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Sputtering of semiconductors, conductors, and dielectrics for the realization of electronics components thin-films

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Abstract:
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, the effect of diver's parameters on the surface structure of thin films are studied in 3D form with the magnetron sputtering process. Inside a vacuum chamber, 10^5 particles of various gas which are Argon (Ar), Xenon (Xe), and Neon (Ne) are injected, the target contained materials used for the manufacturing of electronic components like semiconductors: Silicon (Si) and Germanium (Ge), conductors: Copper (Cu) and dielectric: silicon dioxide (SiO2) materials respectively. The results obtained in this work show that the energies of the particles, the incidence angles, and the gas nature are some of the principles and important parameters which affect the sputtering yield and hence the number of ejected atoms from the target, increasing the energy or incidence angles will increase the total number of ejected atoms, using Xenon gas gives best results comparing to Argon and Neon and also the sputtering yield of the copper conductor is superior to semiconductors and dielectric materials each to each.
Keywords: Thin films deposition, Monte-Carlo simulations, Physical vapor deposition, Sputtering process

1 Introduction

Thin-film manufacturing technology has made it possible to find applications in a large number of industrial sectors, more particularly in the world of electronic components, sensors, optics, or surface protection.

In electronics, nowadays thin films are used in a logic of miniaturization; In this sense, a particular interest is in the resolution of the current problems since they make it possible to combine an economy of material and size with great flexibility of use. For many applications, it is necessary to produce high-quality thin films on substrates of different shapes and characteristics. There are several thin film deposition processes, including sputtering which occupies an important place and is used for the deposition of all kinds of materials, whether conductors, semiconductors, or insulators [1-5].

Various applications and software are handled the study and simulation of the sputtering process and researchers in this field keep looking for more accurate programs when they take into consideration all the phenomena and parameters contributing to the obtained thin films morphology, homogenate, and quality, among them that software based on the Monte-Carlo simulation as TRIDYN (dynamic transport of ions in the matter) [6], ACAT (Computer simulation of Atomic Collision in Amorphous Target) [7], SiMTra (Simulation of the Metal Transport) [8] and SRIM (stopping and range of ion in matter) [9].

In earlier works of our group, we had shown in published papers that the SRIM code is very powerful in higher energies when we compare it with analytical results [2], the influence of energy and angular distribution in the morphology of thin films where satisfying results were obtained and validate our program [3] and the impact of two important parameters which are the pressure and the inter-cathodic distance (between target and substrate) on the total injected and arrived particles and hence to the created thin layers [1]. In this work and with the application of the two software described above (SRIM & SiMTra) in cascade mode, we are interested in the application of the sputtering process in the manufacturing of thin films used in electronics components. The ejected atoms obtained by SRIM with the adjustment of the energy and incidence angles values are injected into the SIMTRA and this later will give us the total arrived particles at the substrate level. A 3D curves will be represented then.

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2 Thin Film Deposition by Sputtering technique

2.1 sputtering Vacuum process

The sputtering deposition is part of the class of physical vapor deposition techniques (PVD) which describes divers vacuum deposition methods and is referring to a process in which the material transforms from a condensed phase to a vapor phase and back to deposit thin films on substrates. This process is widely used in our days in the industry for the manufacturing of new technology devices and their components which includes integrated circuits (IC), solar cells, cell phones, smartwatches, LEDs, and so on [10-13].

vacuum enhances the "mean free path" (the average distance of travel between subsequent collisions) of atoms of material being deposited and it's considered an indispensable tool in All thin film deposition methods. During the travel from source to substrate, the phenomena of atomic or molecular scattering due to the collision of atoms or molecules of all kinds of vapor species and residual gas molecules in the chamber and randomization occur [14].

