PEOPLE’S DEMOCRATIC REPUBLIC OF ALGERIA
MINISTRY OF HIGHER EDUCATION AND SCIENTIFIC RESEARCH
IBN-KHALDOUN UNIVERSITY OF TIARET

FACULTY OF APPLIED SCIENCES

ELECTRICAL ENGINEERING DEPARTMENT

GRADUATION MEMORY

To obtain the Master's degree

Domain: Science and Technology

Field: Electrical engineering

Specialty: Electrical Networks

THEME

Investigation using Monte-Carlo code on the influence of high pressures and temperatures on the thin-films deposition by electrical discharge

Prepared by: BENNAAR YOUCEF

MEFTAHI YOUCEF ABDELAZIZ

Board of Examiners:

Full Name	*Grade*	*Quality*
A. MOKHTARI	**MAA**	**Chairman**
M. BEDOUI	**MCB**	**Examiner**
M. OMARI	**MCB**	**Examiner**
A. BOUAZZA	**MCA**	**Supervisor**

Academic Year: 2021/2022

Praise Allah for giving us the strength and courage to complete this work successfully.

We thank Mr. Abdelkader BOUAZZA, our supervisor, for supervising and directing us throughout the project.

Also, we are grateful to Mr. Mokhtari, Mrs. BEDOUI, and Mr. OMARI for accepting to be members of dissertation jury.

We appreciate our parents' constant encouragement, support, and attention.

Many thanks to our teachers of the electrical engineering department for their high quality of instruction and kindness.

SUMMARY

Summary

General Introduction

General Introduction 1

Chapter I: General notions on thin-films

I.1. Introduction 4
I.2. Definition of thin films 4
I.3. A brief history 5
I.4. Interest and characteristics of thin films 5
I.5. Thin-film applications 6
I.6. Steps of the thin film deposition process 9
I.7. Thin-film deposition techniques 11
I.8. Thin film growth mechanism 15
I.9. Properties of thin films 17
I.10. Types of electronic materials 18
I.11. Thin films importance 19
I.12. Conclusion 20

Chapter II: Deposition by electrical discharge

II.1. Introduction 22
II.2. The Physical Vapor Deposition (PVD) 22
II.3. PVD Advantages and disadvantages 23
II.4. PVD applications 24
II.5. Physical vapor deposition techniques 24
II.5.1. Thermal evaporation 24
II.5.2. Laser Ablation 25
II.5.3. Vacuum evaporation 26

II.5.4. sputtering 26

II.5.4.1. Sputtering history 27

II.5.4.2. Types of sputtering 28

II.5.4.2.1. DC Diode Sputtering 28

II.5.4.2.2. Radiofrequency (RF) sputtering 28

II.5.4.2.1. Magnetron Sputtering 29

II.5.4.2.3. Ion-beam sputtering 30

II.5.4.2.4. Triode-sputtering 31

II.5.4.3. Advantages of sputtering 32

II.5.4.4. Disadvantages of sputtering 32

II.5.4.5. Application of sputtering targets 32

II.6. General information on Monte-Carlo method 33

II.6.1. Monte-Carlo method 33

II.6.2. History of Monte-Carlo method 34

II.6.3. The importance of the Monte-Carlo method 35

II.6.4. Advantages of the Monte-Carlo method 36

II.6.5. Disadvantages of the Monte-Carlo method 36

II.7. Conclusion 37

Chapter III: Results and discussion

III.1. Introduction 39

III.2. The Stopping and Range of Ions in Matter (The SRIM) 39

III.3. The three gases used in the simulation 39

III.4. Monte-Carlo simulation 40

III.5. Operating principal 40

III.6. Sputter yield measurement using the Monte Carlo method..41

III.7. Variation of the sputtering yield according to the incidence angles and energies of particles ……………………………………………………………………………………………41

III.8. Sputtering yield as function of incidence angles..41

III.9. Sputtering yield as function of the energy...43

III.10. Simulation results obtained from the SRIM simulation...45

III.11. Conclusion 46

III.12. Simulation of Metal Transfer (SIMTRA) 46

III.13. The effect of pressure variation on the number of particles arriving in the substrate 47

III.14. The number of atoms arriving on the substrate depends on the applied pressure.................52

III.15. The effect of temperature variation on the number of particles arriving at the substrate 52

III.16. The number of atoms sprayed on the substrate according to temperature........................... 57

III.17. 3D visualization of the ejected atoms reaching the substrate level 58

III.18. Conclusion 60

General Conclusion...62

References

Abstract

List of figures and tables

List of figures

Chapter I

Figure I.01: Thin silicon plates for the production of microcircuits and radio elements with thin-film technology… 5

Figure I.02: Diagram of the thin film deposition process steps… 9

Figure I.03: Techniques and processes for depositing thin-films… 12

Figure I.04: Chemical vapor deposition process… 13

Figure I.05: Spray pyrolysis deposition........ 14

Figure I.06: Various stages of nucleation and growth of thin films… 16

Figure I.07: Conductivity scale for various materials at room temperature 18

Chapter II

Figure II.01: Schematic of physical vapor deposition process… 23

Figure II. 02: applications of Physical vapor deposition........ 24

Figure II.03: The phenomenon of thermal evaporation 25

Figure II.04: Schematic diagram of PLD process… 26

Figure II.05: Schematic diagram of Sputtering 27

Figure II.06: The fundamental components of a DC sputtering system 28

Figure II.07: The fundamental components of a RF sputtering system 29

Figure II.08: Working principle of magnetron-sputtering deposition process… 30

Figure II.09: Schematic diagram of ion beam sputtering system........ 31

Figure II.10: Working principle of the triode-sputtering deposition process… 31

Chapter III

Figure III.01: Sputtering yield as a function of incidence angles for materials (Cu, SiO_2, GaN) bombarded by gasses Argon (Ar), Xenon (Xe) and Oxygen(O_2)… 43

