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Monte Carlo Simulation of the Silver Sputtered Atoms Transport Process

Abderrahmane Settaouti

Electrotechnics Department, University of Sciences and Technology B.P. 1505 Oran EL-M'naouar, Algeria

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Abstract
The simulation of the phenomenons in the sputtering system is necessary in the design optimization. Facing targets sputtering systems are currently being used in various specialities of the nanotechnology. Study the sputtering process and the deposition parameters are important, the direction and energy of the particles at the substrate are the relation with the transport of particles in sputtering system. We present the study on the sputtering process and film deposition with the Monte Carlo method. We followed the trajectory of each sputtered atom separately in the three-dimensional coordinates with the calculation of the scattering angle and if a collision took place the energy loss. With this method we calculate the flux of the atoms at the substrate, direction and energy of each atom. The influences of the geometries of the system and the gas pressure were investigated.

Keywords: *Silver; Monte-Carlo simulations; Sputtering; particle transport.*

1. Introduction

The sputtering techniques are extensively used for thin film deposition of different materials. It is essential to predict the influence of the process parameters on the deposition profile, for the understanding the process and the technological importance. Sputtering is the physical process for a several applications, to protect the substrate and the deposited films from damage by charged particles, in the facing target sputtering system the plasma can be confined between the targets and the substrate placed outside the plasma. [1-8].
In different applications in various technologies, the sputtering process is an established method. The deposition parameters affect highly the properties of the film, for this reason a great attention is given to the study of the sputtering process [9-12]. It is important to model this transport through the background gas, the transport process from the targets to the substrate affect the characteristics of the particles arriving at the substrate.

The complexity of plasma processing, places the Monte Carlo simulation necessary for the research of new materials. To understanding the sputtering process for the interpretation of experiments, and development of processes and new equipment for materials fabrication, the simulation method of the processes in the plasma is necessary. Monte Carlo method can make contributions in the development of the plasma applications.

The Monte Carlo simulation is a kinetic method which agrees well with the gas scattering, transport phase and the deposition process with sputtering. With this method we can obtain various detailed information on the characteristics of the sputtered atoms. For the details on the transport process this method is useful for the design of sputtering systems [13].

Because of its properties the silver thin films have an attracted interest in the scientific and technological fields, and are used in wide applications. In the facing targets sputtering system the transports and deposition on the substrate of sputtered Ag atoms has been studied by the Monte Carlo method. The ejected atoms have a cosine distribution in the transport phase the atoms make several collisions with the atoms of the background gas (argon). With the Monte Carlo method, we have the number of Ag atoms arriving on the substrate, the distribution of the angles and theirs energies. The simulation was carried out for different pressures, the inter targets distance and the substrate target distance.

Corresponding author: settaouti@hotmail.com

2. Numerical procedure

We have developed a three-dimensional Monte Carlo model to investigate the transport phase of the sputtered atoms and deposition on the substrate. This model offers the information on the properties of sputtered particles and deposited on the substrate. In the sputtering transport process and deposition every sputtered atom is followed; the scattering angle and the new energy are calculated after each collision until the substrate.

Inside the argon cell in the facing target sputtering geometry, we utilize the Monte Carlo method for simulating the transport of the sputtered silver atoms. Two targets are placed one facing the others symmetrically, in the facing target sputtering technique, and the substrates on the axis orthogonal to the targets.

The Monte Carlo method in the sputtering transport processes describes the traces of every particle across the background gas in the two targets geometry until the deposition on the substrate. At the intervals determined from the mean free path, the collusions with the background gas atoms (Ar) and the transport of the sputtered Ag atoms are simulated. We utilize the coordinates of the emission points of the sputtered atom in the initial of the simulation. The ejection directions, initial energies of each sputtered atoms, in the transport across the cell are modified by a number of free paths and collisions. We obtain with the Monte Carlo method, the trajectories and the parameters of each sputtered atoms, and the number with theirs angles and energies of atoms reached the substrate at the end of the simulation.

