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Revealing the role of vacuum chamber parameters on the pathways leading to substrate deposition by ejected atoms

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Abstract: The simulation with Monte-Carlo codes represented the efficiency tools that help understand the phenomena inside the vacuum chamber for sputtering. In this work, the impact of temperature and pressure parameters on the surface structure of thin films is studied in 3D with the magnetron sputtering technique. Inside a vacuum chamber, 105 particles of Argon (Ar) gas are injected, the target contains the semi-conductor silicon (Si), and the substrate is placed at a variable distance from the target. The results of this work show that a high temperature, pressure, and long distance between the target and substrate can negatively affect the path of the atoms ejected away from the target, which will cause a decrease in the number of atoms arriving on the substrate.

Key Words: Thin films, Sputtering, Vacuum chamber, Monte-Carlo codes.

1 Introduction

Thin film has become an essential part of human life, so finding a field of activity where it does not exist is challenging. Semiconductor silicon dominates the industry due to its efficient performance and reasonable price; low-mass thin-film solar cells can be integrated into modern compact optoelectronic microcircuits and Si-based devices and can be used in the aerospace industry [1-5].

Several technologies, including the sputtering technique, can be used for producing and disposing of thin films. The properties of the films deposited by the sputtering technique depend on the material and gas used for discharge and deposition parameters such as pressure, target distance, temperature, substrate polarization and chemical composition [6-8].

One of the most commonly used programs to simulate the sputtering process is the SRIM and SIMTRA programs, based on Monte Carlo simulations [9-10].

These two programs are used to study the entire sputtering process, and they allow us to study all the steps that the ejected particles face to create the thin layer [11,12].

In this work, the influence of temperature and high pressure on the path of the atoms ejected was studied with a variation of the distance between the target and substrate using the semiconductor silicon. First SRIM calculates the energy and the direction of the particles that are sputtered away from the targets (Si). The SIMTRA code then handles the transport of these species toward the substrate with a temperature and high-pressure variation. This work aims to deduce the best possible regulation inside the vacuum chamber to achieve the highest number of atoms arriving on the substrate. All the results found will be represented in three-dimensional curves. We aim to participate in the technological development of thin film and offer a result that will allow us to solve several problems in forming cells and thin films.

2 Simulation Methods

Simulation of film growth on time scales of seconds or minutes is possible with the Kinetic Monte Carlo Algorithms [13]; this approach can be used to model different surface processes such as nucleation, growth, and post-deposition structural modification of films [14,15].

The kinetic energy and the number of atoms that arrived at the substrate location are calculated by SRIM and SIMTRA. First, the energy and direction of the particles sputtered away from the target are calculated using SRIM software. In our

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work, we started with SRIM [16]; we applied 10^5 argon ions on the Silicon (Si) with an energy value of 100kev and an angular incidence of 85 degrees. The result was saved on a file and then used on SIMTRA.

The transport of these species to the substrate is then covered by the SIMTRA code [17], considering all collisions occurring in the gas phase. First, we created a vacuum chamber with the dimension of 30cm×30cm×50cm (as shown in Fig.1), taking a distance of 14cm and 20cm between the target and substrate. The magnetron used has a circle shape target with a radius of 2cm and the substrate also has the same shape with a radius of 6cm; we did a temperature and pressure variation on the semiconductor Silicon (Si) on two different distances 14cm and 20cm, the objective is to deduce the influence of temperature and high pressure 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 particles arriving on the substrate, the results will be saved on data files and will be presented by 3D curves.

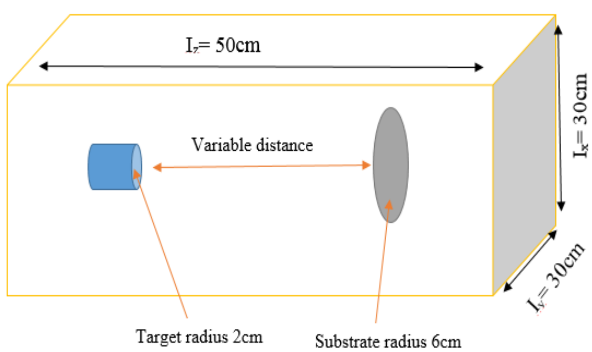

Fig. 1: Model used in the simulation.

