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Monte Carlo method investigation for the transportation of sputtered material atoms from target to substrate

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Abstract

Sputtering as a method for depositing films has received increased attention, as has the investigation of the connection between film qualities and deposition parameters. With the application of Monte Carlo simulation codes represented by SRIM (Stopping and Range of Ion in Matter) and SIMTRA (Simulation of the Metal Transport) software's, the effect of divers parameters on the surface structure of thin films are studied in 3D form with the magnetron sputtering process. Inside a vacuum chamber a 10^5 particles of Argon (Ar) gas are injected, the target contained the semi-conductor silicon (Si), and the substrate is placed with a variable distance from the target. The results obtained in this work show that a high temperature, pressure and a long distance between the target and substrate can negatively affects the path of the atoms ejected away from the target which will cause a decrease in the number of atoms arriving on the substrate.

Keywords: Thin film materials, Sputtering process, Monte-Carlo method, Plasma.

1. Introduction

A thin film has become an essential part of human life, so it is not easy to find a field of activity where it does not exist [1, 5].

Because 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 optoelectronics microcircuits and Si-based devices. They can therefore be used in the aerospace industry [6].

Several technologies can be used for producing and disposing of thin films, among them the sputtering technique. The properties of the films deposited by the sputtering technique depend on the gas material used for discharge and deposition parameters such as pressure, target distance, temperature, substrate polarization, and chemical composition [7–9]. One of the most used programs to simulate the sputtering process is the SRIM and SIMTRA programs, which are based on Monte Carlo simulations. These two programs are used to study the entire sputtering process, and they allow for studying all the steps that the ejected particles face to create the thin layer [10, 11].

This work studied the influence of temperature and high pressure on the atom's ejected path, considering the variation of the distance between the target and substrate using the semiconductor's silicon.

First, SRIM calculates the energy and direction of the sputtered particles from the targets (Si). The SIMTRA code then handles the transport of these atoms toward the substrate, considering variations in two critical parameters: temperature and high pressure. In order to maximize the number of atoms that reach the substrate, this work aims to figure out the ideal vacuum chamber control. All the results found will be represented as three-dimensional curves. Our goal is to participate in the technological development of thin films and offer results that solve several problems related to their formation.

2. Simulation method

Simulation of film growth on time scales of seconds or minutes is possible with the Kinetic Monte Carlo Algorithms [12].This approach can model different surface processes such as nucleation, growth, and post-deposition structural modification [13].

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 work, we started with SRIM [14]; we applied 10^5 ions of argon to the silicon (Si) with an energy value of 100 keV and an angular incidence of 85 degrees; the result was saved on a file and then used on SIMTRA.

The SIMTRA code [15] is then used to cover the transport of these species to the substrate, considering all collisions that occur in the gas phase. First, we created a vacuum chamber with dimensions of 30 cm, 30 cm, and 50 cm (as shown in Fig. 1). A distance of 14 cm and 20 cm between the target and substrate was taken, and the magnetron used has a circle-shaped target with a radius of 2 cm.

he substrate also has the same shape, with a radius of 6 cm. We did a temperature and pressure variation on the semiconductor silicon (Si) at two different distances, 14 cm and 20 cm. The objective is to deduce the influence of temperature and high pressure on the atoms arriving at the substrate and also see 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 onto our target and give the number of particles arriving at the substrate. The results will be saved on data files and presented by 3D curves**.**