The quantities of the angles of the velocity vector and energies of the sputtered atoms starting at the target are obtained from the following equations:

$$\delta = (1/2)\arccos(1-2R_1) \quad (1)$$

$$E^2(R_2-1) + E(2.e_s.R_2) + (e_s)^2.R_2 = 0 \quad (2)$$

Random numbers uniformly distributed between 0 and 1: R_1, and R_2. The angle of the velocity vector with respect to the axial direction is δ. The surface binding energy of the targets material is e_s, where the positive roots give energy *E*.

$$\phi = 2\pi.R_3 \quad (3)$$

$$x = (r).R_4\cos(\phi) \quad (4)$$

$$y = (r).R_4\cos(\phi) \quad (5)$$

The azimuthal ejection angle ϕ is generated uniformly between 0 and 2π by a random number R_3. x and y the coordinates of the starting position are determined by a random number R_4; r the rayon of the targets and z is zero. The diameter of each target used in the simulation has been as 40 mm, *T* the temperature of the sputtering gas utilized in this study is 350 K.

The free path between the ejection position and the successive collisions are calculated using the parameters of the sputtered atoms: impact, deviation, and new energy. Every trajectory of particles in the transport of sputtered atoms process is simulated.
The distance between two successive collisions where the sputtered atom moves is:

$$\lambda_j = -\lambda_m \ln(R_5) \quad (6)$$

λ_m is the mean free path of the sputtered atom and R_5 is a random number uniformly distributed between 0 and 1.

The sputtered atoms enter in collisions with a background gas atom after each λ_j, and during the next step the atoms are followed, this procedure is repeated for all sputtered atoms. With the increases of the background gas pressure, the mean free path decreases, this implies an increase in collisions of the sputtered atoms with the background gas. This implicates the change in the directions and loss of energies of sputtered atoms.

All sputtered atoms from the targets until them deposited on the substrate or thermalized are followed in the Monte Carlo simulation of the sputtering processes. The energy of the sputtered atom is compared with the value of the mean thermal energy of the background gas (0.038 eV for T=350 K). If the atom has energy lower than 0.038 eV after each collision, the sputtered atom is adopted to be thermalized. After another sputtered atom is simulated, in which the sputtered atom follows his trajectory with a random move until it hits the walls or the substrate.

This method was employed to simulate the trajectories of 10000 Ag atoms, at the end of the simulation; we have the total number of deposited atoms on the substrate. We have all properties of the sputtered atoms: positions, directions, energies and number of deposited atoms on the substrate with the Monte Carlo method.

3. Results and discussion

The properties of the deposited thin film are influenced by the background gas pressure, the impact angle and the energy of the deposited sputtered atoms on the substrate. The simulation of these parameters is essential, because we cannot measure the impact angle and the energy of the deposited atoms [9-12]. We can calculate these parameters and the properties of sputtered atoms as a function of time and space with the Monte Carlo method.

The sputtering process has been simulated with the Monte Carlo technique, to know the properties of the deposited film. The pressure of background gas, the inter targets distance and the substrate target distance have been varied in this simulation.

A transport process model of sputtered atoms in the background gas based on the kinetic method simulation was used to observe the trajectories of sputtered atoms and calculate the energy and direction. This enabled to determine the incident energy and the incident angle of the atoms when those reached the substrate. To obtain representative statistical of these data 10000 atoms were simulated. We studied the dependence of the growth of the deposited atoms with the distance between the targets and substrate and the background gas pressure.

With the statistical Monte Carlo technique, we simulate the paths and energies of the sputtered atoms; at the end we obtain the number of deposited atoms, positions, directions and energies for each atom. For the simulation of the trajectories of the each atom we calculated the free path between the ejection of the atom from the target and the first collision, after between two successive collisions. After the impact parameter, deviation of the sputtered atom, losses of energy are determined.

For different pressures and geometries the average energies for the sputtered atoms after their movements from the target to the substrate was determined. The sputtering flux of atoms depends on the sputtering gas pressure which determines the density of plasma; this is an impediment to the transport process of the sputtered atoms from the targets to the substrate.

Figure 1 shows the influence of the distance between the targets and substrate on the growth of the deposited atoms. With the distance inter targets of 50 mm and the distances between the substrate and inter targets which vary from 25 to 40 mm for different pressures of the background gas.