Figure III.02: Sputtering yield as a function of incidence energy for materials (Cu, SiO_2, GaN) bombarded by gasses Argon (Ar), Xenon (Xe) and Oxygen(O_2)… 45

Figure III.03: Depending on the pressure in the chamber, the energy distribution of Cu atoms, SiO2 and GaN arrives at the substrate levels and is bombarded by an Ar ion beam 48

Figure III.04: Depending on the pressure in the chamber, the energy distribution of Cu atoms, SiO2 and GaN arrives at the substrate levels and is bombarded by an O_2 ion beam..........................50

Figure III.05: Depending on the pressure in the chamber, the energy distribution of Cu atoms, SiO2 and GaN arrives at the substrate levels and is bombarded by an Xe ion beam 51

Figure III.06: Depending on the temperature in the chamber, the energy distribution of Cu atoms, SiO2 and GaN arrives at the substrate levels and is bombarded by an Ar ion beam 54

Figure III.07: Depending on the temperature in the chamber, the energy distribution of Cu atoms, SiO2 and GaN arrives at the substrate levels and is bombarded by an O_2 ion beam...........................55

Figure III.08: Depending on the temperature in the chamber, the energy distribution of Cu atoms, SiO2 and GaN arrives at the substrate levels and is bombarded by an Xe ion beam 57

Figure III.09: The location of Cu atoms bombarded with Argon on the substrate according on the variation of temperature of the chambre 58

Figure III.10: The location of SiO_2 atoms bombarded with Argon on the substrate according on the variation of temperature of the chambre 59

Figure III.11: The location of GaN atoms bombarded with Argon on the substrate according on the variation of temperature of the chambre 59

List of tables

Table III.01: Energies, angles and maximum efficiency obtained by SRIM..................................... 46

Table III. 02: total number of atoms sprayed on the substrate depending to the pressure 52

Table III. 03: total number of atoms sprayed on the substrate depending to the temperature 57

list of abbreviations

List of abbreviations

Abbreviation	Meaning
Ar	Argon
Ar^+	Argon ion
BCA	Binary Collision Approximation
CVD	Chemical vapor deposition
Cu	Copper
CIGS	Copper Indium Gallium Selenide
DC	Direct current
GaN	Gallium Nitride
IBS	Ion-beam sputtering
K	Kelvin
KeV	Kiloelectronvolt
LEDs	Light-emitting diodes
MC	Monte-Carlo
MCMC	Markov Chain Monte Carlo
O_2	Oxygen
PVD	Physical vapor deposition
Pa	Pascal
PLA	pulsed laser ablation
RFID	Radio Frequency Identification
RF	Radiofrequency
SRIM	Stopping and range of ions in matter
SIMTRA	Simulation of Metal Transfer
Xe	Xenon
Y	Sputtering performance
θ	Angle

General Introduction

General Introduction

Decades of research have enabled humanity to benefit from a multifaceted technological development. Thin films are prominent in producing components such as microprocessors and integrated circuits, various screens, packaging, and the manufacture of optical materials. This technology is being used in an increasing number of industrial applications as it is beneficial for creating compounds that are impossible to produce using mass chemistry (traditional processes, such as foundry). [1]

In recent years, many thin-film deposition techniques have been developed. Among the techniques used, there is sputtering deposition, which is used for the deposition of all materials, whether they are conductors, semiconductors, or insulators, the sputtering technique is one of the best methods for the practical preparation of thin films. It has been shown that sputtering offers more flexibility to the process and gives good quality films with reproducible performance [2]. Some reasons for using the sputtering technique are excellent uniformity of the film, especially on large surfaces, surfaceand thickness control, good adhesion, high-speed deposition, and versatility.

The work with the two cascade simulation software (SRIM 2013 and SIMTRA) makes it possible to consider the parameters of the sputtering system. Therefore, the motivation of this study is to study the influence of specific parameters (energy, angle of incidence, gas used for the bombardment and the material used, high pressure, and high temperature).

In this dissertation, we have chosen to simulate sputtering and calculate its performance for semiconductor (Gallium Nitride (GaN)) and conductor (copper (Cu)) and insulator (silicon dioxide (SiO_2)), submitted bombardment by ion beams of gases such as Xenon (Xe), Argon and Oxygen (O_2).

Our work is divided into three chapters:

— In the first chapter, we will present general information on thin films, then describe the thin film deposition techniques, the growth mechanisms, and their application. Finally, we will present the materials used in the simulation and the importance of thin films.

— he second chapter is about electrical discharge deposition. In this chapter, we will focus on the sputtering deposition and the different sputtering techniques. Finally, we will present the Monte Carlo method.