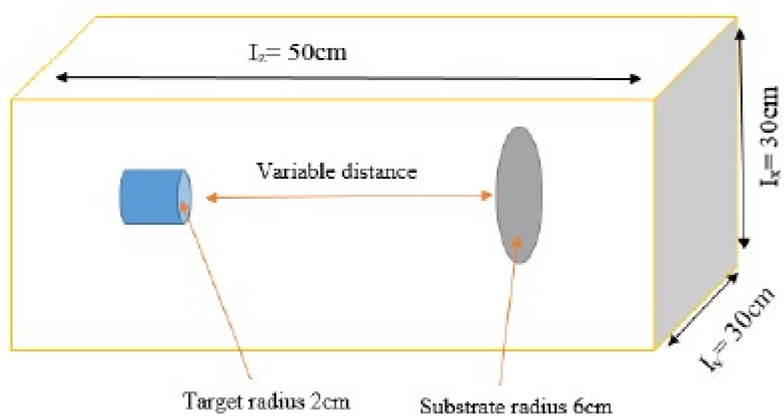

Fig. 1. Model used on the simulation

3. Results and discussion

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

3.1.1 Variation of temperature with fixed pressure on 14cm distance

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

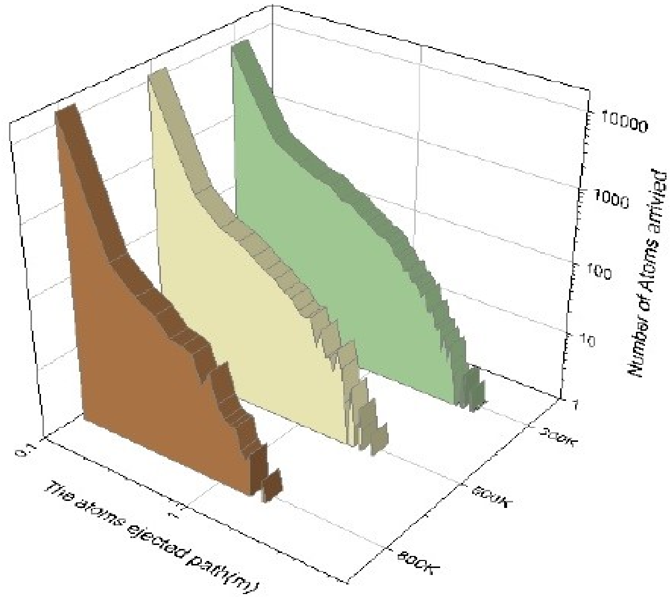

Fig. 2. Number of Si atoms arrived as function of the path using three different temperatures T= [300K, 500K, 800K] on 14cm distance

As shown in the figures above, the number of atoms arrived on the substrate are different on each temperature, when we applied a temperature of 300k the number of atoms arrived reached a value of 10K, every time we raise the temperature the ejected atoms cross the substrate with less distance.

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

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

For this time, we will use three different pressures [0.5, 3, and 6 Pa], and a temperature of 300 K will be applied inside the chamber. The same gas and material will be used to bombard our target. The results are presented on the following figures:

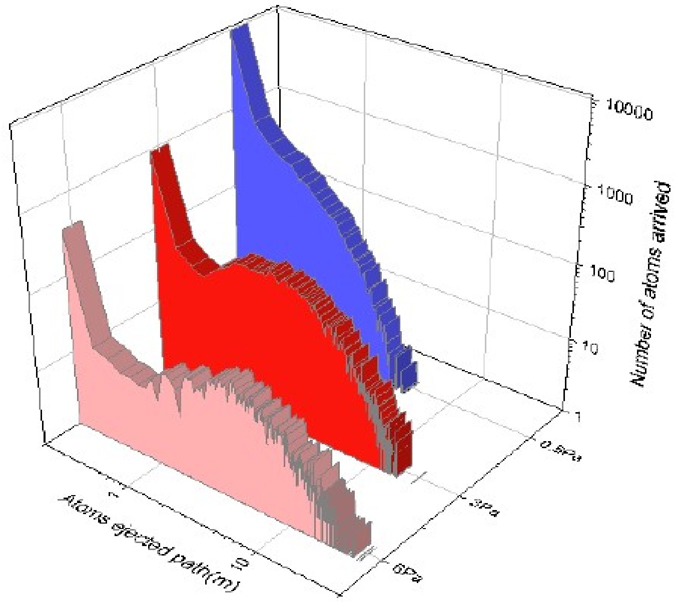

Fig. 3. Number of Si atoms arrived as function of the path using three different pressures P= [0.5Pa, 3Pa, 6PA] on 14cm distance

Pressure has a very big influence on the number of atoms, when we apply a pressure of 0. 5Pa we get a value of 10K for the target Si, after applying a pressure of 2Pa and 5Pa, there is a very large 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 rise the pressure inside the vacuum chamber it will create a very large number of collisions and a large decrease in particle mobility, the ejected atoms will face a difficult path to reach the substrate, the atoms collide with the argon ions which will decrease their kinetic energy and they will not be able to reach the substrate.