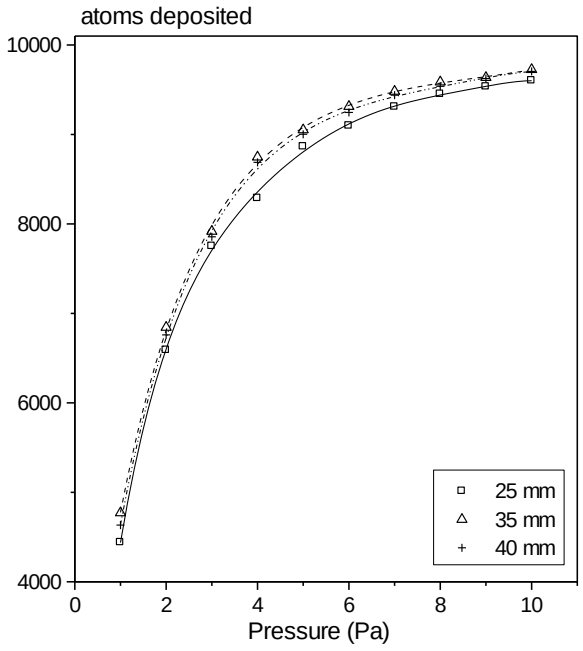

Figure 1 deposited Atoms as a function of pressure for different distances inter targets to substrate (two targets).

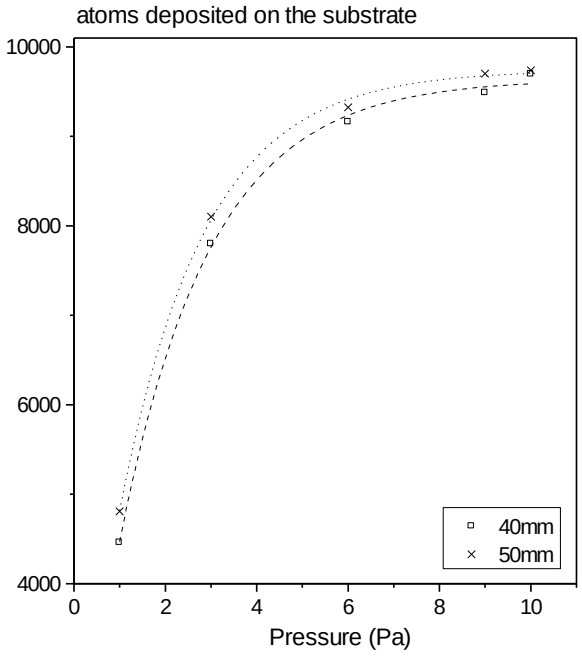

Figure 2. Influence of the pressure for different inter targets distances on the deposited atoms (two targets).

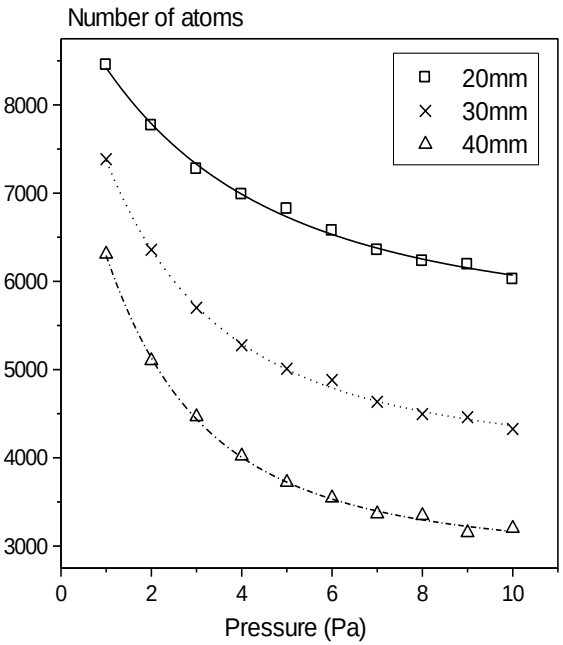

Figure 3. Influence of pressure on deposited atoms in the one target sputtering configuration.

