_c$$

With Y_m, Y_r and Y_c the corresponding sputter yields of the different fractions. It will be assumed that the compounds formed by chemisorption or by subsurface reaction are identical, so it can be stated that $Y_r = Y_c$. The speed v_s with which the surface recedes due to sputtering, is defined as:

$$v_s = \frac{J_{\text{ion}} Y_s}{n_0}$$

Where J_{ion} is the ion current density and n_0 is the atomic metal density of the target surface. Because of the receding surface, subsurface compound molecules are transported to the surface region. As the fraction θr remains in steady state constant, the following continuity equation is valid [22,23].

$$v_s\theta_b n_0 = J_{\text{ion}} Y_r\theta_r$$

Substrate

The substrate is defined as the whole of surfaces where sputtered material is deposited, except the target. The sputtered material is deposited on this substrate according to a certain deposition profile. Knowledge of a deposition profile allows to treat the substrate in a multi-cell approach.

This equation allows to calculate the full substrate condition, described by the individual fractions $\theta_{s,i}$

$$J_{\text{ion}} A_t Y_m \theta_m \theta_{s,i} \varepsilon_i = \\ \frac{2}{z}\alpha_s F_r\left(1-\theta_{s,i}\right)A_{s,i} + J_{\text{ion}} A_t\left(Y_c\theta_c + Y_r\theta_r\right)\left(1-\theta_{s,i}\right)\varepsilon_i$$

Where A_t is the racetrack area, ε_i represent the weighting factor, F the flux of reactive lecules toward the target and z the stoichiometric factor.

Chamber

During reactive sputtering a given flow rate Qin (molecules per second) of reactive gas is introduced in the vacuum chamber. This reactive gas flow can be consumed in three ways: by reaction on the target Q_t, by reaction on the substrate Q s or by the action of the vacuum pump Q_p. The steady state condition requires then that

$$Q_{\text{in}} = Q_t + Q_s + Q_p$$

The gas consumption by the target Q_t and by the substrate, Qs, depends on the target and the substrate condition, respectively, as explained in the sections above. The consumption by the vacuum pump is defined by:

$$Q_p = \frac{P_r S}{k_B T}$$

With S as the pumping speed (in $\mathrm{m}^3\ \mathrm{s}^{-1}$) [24-26]. For the flow toward the substrate in the multi-cell approach, it is given by

$$Q_s = \sum_i Q_{s,i}$$

$$Q_{s,i} = \alpha_s F_r\left(1-\theta_{s,i}\right)A_{s,i}$$

Simulation method

Simulation of film growth on time scales of seconds or minutes is possible with the Kinetic Monte Carlo Algorithms [27, 28], this approach can be used to model different surface processes such as nucleation, growth, post-deposition structural modification of films [29, 30], the kinetic energy and the number of atoms arrived at the substrate location are calculated by SRIM and SIMTRA software.

These programs offer a choice of bombardment energy and configuration of values such as temperature and pressure with no limit, that's why it is necessary to do research concerning the limit of value used because exceeded this value will give an impossible result to test on the practical side, so the choice of these values to use in our work was based on research already done regarding the choice limitation [31-34].

First we have created a vacuum chamber which has dimension of 25cm×25cm×40cm (as shown in Fig.1), three different distance (5cm, 8cm and 14cm) between target and substrate was taken, the magnetron used has a circle shape target with a radius of 4cm and the substrate has a 10cmx10cm rectangle shape, we applied a constant temperature, pressure and a 10^4 ions of argon on the semiconductors (Si and Ge) with an energy value of 1.5kev and an angular incidence of 75 degree, the objective is to deduce the influence of the distance on the atoms arriving on the substrate and to see also the thickness of the thin-films built, after all this configuration we can start the simulation this model will calculate the ejection of sputtered atoms on our target and gives the number of particle arriving on the substrate, the results will be saved on data files and will be presented by 3D curves.

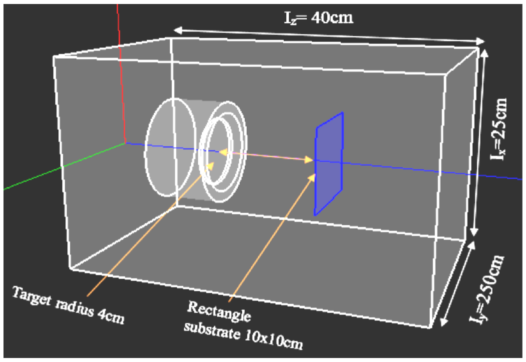

Fig. 1: Model used on the simulation

2 Results and discussion

A. Number of the atom's collision between emission and deposition

Inside the vacuum chamber, the target which contained materials (Si and Ge) is being bombarded by Argon gas ions with a fixed pressure and temperature of 0.5 Pa and 300 k on three different distance value between the target and substrate (5cm, 8cm and 14cm).