— The last chapter is divided into two parts. Part one is for the calculation of the sputtering yield using the simulation with SRIM 2013. Next, part two is for the transport of the ejected particles to the substrate with SIMTRA. The results obtained by the first part of the simulation are inserted in the following one in order to obtain appropriate models

Chapter I

General notions of thin films

I.1. Introduction

Technologies based on exploring the specific properties of thin films developed strongly at the end of the 20th century and became one of the most important paths of progress both in terms of the theoretical understanding of the properties of matter condensed through miniaturization and the development of new applications, the realization of which could not be done without this technology. Thin films find many practical applications in various fields such as optics, electronics, sensors, and mechanics. [3]

This chapter covers the fundamentals of thin-film technology, including deposition techniques, characterization techniques, and applications. Due to the exceptional diversity of thin films and the large range of applications, it is not very easy to cover in detail all the areas. However, as many thin films share several features in all steps of the production process, characterization, and even applications, it is possible to treat them from a general perspective.

I.2. Definition of thin films

A thin film is a layer or layers (a stack of thin films is called a multilayer) of material ranging from nanometers (monolayer) to several micrometers in thickness. The thin-film deposits on the substrate for different purposes, like protecting the substrate, changing its appearance (for decorative purposes), changing the substrate's optical or electrical properties, etc. The thin film deposition process is a fundamental step in many applications, which refers to applying a thin film of any substance on a surface, whether a substrate or already deposited layers.

Whether the process is primarily physical or chemical, thin-film applications are undeniable, and a simple example is a mirror we use daily to see ourselves.

The mirrors typically consist of a sheet of glass covered by a thin film of metals such as aluminum or silver, using deposition techniques such as sputtering to form a reflective surface. Due to the advances in thin film deposition techniques during the 20th century, there has been a wide range of technological breakthroughs in various areas, such as optical coatings (such as anti-reflective coatings), electronic semiconductor devices, hard coatings on cutting tools, magnetic recording media, integrated passive devices, LEDs, and energy generation (e.g., thin-film solar cells) and storage (thin-film batteries) [4].

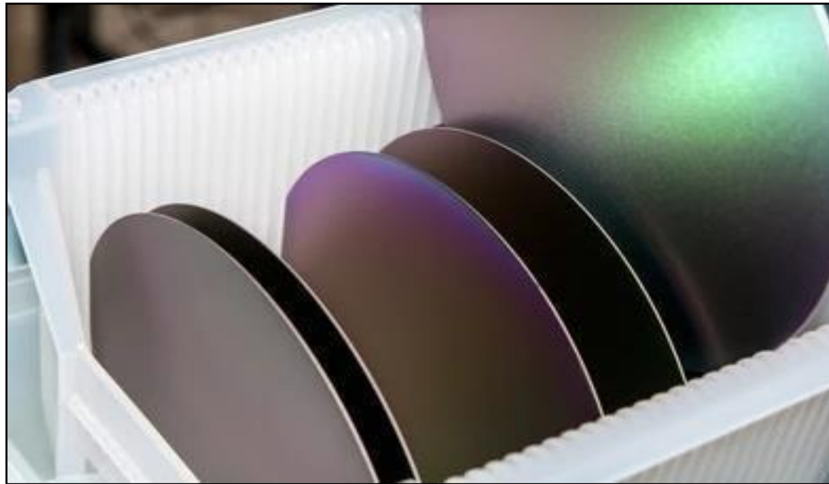


Figure I.01: Thin silicon discs for the production of microcircuits and radioelements with thin-film technology.

I.3. A Brief History

Thin-film usage dates back over 5,000 years, when precious items were coated in gold for preservative and decorative purposes. Although these ancient methods for creating thin films are much different than what is commonly used today, it is interesting to note the prominence thin films have had on many cultures throughout history. It was not until the advancements in vacuum technologies in the 1800s that thin films became popular in our modern society.

They are used for numerous applications, such as protective coatings, optical filters, semiconductors, visual decor, and more [5].

I.4. Interest and characteristics of thin films

The interest in thin films comes mainly from the economical use of materials with the physical properties and the simplicity of the technologies implemented for their production (easy development, inexpensive). A wide variety of materials are used to produce these thin films.

These include metals, alloys (possibility of making several alloys: binary, ternary, quaternary), refractory compounds (oxides, nitrides, carbides), intermetallic compounds, and polymers.

The second essential characteristic of a thin film is that, whatever the process used for its

manufacture, a thin film is always attached to a support on which it is constructed (even if it sometimes happens that the film is separated thin from said support).

Consequently, it is imperative to consider this major fact in the design, namely that the support strongly influences the structural properties of the film deposited on it. Thus, a thin film of the same material and thickness may have significantly different physical properties.

Depending on whether it will be deposited on an amorphous insulating substrate such as glass or a monocrystalline silicon substrate, for example. The following consequence results from these two essential characteristics of a thin film: A thin film is anisotropic by construction. [6].