From the kinetic theory of gas, this mean free path is calculated as:

$$mfp = \frac{KT}{Pr^2 \cdot \pi \cdot \sqrt{2}} \tag{1}$$

Where:

- K is Boltzmann constant,
- T is absolute temperature,
- r is molecular diameter,
- P is pressure in Pascal
- π is a constant =3.14

This mfp is directly proportional to the temperature of the gas and inversely proportional to the pressure and square of the molecular diameter. The scattering probability is given as fraction $\frac{N}{N_0}$ of molecules that are scattered in distance "d" during their travel through the gas.

$$\frac{N}{N_0} = 1.e^{\frac{d}{\lambda}} \tag{2}$$

The equation (2) of the mean free path shown above is illustrated in the following where:

- N_o is the total number of molecules
- N is the number of molecules that suffers collisions
- d is the distance between source and substrate
- λ the free path

At the pressure of 10^{-4} Pascal, only 0.3% of molecules will suffer collisions i.e., during evaporation molecular motion is non-randomized. Here we have seen that to have greater lambda, pressure should be reduced and a high lambda gives the least scattering probability, and thus the film deposition rate will be high also because of the less scattering, most molecules get from source to substrate [14].

2.2 Sputtering Yield measurement

For a long time, many research groups have worked to calculate the sputtering yields for divers materials [15–18]. Besides the analytic approach by Sigmund [15,16] many sputtering yields have been calculated with computer programs based on the binary collision approximation. A large number of yields have been provided mainly by Yamamura [19, 20] with his program ACAT [7,21] and by Eckstein [22] with the program TRIM.SP [23, 24].

Sputtering yield depends on several factors including ion mass, ion energy, ion angle of incidence, the atomic mass of target atoms, target atomic structure (crystal orientation/lattice system and whether the target is polycrystalline, amorphous, or comprised of a single crystal), target surface binding energy, and target texture relating to the incident ion and target material [2,3,25-27].

When the threshold energy of the bombarded surface is lower than the energy of the incidence ion, this will eject a large number of atoms from the target which will move toward the substrate, the sputter yield (S) then will define the average number of atoms ejected from the surface by the impact of primary ions.

$$S = \frac{\text{number of atoms emitted}}{\text{number of projectiles}} \tag{3}$$

3 SRIM and SiMTra codes based on the Monte-Carlo method

SRIM, Stopping and Range of Ions in Matter, is a collection of computer software that simulates the interaction of incident ions with the matter, all ion/atom collisions are handled by quantum mechanics. The arrest and distribution of ions in the solid can be calculated, in principle, in the energy range 10 eV – 2 GeV/amu. The programs were developed by James F. Ziegler and Jochen P. Biersack in the 1980s.

Since its introduction in 1985, significant improvements and corrections have been made every six years on the basis of new experimental data. Currently, over 700 scientific citations are made in relation to SRIM each year. The program allows a quick calculation of the implantation and sputtering [28-29].

SiMTra, Simulation of the Metal Transport, was developed by Koen Van Aeken for the simulation of trajectories of gas-phase particles in a definable 3D configuration where the interatomic collision modeling, the potentials, and thermal motion of the background atoms are included in the code. It's known as a binary collision Monte Carlo program that allows the simulation of the transport of sputtered particles through the gas phase flux during sputtering.

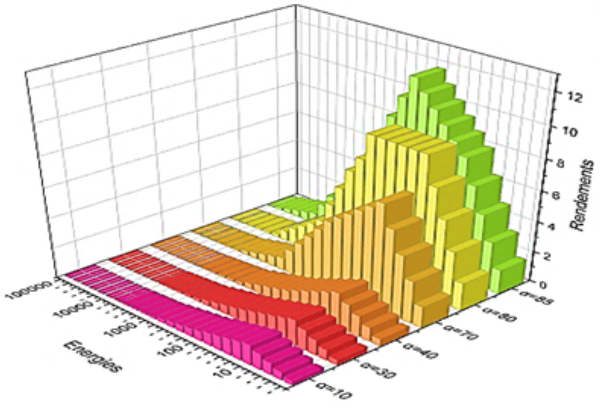
4 Results and discussion

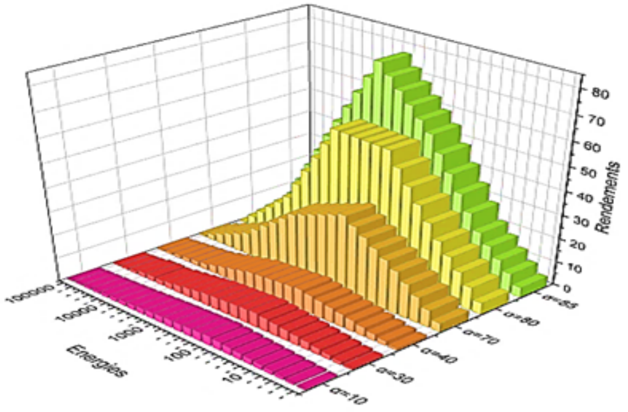
4.1 Part 1: Sputtering

4.1.1 Sputtering yield calculation

The aim of studying the sputtering yields is to control the amount of material deposited. In the figures below, we present the results of the sputtering yield calculations obtained by SRIM simulation, for different materials as a function of the impact energy at incidence angles θ = [10, 30, 40, 70, 80,85].