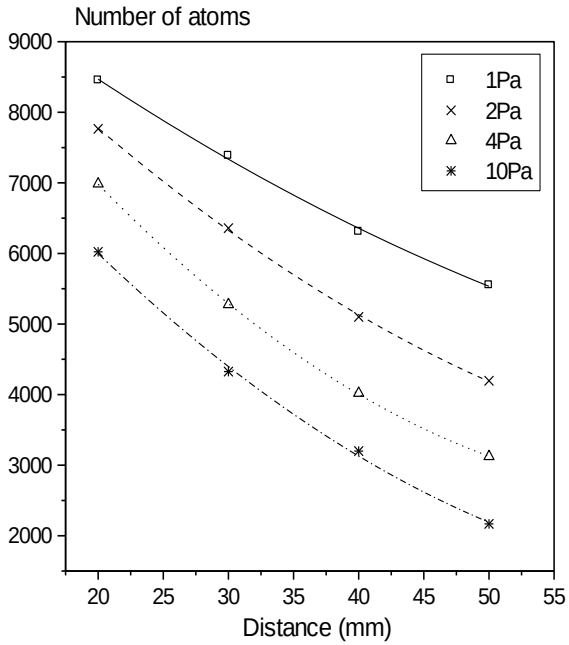

Figure 4. Influence of distance on deposited atoms in the one target sputtering configuration.

The number of atoms reaching the substrate indicates the influence of the transport processes of sputtered atoms (Figure 1 and Figure 2). We remark with the increase of the pressure gas the number of deposited atoms on the substrate increases. It is not observed in the diode sputtering configuration (one target with substrate), where the number of deposited atoms decreases with the pressure (Figure 3 and Figure 4).

The trajectories and energies of the sputtered atoms change when the collisions occur with the background gas. In the facing target sputtering configuration, the diffusion of the sputtered atoms is perpendicular to the targets axis, this implicates that the sputtered atoms have a great probability to deposit on the substrate.
A significant increase has been observed of the deposited atoms with the pressures from 1 to 4 Pa, and the value of the increase of the atoms reaching the substrate is reduced for the pressures from 4 to 8 Pa, and this augmentation of deposited atoms continuous to reduce after the pressure 8 Pa.

Figure 2 shows the results of the kinetic simulation of the transport of sputtered atoms reaching the substrate for different inter-targets spacing, and background pressures gas, for the distance between the substrate and inter-targets of 30 mm. The number of the deposited atoms on the substrate increase with the pressure gas. A great increase of sputtered atoms reaching the substrate for the pressure gas from 1 to 7 Pa and a less significant increase after the background pressure gas of 7 Pa.

In the sputtering system of facing targets the movement of sputtered atoms perpendicular to the axis of inter-targets has a great influence on the efficiency of the number of deposited atoms. This implies for the background pressure gas 10 Pa a great number of sputtered atoms are deposited on the substrate.

The Figs. 5 and 6 show spatial distributions of the deposited atoms on the substrate calculated with the Monte Carlo technique. The number of collisions of the sputtered atoms with the background gas is affected by the increasing of the pressure gas. This implicates the increase in the deposition of sputtered atoms on the substrate, and the increase of the pressure implies a great number of sputtered atoms deposited on the substrate nearby to the targets. That induces in non uniformity of the deposited film; the uniformity of the film becomes better with the increasing of the background pressure gas. The deposited film of sputtered atoms at the pressure 1 Pa has a uniform distribution compared with that at 10 Pa. Due to the number of collisions with the background gas for the pressure 10 Pa the sputtered atoms deposited on the substrate are concentrated on the side of the targets. The number of collisions of the sputtered atoms with the background gas at the pressure 1 Pa is less than at 10 Pa, this implicates the distribution of the deposited atoms on the totality of the substrate and this induces a uniformity of the deposited film.

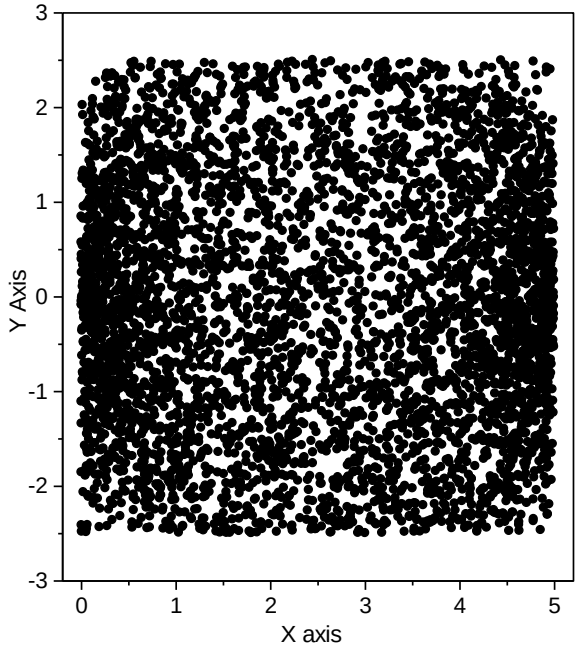

Figure 5. Distribution of deposited atoms on the substrate at pressure 1 Pa.