I.5. Thin-film applications

The following general categories can be identified by considering the different applications of deposited thin films: [7]

a) Semiconductors

The semiconductor industry has relied on flat, two-dimensional chips upon which to grow and etch the thin films of material that become electronic circuits for computers and other electronic devices. They can be transferred to glass, plastic, or other flexible materials and electronics. Solar cells, smart cards, radio frequency identification (RFID) tags, medical applications, and active-matrix flat panel displays could benefit from the development.

b) Electronic Components

Fabricating electronic components, especially solid-state devices and microelectronic integrated circuits, has been found to have the widest and most demanding applications for thin-film depositions. These films typically consist of semiconductor materials, dielectric and metal or refractory silicide conductors.

c) Electronic Displays

Electronic displays are used for electronic interfacing equipment with human operators. Different components and device structures are required, such as:

- Liquid-crystal displays
- Light-emitting diodes (LEDs)
- Electroluminescent displays
- Plasma and fluorescent displays
- Electrochromic displays

Fabricating these displays requires conductive films, transparent and conductive films, luminescent or fluorescent films, and dielectric and insulating films.

d) Gas Sensors

Various gas sensing elements have been developed during the past years, of which resistive metal oxide sensors comprise a significant part. These properties make them candidates for building blocks of active materials in nanoelectronics, field emission devices, gas storage, and gas sensors.

e) Optical Coatings

Optical coatings are applied for antireflection purposes, as interference filters on solar panels, plate glass infrared solar reflectors, and laser optics. In the fabrication of filter optics, thin films with refractive index gradients are deposited on the substrates from which the optical fibers are drawn.

These coatings require dielectric materials with precisely defined indices of refraction and absorption coefficients. Laser optics requires reflective metal coatings that can withstand high radiation intensities without degradation. Infrared reflecting coatings are applied to filament lamps to increase the luminous flux intensity.

f) Magnetic Films for Data Storage

Thin films of magnetic materials have found wide commercial applications for data storage in computers and control systems. The substrates can be metal, glass, or plastic polymeric materials.

Thin-film deposition processes for magnetic materials and materials with a high degree of hardness are required.

g) Optical Data Storage Devices

Thin films are increasingly commercially used for optical data storage devices in compact disks and computer memory applications. Processes for the deposition of organic polymer materials as storage media and as protective overcoats are required for this technology.

h) Anti-static Coatings

Thin films of conductive or semi-conductive materials are deposited to protect them from electrostatic discharges.

i) Hard Surface Coatings

Thin-film coatings of carbides, silicide, nitrides, and borides have improved the wear characteristics of metal surfaces for tools, bearings, and machine parts. Particular current interest is films of diamond-like carbon because of this material's heat dissipation properties, electrical insulation, hardness, and resistance to high-temperature and high-energy radiation.

j) Thin-film photovoltaic cells

Thin-film technologies are also being developed to reduce the cost of solar cells substantially. The rationale is that thin-film solar cells are cheaper to manufacture owing to their reduced material costs, energy costs, handling costs, and capital costs; this is especially true in printed electronics (roll-to-roll) processes. Other thin-film technologies that are still in an early stage of ongoing research or with

limited commercial availability are often classified as emerging or third-generation photovoltaic cells and include organic, dye-sensitized, and copper zinc tin sulfide, nanocrystal, and perovskite solar cells. [8-9].

k) Thin-film batteries

Thin-film printing technology is being used to apply solid-state lithium polymers to various substrates to create unique batteries for specialized applications. Thin-film batteries can be deposited directly onto chips or chip packages in any shape or size. Flexible batteries can be made by printing onto plastic, thin metal foil, or paper.

I.6. Steps of the thin film deposition process

All thin film deposition processes contain four successive steps, as shown in Figure I.02.