The chosen targets are semiconductors (silicon (Si), germanium (Ge)), conductor (copper (Cu)), and dielectric (silicon dioxide (SiO_2)): they are subjected to the bombardment of xenon (Xe), argon (Ar) and neon (Ne) particles.





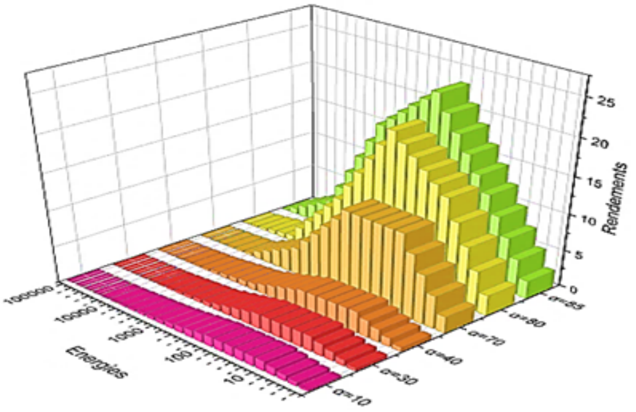
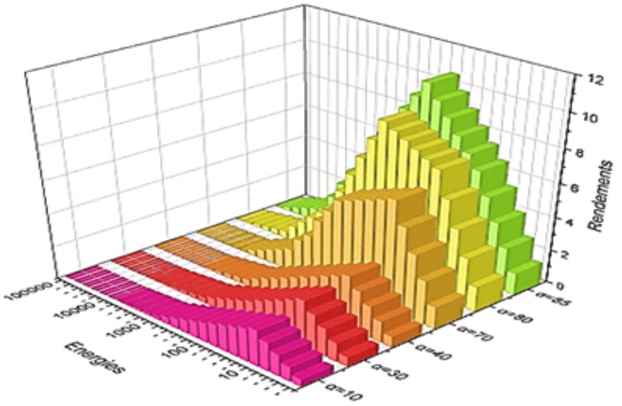
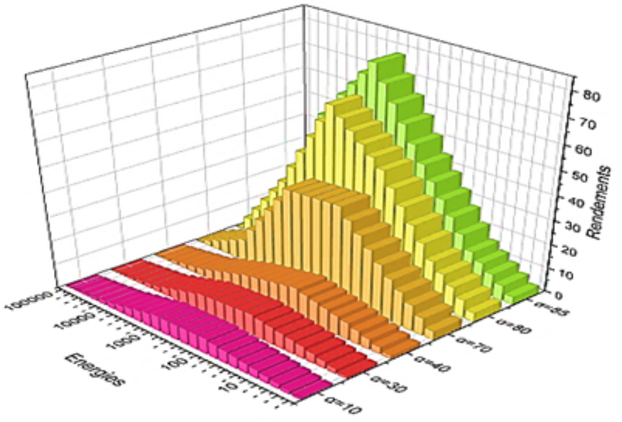


Figure 1. Sputtering Yield in incidences of 10 °, 30 °, 40 °, 70 °, 80 °, 85 ° calculated by SRIM for silicon (Si) as a function of the energy of the bombardment ions for a) Neon, b) Xenon and c) Argon