3 Results and Discussion

3.1. Influence of temperature and high pressure on the atoms sputtered arriving on the substrate on a 14 cm and 20 cm of target-substrate distance

3.1.1. Variation of temperature with fixed pressure on 14 cm of distance

The following figure represents the path and number of atoms that sputtered and arrived on the substrate; three different temperatures (300 K, 500 K, and 800 K) are used with a pressure value of 0.5 Pa inside the vacuum chamber, the target (Si) is being bombarded by Argon ions.

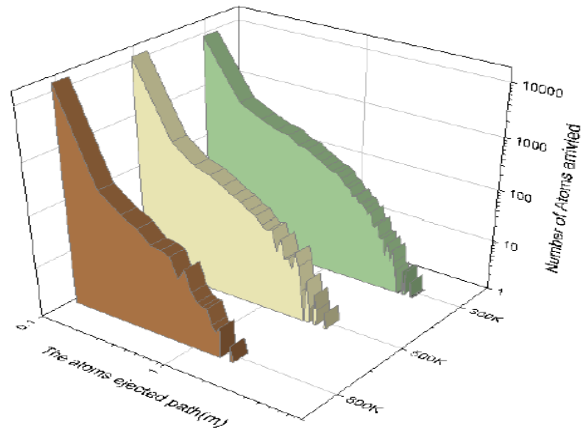

Fig. 2: Number of Si atoms arrived as a function of the path using three different temperatures T= [300 K, 500 K, 800 K] on 14 cm of distance.

As shown in the figures above, the number of atoms arriving on the substrate differs at each temperature. When we applied a temperature of 300k, the number of atoms that arrived reached a value of 10K, and every time we raised the temperature, the ejected atoms crossed the substrate with less distance.

The increase in temperature will create heat inside the vacuum chamber that will give high mobility to the particles, the argon ions will bombard the target with great energy, and the atoms ejected will get great kinetic energy that will help them to reach the substrate faster.

3.1.2. Variation of pressure with a fixed temperature on 14 cm of distance

At this time, we will use three different pressure P= [0.5Pa, 3PA, 6Pa], and a temperature of 300k will be applied inside the chamber, the same gas and material will be used to bombard our target, and the results are presented on the following figures:

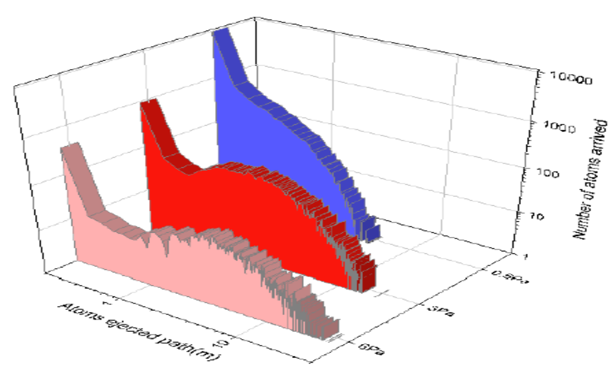

Fig. 3: Number of Si atoms arrived as a function of the path using three different pressures P= [0.5 Pa, 3 Pa, 6 PA] on 14cm of distance.

Pressure has a significant influence on the number of atoms. When we apply a pressure of 0. 5 Pa, we get a value of 10 K for the target Si; after applying a pressure of 2 Pa and 5 Pa, there is a considerable decrease in the number of atoms reaching the substrate, and we notice that the atoms ejected will arrive into the substrate with higher path.

When we raise the pressure inside the vacuum chamber, it will create a vast number of collisions and a significant decrease in particle mobility, the ejected atoms will face a difficult path to reach the substrate, and the atoms collide with the argon ions, which will decrease their kinetic energy. They will not be able to reach the substrate.

3.1.3. Variation of temperature with fixed pressure on 20 cm of distance

The same procedure will be carried out except for this case, we have changed the distance between the target and substrate from 14 cm to 20 cm, the temperatures used are the same T= [300 K, 500 K, 800 K], and the results are shown on the following curves.