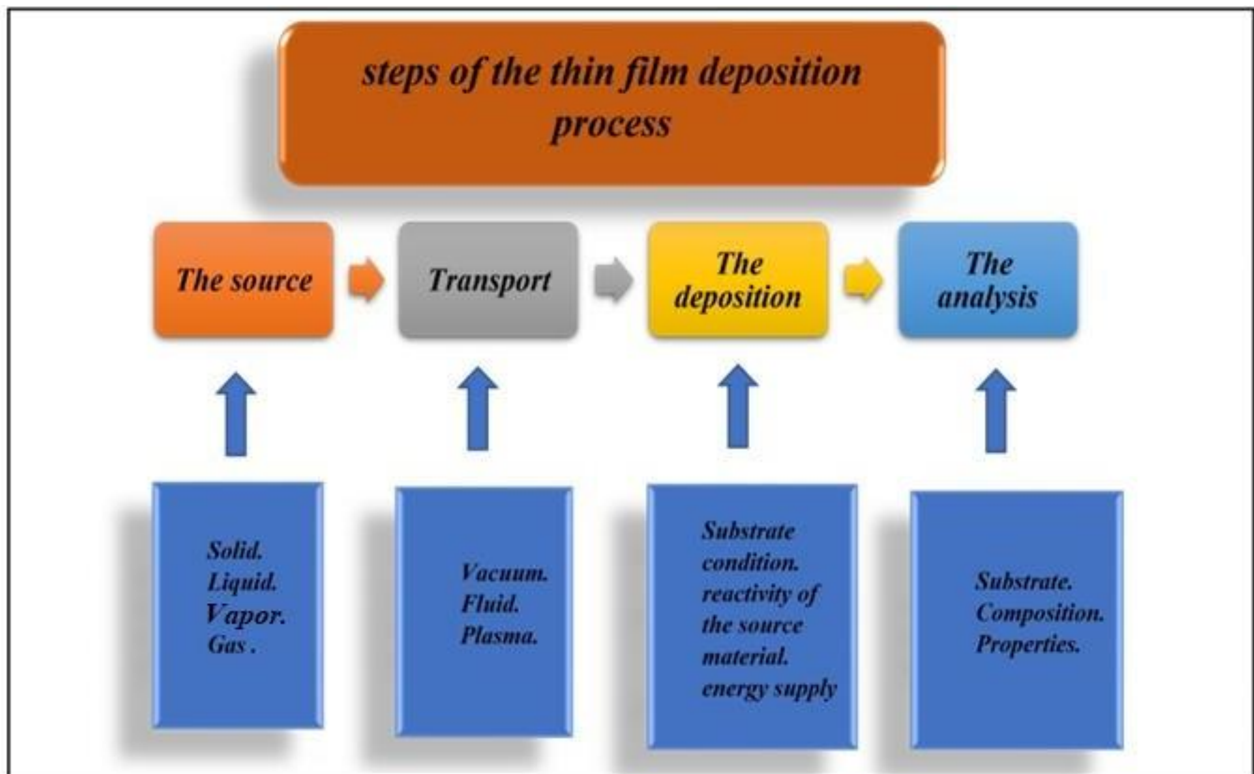


Figure I.02: Diagram of the thin film deposition process steps

I.6.1. The source

The source constitutes the basic material of the thin film to be produced. It can be a solid, a liquid, a vapor or a gas. When the material is solid, it is transported to the substrate by vaporization. It can be achieved by thermal evaporation, electron gun, laser ablation, or positive ion "spray." All of these methods are classified under the name of physical vapor deposition (PVD). The reliable source is occasionally transformed into vapor by chemical means. In other cases, the base material is in the form of a gas or liquid with sufficient vapor pressure to be transported at moderate temperatures. Processes that use gases, evaporated liquids, or chemically evaporated solids as a base material are known as chemical vapor deposition, or CVD. [10].

I.6.2. The transport

In the transport stage, the uniformity of the flow of species arriving on the surface of the substrate is an important element, and several factors can affect this uniformity and depend on the medium in which the transport takes place, a high vacuum or a fluid "mainly gases."

In the case of a high vacuum, the molecules coming from the source and going towards the substrate cross the medium in straight lines, whereas in a fluid medium, they undergo several collisions during their transport.

Consequently, in a vacuum, the uniformity of the flow that arrives on the substrate is determined by the geometry of the reaction, while in a fluid, it is determined by the flow of the gas and by the diffusion of the molecules of the source in the other present gases.

Often, the processes that use a high vacuum are equivalent to PVD processes, while those that use fluid flow are CVD processes. This definition is not always confirmed. Several physical vapor deposition processes operate in a high vacuum; others, such as laser ablation and sputtering, often operate at high fluid pressures.

Similarly, most CVD processes are found to operate at moderate pressures, while chemical beam epitaxy operates in a vacuum.

In this phase, several thin film deposition processes use a plasma medium. Indeed, the large amount of energy contained in this medium allows, at low temperatures, the activation of the formation of films. The working pressure of plasma can be that of a fluid. [11]

I.6.3. The deposition

The third step in the thin film process is the deposition of the film on the substrate surface. The deposition process is determined by the substrate surface's source, transport, and three main conditions. The latter is the surface conditions the reactivity of the incoming material on this surface "roughness, contamination level, degree of chemical bonding with the incoming material,", and the energy deposited on the surface "substrate temperature, photons, positive ions" [12].

I.6.4. The analysis

The fourth step in the manufacturing process is analyzing the obtained film. The first control over materials is to make direct measurements of their important properties.

If the results of the analysis are insufficient, it is necessary to resort to certain experiments that make it possible to remove the possible ambiguity of a particular process. [12].

I.7. Thin-film deposition techniques

The thin film deposition techniques are divided into three major categories: Physical Vapor Deposition (PVD), Chemical Vapor Deposition (CVD), and wet deposition techniques. In Figure I.03, the thin film deposition techniques and their subcategories [13].

Physical deposition methods are generally used in research, while chemical methods are also used industrially because of their better performance and the quality of the films obtained.

In this chapter we will explain CVD, and in the second chapter we will explain PVD.