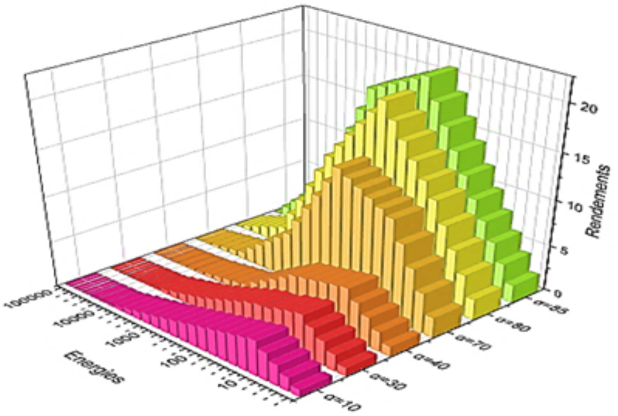
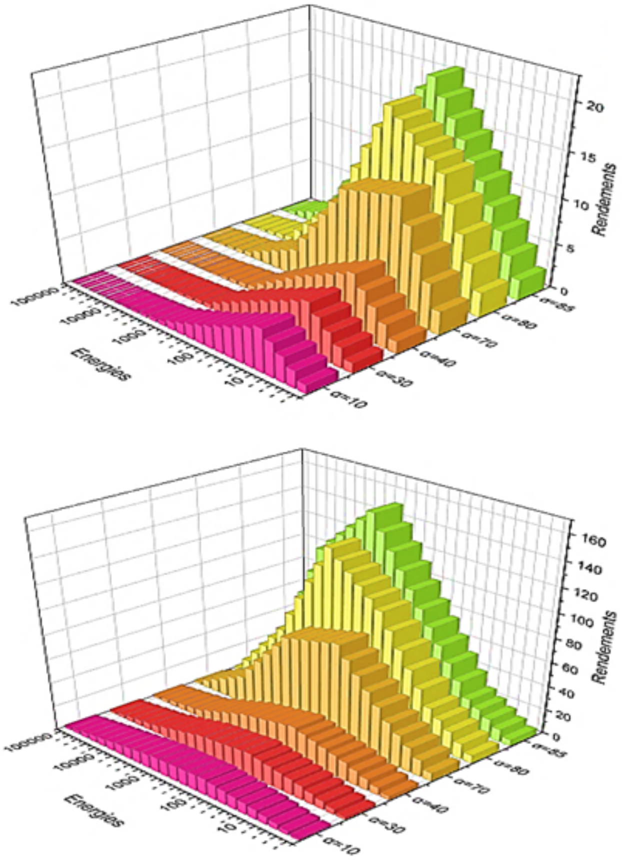


Figure 2. Sputtering Yield in incidences of 10 °, 30 °, 40 °, 70 °, 80 °, 85 ° calculated by SRIM for Germanium (Ge) as a function of the energy of the bombardment ions for a) Neon, b) Xenon and c) Argon



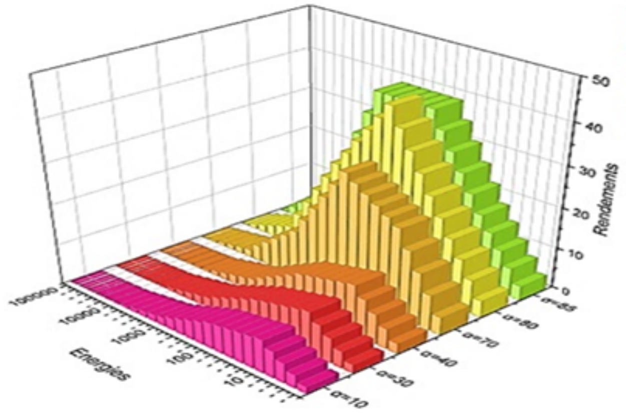
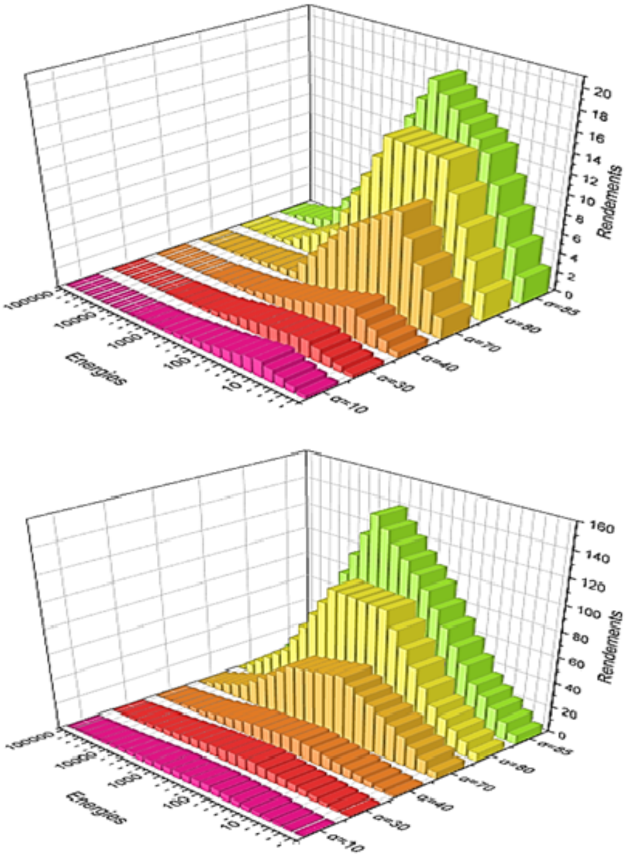