The following figures represents the number of the atom's collision sputtered and arrived on the substrate for each distance.

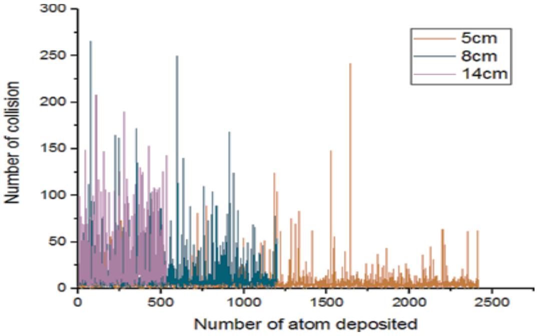

Fig. 2: Number of collisions as a function of the silicon (Si) atoms ejected using three different distance d= [5cm, 8cm, 14cm]

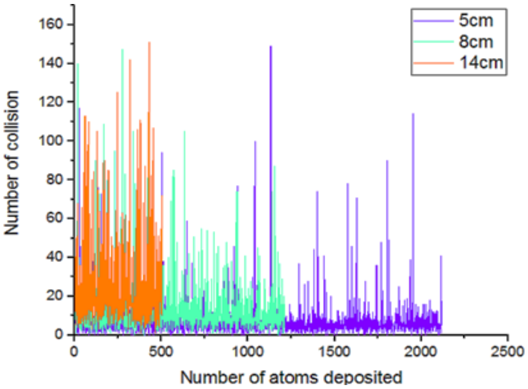

Fig. 3: Number of collisions as a function of the germanium (Ge) atoms ejected using three different distance d= [5cm, 8cm, 14cm]

As shown in the figures above, if we expand the distance between the target and substrate the number of collisions will rise, and we will obtain less atoms arrived on the substrate.

On the distance 5 cm we notice that the number of collisions is very low comparing to the other distances, we have obtained more than 2000 atoms on the semiconductor targets, and on the distance 8cm and 14cm we observe that the number of atoms arrived diminished, and the number of collisions grow.

By increasing the distance, the atoms ejected from the target will have a longer distance to travel so they will face a hard path to reach the substrate, applying a long distance will grow the possibility of atoms colliding with each other or between ions which will make a lot of atoms ejected not reaching the substrate.

B. Analysis of the thin layer created by the deposition of the atoms ejected

The same procedure will be carried out, but for this time we will analyses the deposition of the atoms ejected into the substrate using the same materials as target (Si and Ge).

This figure illustrates the formation of the thin film for each sputtered material on three different distances (5cm, 8cm and 14cm)

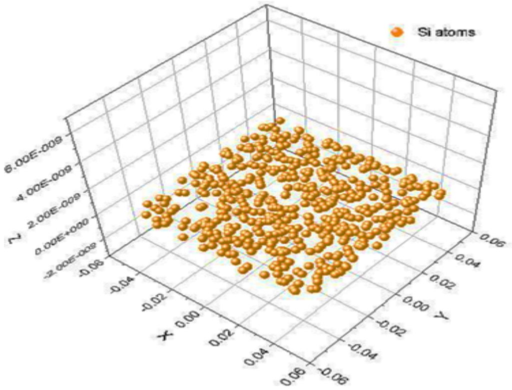

Fig. 4: Deposition of the atoms ejected on the substrate for the semiconductor (Si) using 14cm distance.

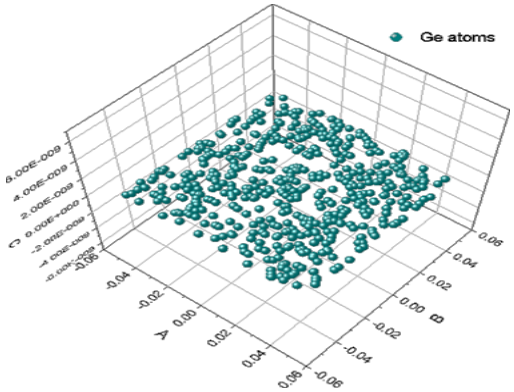

Fig. 5: Deposition of the atoms ejected on the substrate for the semiconductor (Ge) using 14cm distance.

For each materiel used we can distinguish an emptiness between the atoms deposited on the substrate, this means that the formed thin layer is not well coated, using a 14cm distance between the target and substrate will lead to a bad coating, a lot of atoms ejected will not reach the substrate due to the high number of collisions that they will face.