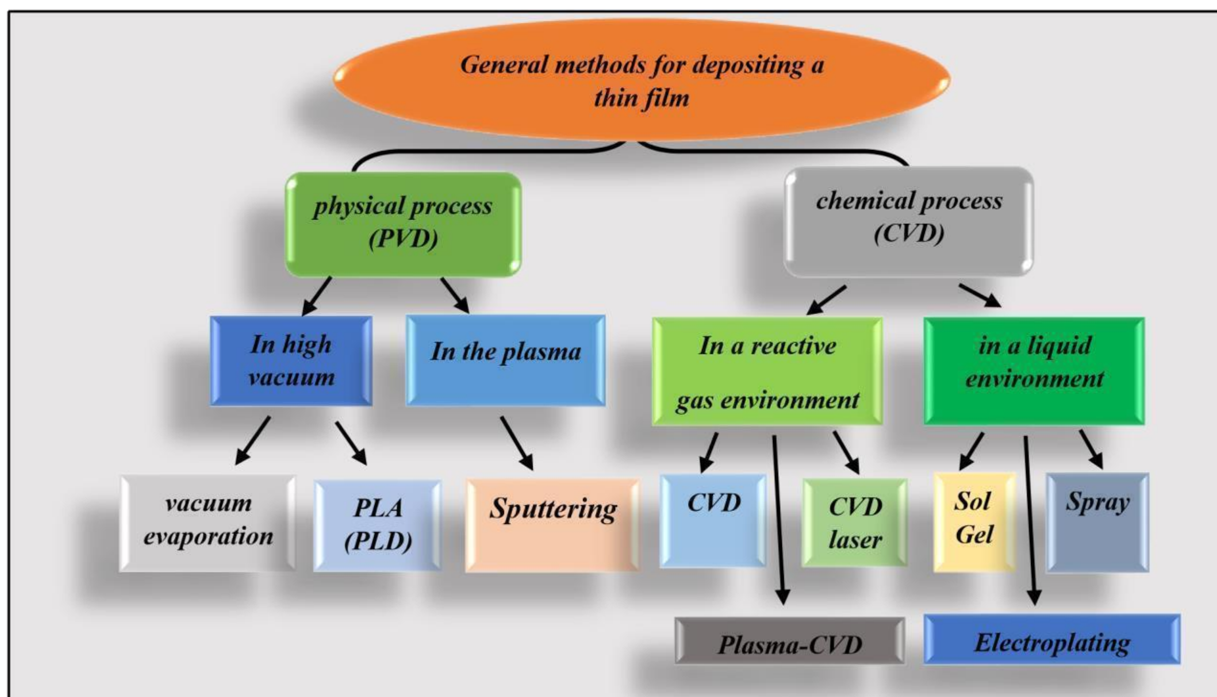


Figure I.03: Techniques and processes for depositing thin-films

I.7.1. The chemical Vapor Deposition (CVD)

CVD is a deposition method where a volatile compound of a pre-established substance is introduced into a reactor, usually with inert gas, to induce a chemical reaction that produces a solid thin film on a substrate at an elevated temperature. This technique, unlike PVD, must not produce the reaction. It must not be produced under vacuum conditions. Due to its versatility in working with a broad range of reactants and precursors, this technique enables the deposition of various structures, including metal alloys and compound semiconductors, with excellent control of purity and doping (stoichiometric film) [14]. Compared to PVD, this technique offers higher deposition rates, better conformance in rough substrates, easy deposition onto complex surfaces, and high throughput. However, some disadvantages, such as high substrate temperatures and the toxicity and flammability of the reactive gases, have prevented it from being used in low-scaled developments but are well justified in applications where high throughput is required, i.e., the semiconductor industry. The CVD processes can be classified based on the source employed to initiate the chemical reaction, the range of pressure under which the deposition is carried out, and the type of reactant used. The Chemical Vapor Deposition process is shown in Figure I.04.

We will talk a little about these methods: Thermal CVD, Chemical Thermal Spray Method (Spray Pyrolysis), and the laser CVD technique (CVD Laser).

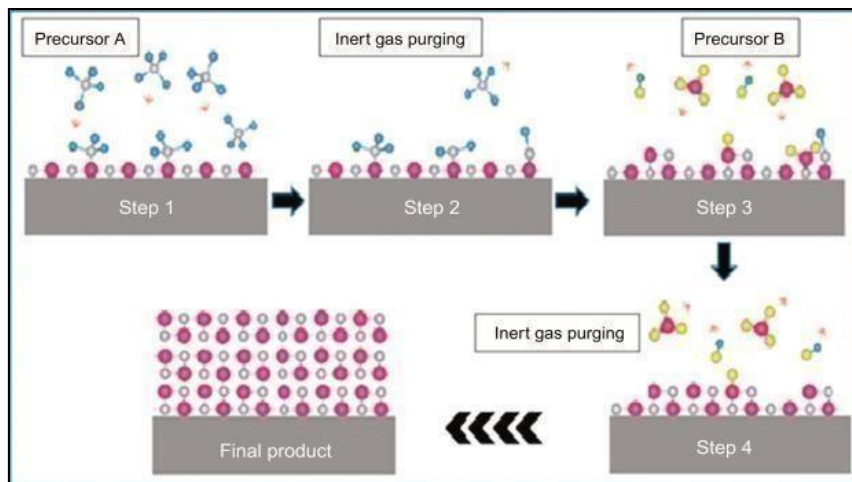


Figure I.04: Chemical vapor deposition process

a) Thermal CVD

Thermal CVD uses higher temperatures to provide the energy necessary for a chemical reaction that forms a thin film on the substrate. In atmospheric-pressure thermal CVD processes, the gaseous reactants are carried by an inert gas such as nitrogen into the reactor chamber. Chemical vapor deposition is generally carried out at high temperatures for enhanced deposition rates, improved crystallinity, greater density, and the promotion of otherwise impossible reactions. It is noteworthy that some properties of the film are difficult to achieve when it is deposited at low temperatures, followed by post-annealing at elevated temperatures. High-temperature deposition's major drawbacks are:

- Stress formation
- higher diffusion rates for elements from the substrate into the film.
- The possible degradation of the substrate

Low-temperature CVD at atmospheric pressure is generally used for metallization with gold, aluminum, etc. [15].

b) Chemical Thermal Spray Method (Spray Pyrolysis):

Spray pyrolysis is a simple, low-cost aerobic decomposition method and pulverization technology based on the pyrolysis of a liquid sample produced by spray pyrolysis [16]. This technology is a chemical method developed in the 1960s due to the urgent need to prepare thin films with large surface areas in the photovoltaic industry. Spray pyrolysis deposition is shown in Figure I.05.