Figure 3. Sputtering Yield in incidences of 10 °, 30 °, 40 °, 70 °, 80 °, 85 ° calculated by SRIM for Copper (Cu) as a function of the energy of the bombardment ions for a) Neon, b) Xenon and c) Argon



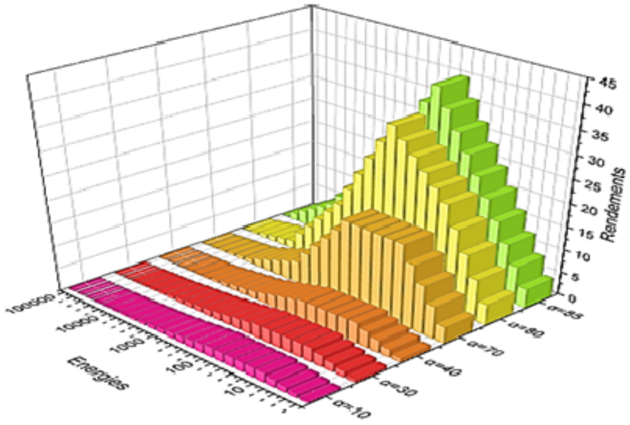


Figure 4. Sputtering Yield in incidences of 10 °, 30 °, 40 °, 70 °, 80 °, 85 ° calculated by SRIM for silicon dioxide (SiO2) as a function of the energy of the bombardment ions for a) Neon, b) Xenon and c) Argon

Figures (1, 2,.3, and 4) represent respectively the number of sputtered atoms, or the sputtering yield for semiconductor (silicon (Si), Germanium (Ge)), conductor (copper (Cu)), and insulator (silicon dioxide (SiO_2)) according to their energies and their incidence angles.

We can distinguish 3 main sections in all the previous figures which can be represented by the figure 5 below:

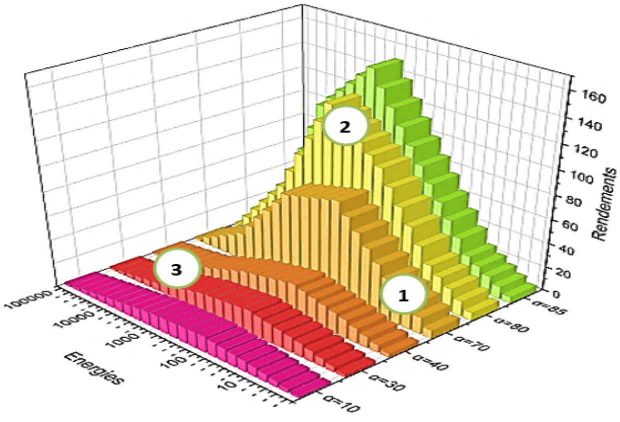
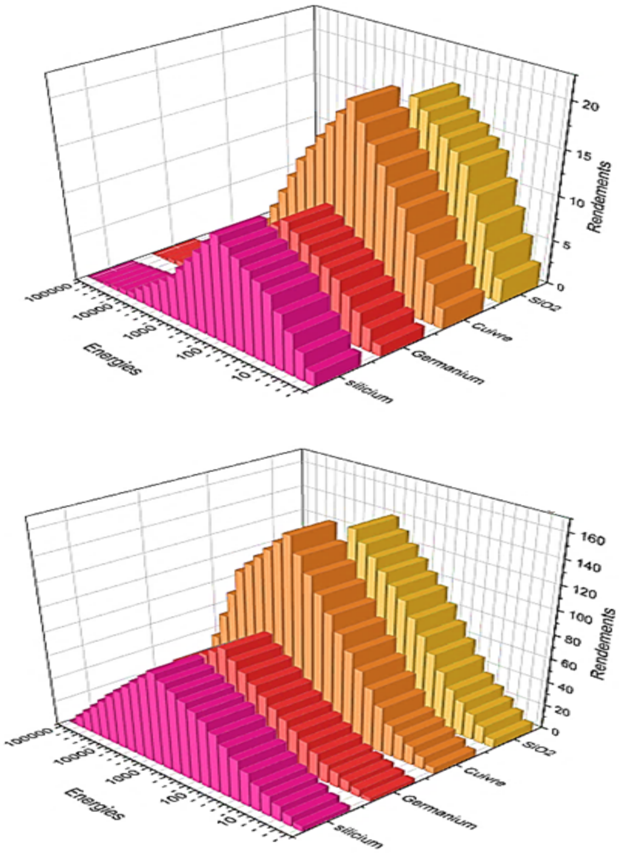