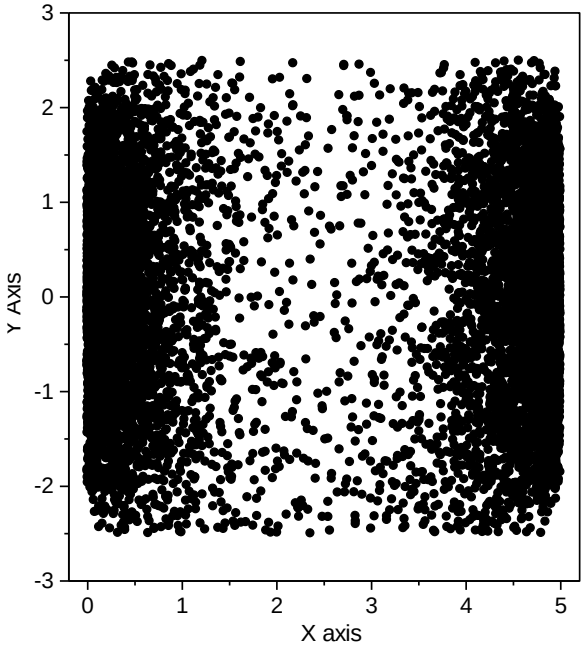

Figure 6. Distribution of deposited atoms on the substrate at the pressure 10 Pa.

The impact angles of the sputtered atoms on the substrate depend of the transport process and have a large influence on the properties of the morphological of deposited films. That implies in sputtering technology it is essential to study the angular distributions of deposited atoms. The effects of the geometries of the system and the background gas pressures on the incident angle of the sputtered atoms on the substrate with the consideration to the substrate tangent have been calculated.

The calculated distributions of the incident angles of sputtered atoms deposited on the substrate with respect the substrate tangent, with the Monte Carlo technique for different pressures and geometries are shown in figures 7 and 8. The impact angles have the same distributions for all geometries and pressures of background gas. We remark normal distributions, which imply an isotropic velocity distribution. The distributions of the impact angle on the substrate have two peaks around 45° and 135° for different pressures.