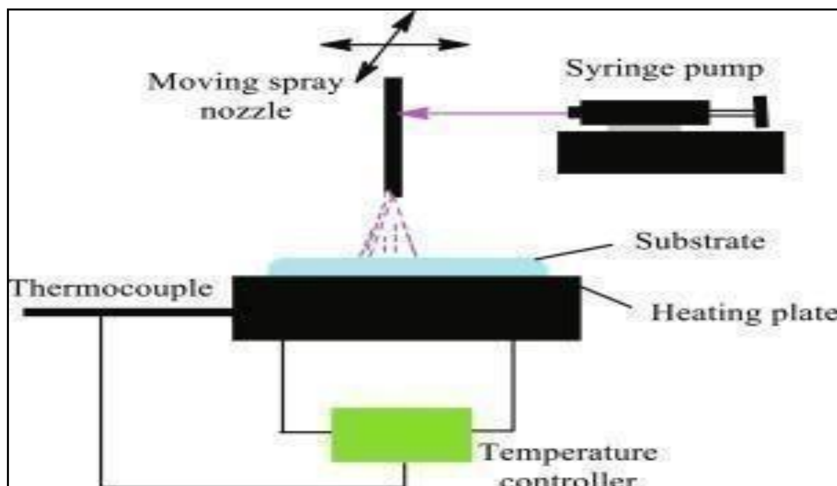


Figure I.05: Spray pyrolysis deposition

c) The laser CVD technique (CVD Laser)

This technique consists of irradiating, using a continuous or pulsed laser beam, either very locally on the surface of the substrate (in which case the chemical reaction takes place by simple activation thermal) or in the vapor phase to cause the excitation of the molecules and thus increase the reactivity of the gaseous species. In the first case, the rise in temperature being very localized, it is considered that we are dealing with a low-temperature process. This technique also obtains deposits in very localized areas, particularly in microelectronics. This process is still very limited industrially because of its high cost. [17].

I.8. Thin film growth mechanism

The growth of a thin film takes place in several stages:

- The arrival or adsorption of atoms (or molecules) on the surface of the substrate.
- Surface diffusion of atoms.
- The stability of the interaction between the deposited atoms and/or those of the substrate for forming bonds is ensured.
- Film nucleation.
- volume growth.
- The diffusion of the atoms in volume in the film and/or in the substrate.

Various physicochemical processes and several growth modes can occur during these growth stages. They depend in particular on the parameters relating to the film production process (energy of the species, deposition temperature, etc.) and the materials involved (deposited atoms and substrate). Different approaches to describing these mechanisms depend on the scale considered, from the macroscopic to the microscopic, and the growth stage is considered. [18]

a) The nucleation

It is the phenomenon that accompanies changes in the state of matter and consists of the appearance, within a given medium, of points of transformation from which a new physical or chemical structure develops. The sputtered atoms arriving at the substrate lose their components normal to the substrate of their velocity and are physically adsorbed by the surface of the substrate. These species are not thermodynamically in equilibrium with the substrate and move over its entire surface. They interact with each other in this state and form "clusters." These "clusters," also called nuclei, are unstable and tend to desorb.

Under certain deposition conditions, they collide with other adsorbed species and begin to grow. These clusters become thermodynamically stable after reaching a critical size, and the nucleation barrier is crossed.

b) The coalescence

The nuclei grow in size and number until they reach a maximum nucleation density. This one, as well as the average size of these nuclei, also called islands, depends on several parameters, such as the energy of the sputtered species, the sputtering rate, the activation energy, the adsorption energy, the desorption energy, the thermal diffusion, the substrate temperature, the topography, and the chemical nature of the substrates.

A core can grow parallel to the substrate by a phenomenon of surface diffusion of the sputtered species. It can also grow perpendicularly to the substrate by adding sprayed species. In general, the lateral growth in this step is much more critical than perpendicular growth.

c) The growth

The last step in the film manufacturing process is the coalescence step, in which the islets begin to group. This tendency to form larger islands is called possesses the terminology of agglomeration and is enhanced by the growth of the surface mobility of the adsorbed species. This improvement is obtainedby increasing the temperature of the substrate.

These larger islands are still growing, leaving channels and holes in the substrate. The film structure in this step changes from a discontinuous island type to a porous network type. A continuous film is formed by filling the channels and holes. [19] The steps of nucleation and growth of thin films are represented in the following figure I.06.

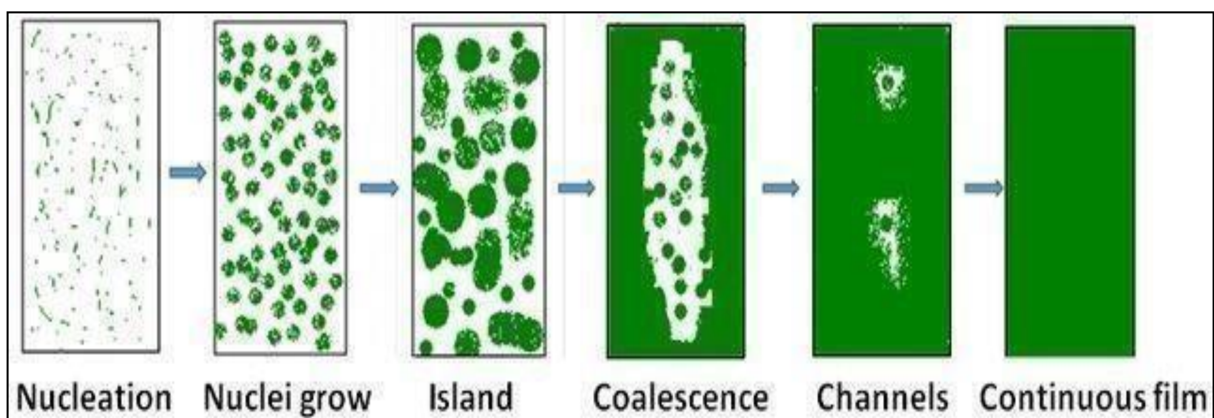


Figure I.06. Various stages of nucleation and growth of thin films

I.9. Properties of thin films

a) Optical properties

Optical experiments provide a good way of examining the properties of semiconductors.