Figure 5. Sputtering Yield sections representation

- The sputtering yield is not clearly visible in the first section due to the modest energy value and also for incidence angles near to the normal ($\alpha=0$) of the incident particles hence the atoms cannot smash the binding surface of the materials.
- Increasing the incidence of particles energies and moving away from the angles from the normal in the second section will greatly influence the sputtering yield and the deposition becomes possible. This coefficient achieved a maximum that represented the highest ejected atoms at the end of this section
- The decrease of the number of particles and hence the sputtering yield in the third section despite the increase of energy is resulting from the profound penetration of the incident particles into the target surface Leading to the diminution of the ejected particles.

4.1.2 Comparison of materials

Figure 6 below presents a comparison of the sputtering yield results obtained with the application of a fixed angle of incidence at 85 degrees for different materials in order to know the impact of the energy and vacuum chamber gases (Xenon, Neon, and Argon) on the sputtering phenomenon and consequently on the characteristics and morphology of thin layers



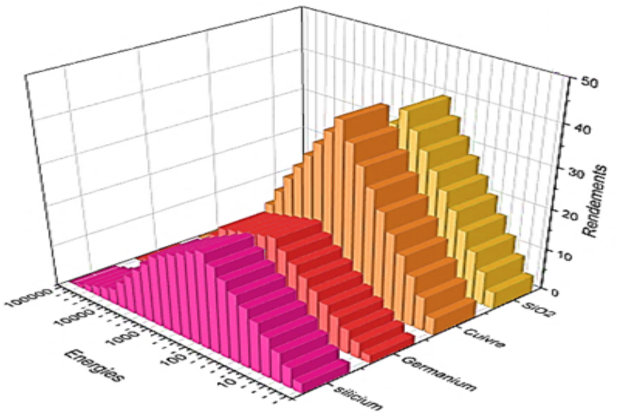


Figure 6. Sputtering Yield of materials (Silicon, Germanium, copper, silicon dioxide) at an incidence angle of 85^0 calculated by SRIM as a function of the energy of the bombardment ions for a) Neon, b) Xenon and c) Argon

Copper and silicon dioxide give a high yield with xenon, Argon, and Neon ions bombardment respectively compared to silicon and germanium. The yield always goes through a maximum and enfeeble after consumption of the total amount.

4.2 Part 2: Transportation of pulverized particles

The ejected particles from the target surface can collide with the gas atoms present in the vacuum chamber during transportation to the substrate. The paths of the pulverized atoms from the target to the deposition on the substrate through the gas are surrounded by the number of collisions however film deposition is dependent on the number of arrived particles during the transport.

SiMTra is a binary collision Monte Carlo program that allows the user to simulate the transport of sputtered particles through the gas phase flow during sputtering. The user is able to define the simulation configuration, and therefore imitate the experimental configuration. Not only the profile and the rate of deposition but also the properties of the metal flow like the Pressure, temperature, distance between target and substrate, direction …..etc.

In this work, we have chosen the optimal values of the program so the pressure was fixed to 0.5 Pa, the temperature 300K, and 50 cm of target-substrate distance.

