Influence of temperature and pressure on the atoms ejected path during thin films deposition

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Abstract: The simulation with Monte-Carlo codes represented the efficiency tools which helps knowing the phenomena that occur inside the vacuum chamber for sputtering process. In this work, the impact of temperature and pressure parameters on the surface structure of thin films are studied in 3D form with the magnetron sputtering technique. 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 atom arriving on the substrate.

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

1. Introduction

Thin film has become an essential part of human life, so it is difficult to find a field of activity where it does not exist [1-4], the semiconductor silicon dominate the industry due to the efficient performance it provides and its reasonable price, low-mass thin-film solar cells can be integrated into modern compact optoelectronic microcircuits and Si-based devices and can therefore be used in the aerospace industry [5]. There are several technologies that can be used for the production and disposition of thin films, among them the technique of sputtering, the properties of the films deposited by the sputtering technique depend on the material the gas used for discharge and deposition parameters such as pressure, target distance, temperature, substrate polarization and chemical composition[6-8], One of the most used programs to simulate the sputtering process is SRIM and SIMTRA program which is based on Monte Carlo simulations, 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[9,12].

On 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 target and substrate using the semi-conductors silicon, first SRIM is used to calculate the energy and the direction of the particles that are sputtered away from the targets (Si). The transport of these species toward the substrate is then handled by the SIMTRA code with a temperature and high pressure variation, the objective of this work is to deduce the best possible regulation inside the vacuum chamber to achieve the highest number of atoms arrived on substrate, all the results found will be represented in a three-dimensional curves using Origin software. Our goal is to participate on the technology development of thin film and to offer a result that will allow us to solve several problems on the formation of cells and thin films.

2. Simulation method

Simulation of film growth on time scales of seconds or minutes is possible with the Kinetic Monte Carlo Algorithms [13,14], this approach can be used to model different surface processes such as nucleation, growth, post-deposition structural modification of films [15,16].

The kinetic energy and the number of atoms arrived at the substrate location are calculated by SRIM and SIMSTRA, first the energy and the direction of the particles that are sputtered away from the target are calculated by using SRIM software, in our work we started with SRIM [16-20], we applied a 10^5 ions of argon on the Silicon (Si) with an energy value of 100kev and an angular incidence of 85 degree, the result was saved on a file then used on SIMTRA.

The transport of these species to the substrate is then covered by the SIMTRA code[12],taking into account all collisions occurring in the gas phase, first we have created a vacuum chamber which has dimension of 30cm×30cm×50cm (as shown in Fig.1), a distance of 14cm and 20cm between target and substrate was taken, 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 distance 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 particle arriving on the substrate, the results will be saved on data files and will be presented by 3D curves.

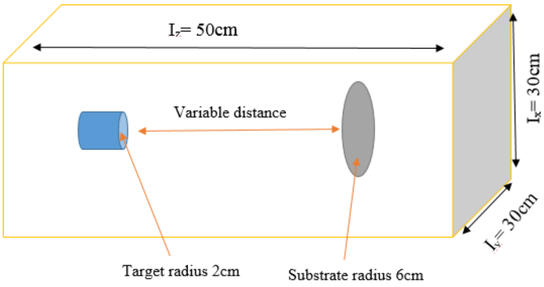

Fig. 1. Model used on the simulation

3. Results and discussion

3.1 Influence of temperature and high pressure on the atoms ejected path

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 temperature (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.

The choice of these temperatures gives us three cases to study inside the vacuum chamber which are warm, hot and extremely hot, the result will help us to make a comparison between them to see how the atoms ejected will act on every case.

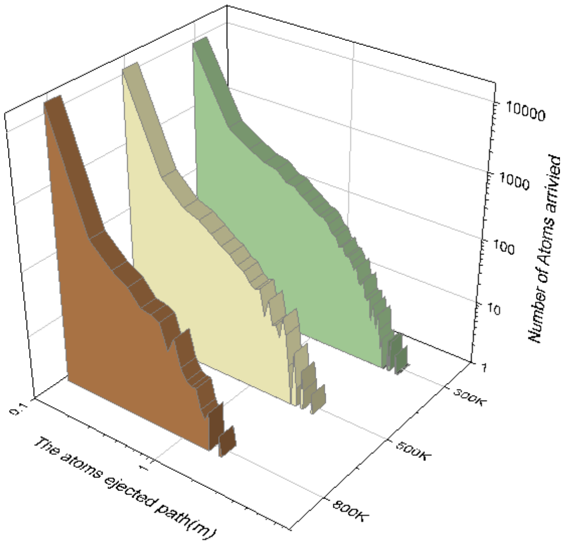

Fig. 2. Number of Si atoms arrived as function of the path using three different temperatures T= [300K, 500K, 800K] on 14cm distance

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.