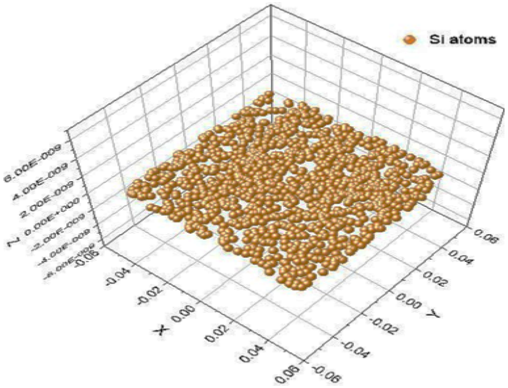

Fig. 6: Deposition of the atoms ejected on the substrate for the semiconductor (Si) using 8cm distance.

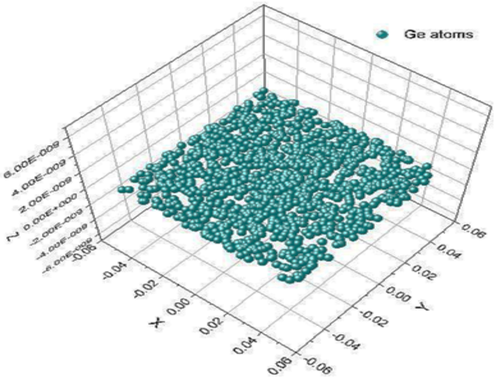

Fig. 7: Deposition of the atoms ejected on the substrate for the semiconductor (Ge) using 8cm distance.

For this time, we can perceive that applying a distance of 8cm between the target and the substrate the gap between the atoms begins to fill, we can observe that the coating is better, the thin layer formed may be usable, but it still needs more atoms to be deposited to reach the perfect coating.

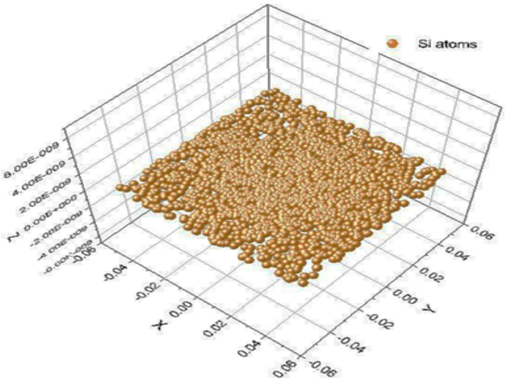

Fig. 8: Deposition of the atoms ejected on the substrate for the semiconductor (Si) using 5cm distance.

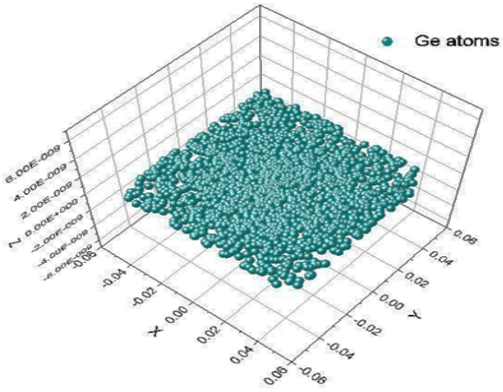

Fig. 9: Deposition of the atoms ejected on the substrate for the semiconductor (Ge) using 5cm distance.

Now, we can see the thickness on the formed thin layer, there is no void between the atoms, with the use of 5cm distance between target and substrate a huge number of atoms ejected will be deposited on the substrate, the atoms ejected will face less collision which will make them reach the substrate easily, therefor the coating is perfectly done.

3 Conclusion

PVD techniques are constantly evolving, with the emergence of new technologies that are adapted to the processes. They also meet the growing demands of the industry. Researchers have also concentrated in recent years on improving reactors and improving the use of external devices to the detriment of improving the properties of films, which has moved to the background, depending on the needs of the industry.

The choice of deposition process is dependent upon several factors with the help of SIMTRA software we have analysed the deposition of the atoms ejected on the substrate, using a Monte Carlo code we have simulated several cases using the semiconductors (Si and Ge) as a target, the variations in distance between target and substrate have given the following important information about the disposition of thin films.

Applying a long distance will grow the possibility of atoms colliding with each other or between ions which will make a lot of atoms ejected not reaching the substrate.

Utilizing a distance of 5cm between the target and substrate is the best choice to get a thick coating and the highest number of deposited atoms. Choosing a wrong configuration inside the vacuum chamber will lead you to a bad coating quality.

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