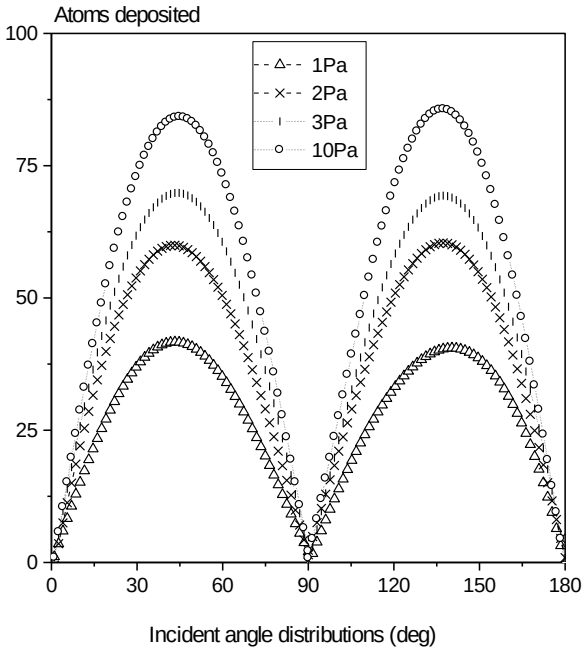

Figure 7. Distributions of the incident angles, distance targets-substrate=30 mm

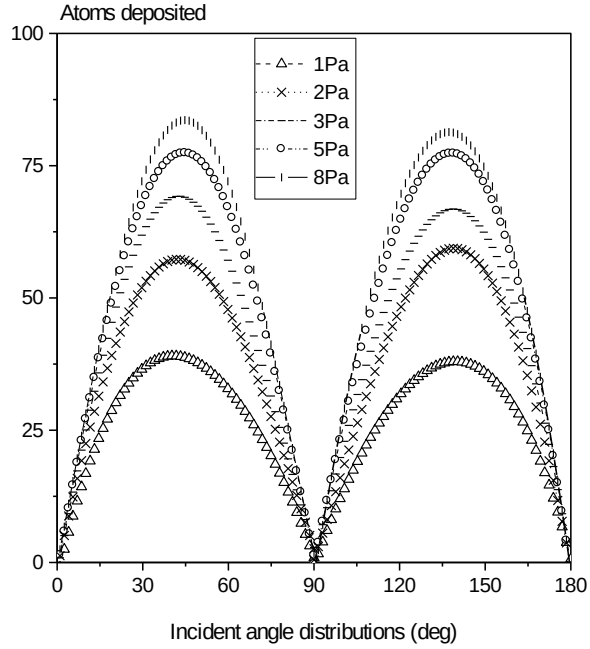

Figure 8. Distributions of the incident angles distance targets-substrate=40 mm.

The energy and the incident angle of the deposited atoms is function of the transport process in the sputtered system. The properties of the layer of the deposited atoms are highly affected by the direction of the impact and energy of the deposited atoms.

The figures 9-12 indicating at different pressures and geometries, the energies of sputtered atoms deposited on the substrate. The number of collisions with the background gas decreases the energies of the sputtered atoms by the transfer of energies from the sputtered atoms to the thermalized background gas, this implies solely a few sputtered atoms depositing on the substrate with a high energy. The frequency of collision with the background gas conduct to reduce the energies of the deposited sputtered atoms, this frequency is function with the pressure. The curves of the energies of deposited atoms have a maximum around 1.5 eV. The distribution of energies of deposited atoms presents a Maxwelian curve, and an asymptotic extremity for the high-energy. The peaks of the energies of deposited atoms are reduced when the background gas pressure decreases. And the increase in the energies of the deposited atoms with the decrease in the background gas pressure, this is due to the few of collisions of the sputtered atoms in the transport phase.

The results of the transport of sputtered atoms simulated by the Monte Carlo technique indicate the effect of process parameters on transport and finally on the properties of the deposited films. With this method we can simulate the influence of the geometries of the sputtering systems and also the influence of the background pressure gas on the transport process. The geometry of the sputtering system is important in the composition and the uniformity of the deposited film on the substrate.

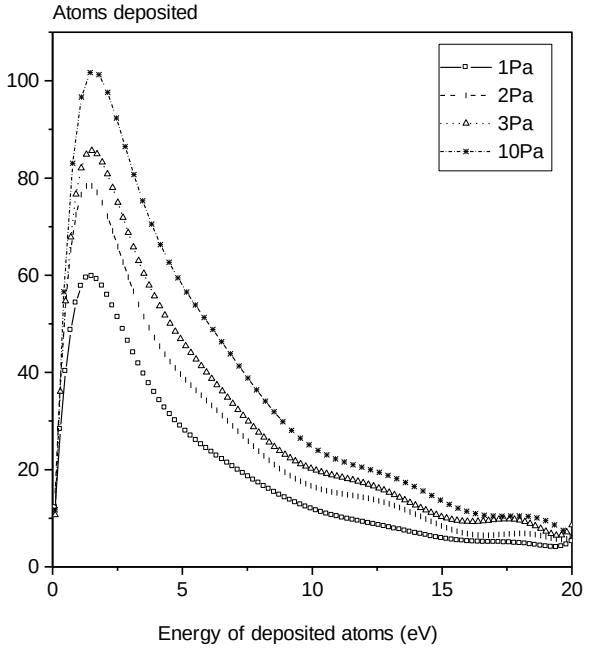

Figure 9. Energy distributions of deposited atoms as function of pressure (targets-substrate=20 mm).