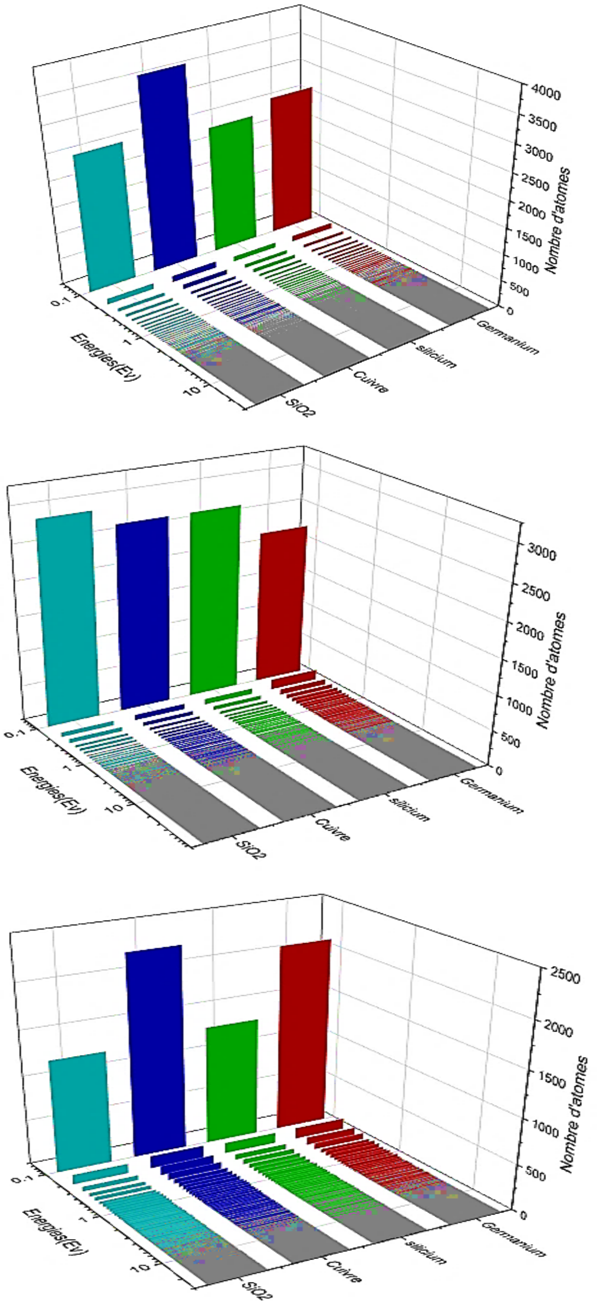


Figure 7. The energy distribution of silicon dioxide, copper, silicon, and germanium atoms arriving at the substrate and bombarded by ion beam for a) Argon, b) Neon and c) Xenon

Figure 7. below represents the energy distribution of arriving at the substrate atoms for different materials, it then shows the simulation results of the ejected materials atoms (Si, Ge, Cu, SiO_2) arriving at the substrate level as a function of their energies.

As shown in the figures above (Fig.7 a, b, and c), the numbers of atoms that reached the substrate are different for each material and for diver's gases.

5 Conclusions

The results obtained by the SRIM simulation show:

1. The maximum sputtering yield for the ejected particles from the materials (Si, Ge, Cu, and SiO2) is achieved (with different values) at an angle of incidence of approximately 85 degrees by varying the energies of the plasma ions. The figures look almost the same, it starts with low yields values at the beginning due to the ion energy threshold that has not yet been reached, and after a maximum and a decrease due to penetration or the exhaustion of the target.

2. From these results it can be seen that the Yield inferred from the Xenon (Xe) ions is quite large compared to Argon (Ar) and Neon (Ne) but as the Xenon gas is a very expensive and rare gas so the Argon is the dominant gas.

3. Semiconductors (silicon, Germanium) give almost the same yield amount.

4. The insulator (silicon dioxide) and conductor (copper) performance are satisfactory compared to the semiconductors.

The results obtained by the SIMTRA simulation show that:

1. The maximum number of atoms arriving at the substrate with low energies ensures at the end a uniform film deposition and contributes to the creation of thin films with the desired morphology.

2. The number of the arriving atoms can be reached with great value when bombarding by the Argon ion beam.

3. Neon gives convergent results with the four materials.

According to the obtained results, copper has some excellent properties, this is why it is much more commonly used in electronics.

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