It is also necessary to know that the excessive increase of temperature can cause damage to the materials used, before choosing the temperature it is necessary to do research on their ability to resist temperature.

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

For this time we will use three deferent 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.

We chose these three different pressures which are normal pressure, high and extreme high to create a comparison between them that will help us to see how the atoms ejected will act on every case, the results are presented on the following figures:

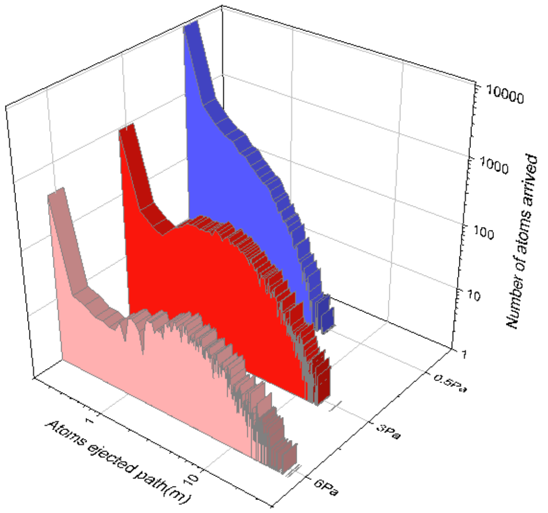

Fig. 3. Number of Si atoms arrived as function of the path using three different pressures P= [0.5Pa, 3Pa, 6PA] on 14cm distance

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

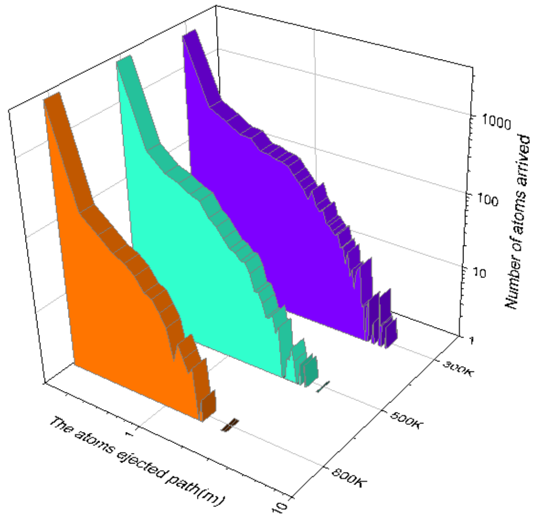

Fig. 4. Number of Si atoms arrived as function of the path using three different temperatures T= [300K, 500K, 800K] on 20cm distance

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.

Widening the distance will cause several problems, a large amount of atoms ejected will not survive and won't be able 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].

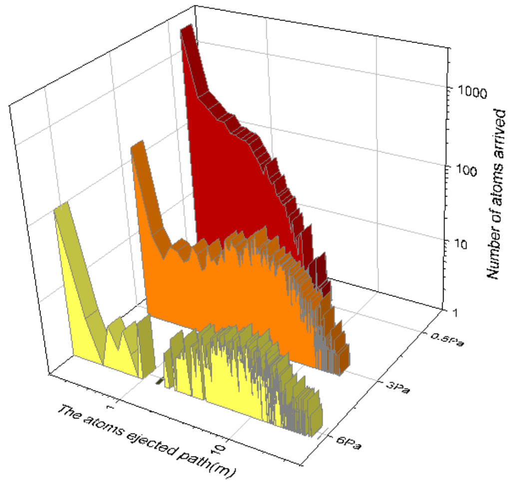

Fig. 5. Number of Si atoms arrived as function of the path using three different pressures P= [0.5Pa, 3Pa, 6PA] on 20cm distance

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.

5. 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 collision 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 amount of atoms ejected will not survive and won't reach the substrate.

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