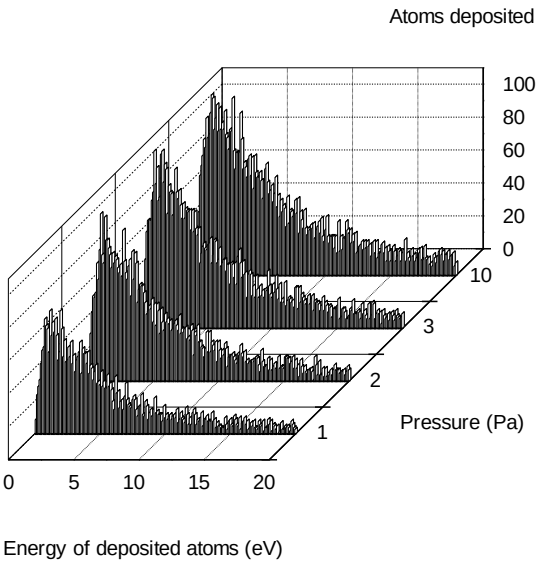

Figure 10. Energy distributions of deposited atoms as function of pressure (targets-substrate=30 mm).

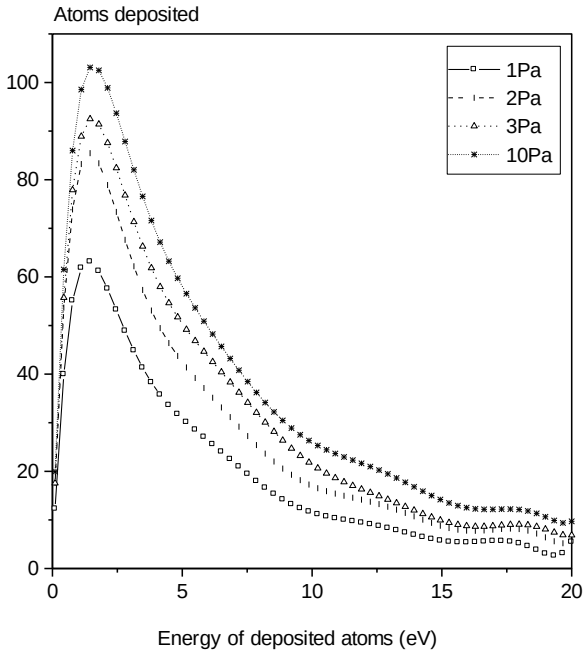

Figure 11. Energy distributions of deposited atoms as function of pressure (targets-substrate=40 mm).

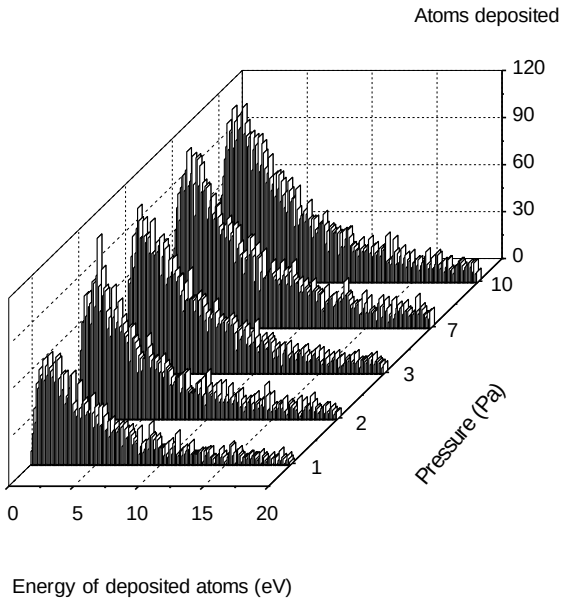

Figure 12. Energy distributions of deposited atoms as function of pressure (targets-substrate=40 mm).

4. Conclusions

The Monte Carlo simulation enables us to know the properties of the atoms in the space and the time, and we can with this technique calculate the directions and energies of the sputtered atoms. To simulate the transports of sputtered atoms in a facing targets sputtering system we utilize the Monte Carlo technique. The characteristics of the deposited particles and the growth of the thin films on the substrate by sputtering, depend from the target, the geometry of the sputtering system, the working gas and the pressure.

The Monte Carlo simulation allows knowing the information about the thermalized atoms and the deposited atoms on the substrate. The results permit to understand the influence of transport process of the sputtered atoms, which has the effects on the deposited film. These studies indicate the transport process of the sputtered atoms has an important part on the properties of the deposited film.

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