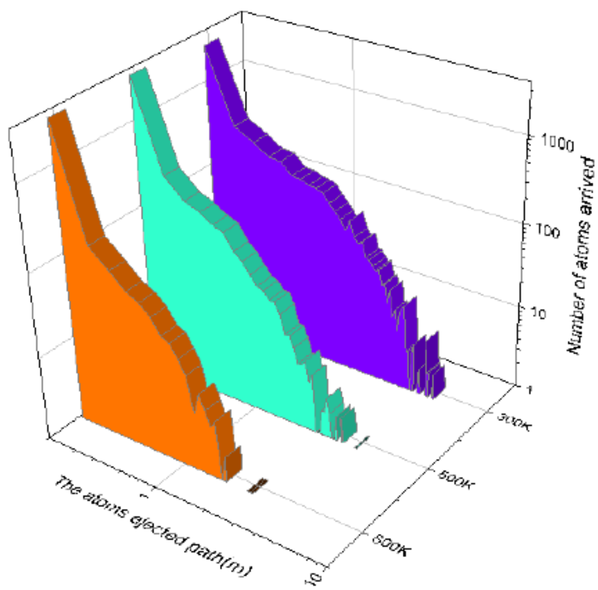

Fig. 4: Number of Si atoms arrived as a function of the path using three different temperatures T= [300 K, 500 K, 800 K] on 20 cm of distance.

Changing the distance from 14cm to 20cm will significantly decrease the number of atoms that arrive on the substrate. An applied temperature of 300k gives 3K of atoms ejected on the material Si, while with argon ions, it gave 10 K.

Widening the distance will cause several problems; many atoms ejected will not survive or reach the substrate.

3.1.4. Variation of pressure with a fixed temperature on 20 cm of distance

This time we used the vacuum chamber with a 20 cm distance between the target and substrate and a pressure variation P= [0.5 Pa, 3 Pa, 6 Pa].

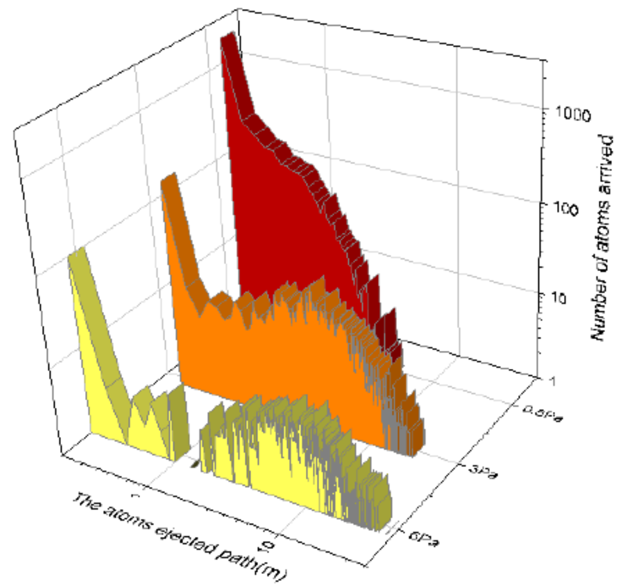

Fig. 5: Number of Si atoms arrived as a function of the path using three different pressures P= [0.5 Pa, 3 Pa, 6 Pa] on 20cm of distance.

As shown in the above figures, applying a 20 cm distance inside the vacuum chamber gives the same result, except that the atom that arrived in the substrate has dramatically diminished; it will create a less thick, thin layer with low quality.

4 Conclusions

The choice of the deposition process is dependent upon several factors. With the help of SIMTRA software, we have studied the influence of temperature and high pressure on the magnetron sputtering; using a Monte Carlo code, we have simulated several cases using silicon as a target, variations in temperature and pressure, and distance between target and substrate have given the following important information about the disposition of thin films.

The temperature increase gives the particle kinetic energy, increasing their mobility inside the chamber. The atoms ejected will travel a shorter distance because they will face less collision.

On the other hand, the increase in pressure will decrease the particles' kinetic energy, creating several collisions, so the ejected particles will have a hard path to reach the substrate.

Finally, we have shown that widening the distance will cause several problems; many atoms ejected will not survive and will not reach the substrate.

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