3.1.3Variation of temperature with fixed pressure on 20cm distance

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

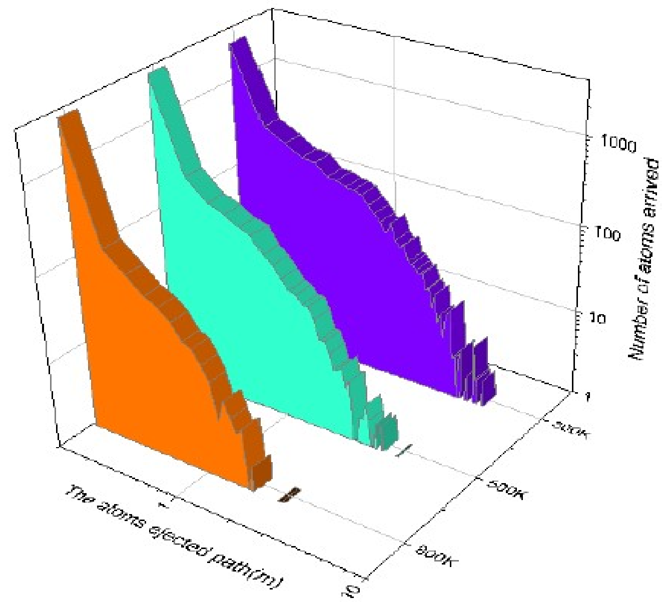

Fig. 4. Number of Si atoms arrived as function of the path using three different temperatures T= [300K, 500K, 800K] on 20cm distance

Changing the distance from 14cm to 20cm will result into a large decrease to the number of atoms arrived on the substrate, an applied temperature of 300k gives 3K of atom ejected on the material Si while with argon ions it gave 10K.

Widening the distance will cause several problems, a large number of atoms ejected will not survive and won't reach the substrate.

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

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

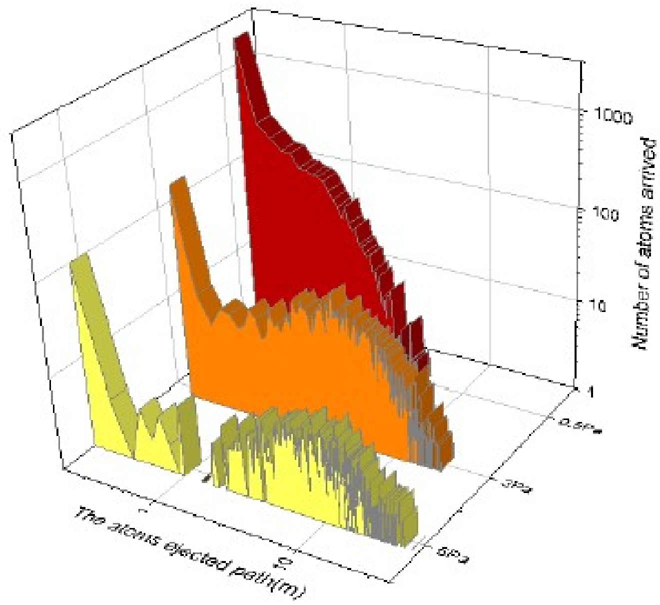

Fig. 5. Number of Si atoms arrived as function of the path using three different pressures P= [0.5Pa, 3Pa, 6PA] on 20cm distance

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

4. Conclusion

The choice of 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 kinetic energy to the particle which increases 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 of pressure will decrease the kinetic energy of the particles which will create 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, a large number of atoms ejected will not survive and won't reach the substrate.

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