In particular, measuring the absorption coefficient for various energies gives information about the band gaps of the material. Knowledge of these band gaps is vital for understanding the electrical properties of a semiconductor and is, therefore, of great practical interest [20].

b) Mechanical properties

The mechanical properties of thin films often differ from those of bulk materials, and this can be partially explained by the nanostructure of thin films and the fact that these films are attached to a substrate. Due to their typically high yield strengths, thin films can support very high residual stresses. This residual stress can be relieved later during processing or the actual device operation through plastic deformation, thin-film fracture, or interfacial delamination. Both elastic and plastic properties are essential for thin-film characterization. Thin-film mechanical properties can be measured by tensile testing of freestanding films and by the microbeam cantilever deflection technique. However, the easiest way is to use nano indentation since no special sample preparation is required. The tests can beperformed quickly and inexpensively [21].

c) Electrical properties

There are three types of electronic materials: conductors, semiconductors, and insulators. The electrical transport nature is different in all types of materials. Therefore, it is impossible to describe them all together. However, in the thin film form, scaling effects begin to influence the electrical properties of materials similarly. The film thickness, the lattice dimensions, the purity, the surface roughness, and the layer's imperfect level are significant parameters to define the type, mechanism, and stability of the electrical transport [22]. Figure I.07 shows the conductivity scale for various materials at room temperature.

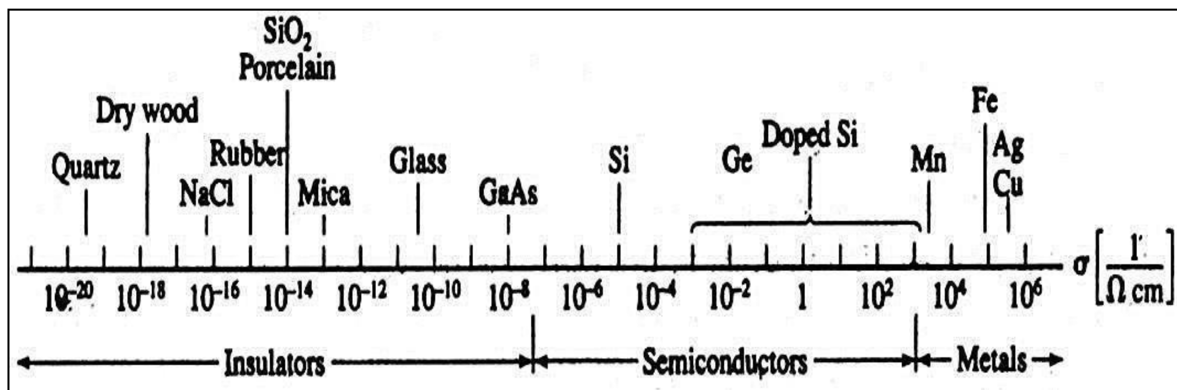


Figure I.07: Conductivity scale for various materials at room temperature

I.10. Types of electronic materials

There are many types of solids, such as semiconductors, insulators, and conductors, and we will explain how to define each type below [23].

I.10.1. Conductors (metals)

The materials with the lowest resistivity at room temperature, typically less than 10^{-5} Ωcm, are metals (copper, gold, silver, aluminum, etc.). Free electrons essentially carry out electrical conduction, the concentration of which differs little from one metal to another (from 10^{22} to 10^{23} cm^{-3}) regardless of its purity. An increase in temperature causes a slight increase in resistivity, which can be explained by the fact that the free electrons are gêner in their movement by the vibrations (increasing with temperature) of the metal atoms.

In the simulation, copper (Cu) was chosen because of its superior conductivity and excellent electrical current conductor. It is relatively inexpensive compared to gold, silver, and most other metals that do not conduct electricity quite as well as copper.

I.10.2. Insulators

Materials whose resistivity is typically greater than 10^{8} Ωcm are considered insulators; this is the case for glass, mica, silica (SiO_2), and carbon (diamond). This time, the increase in temperature can cause

the release of electrons (as well as "holes"), which can participate in electrical conduction, which causes a drop in resistivity with temperature.

Silicon dioxide is a chemical compound with the formula SiO_2. It is a very abundant mineral in the earth's crust (55% by mass). That is why we chose it in simulation. SiO_2 is widely used as a thin film to improve the surface properties of materials because it is anti-resistance, hardness, corrosion resistance, dielectric, optical transparency, etc. In addition to these excellent performances, silicon oxide thin films are used in many fields.

I.10.3. Semi-conductors

Between metals and insulators are semiconductors (SC) whose resistivity varies from 10^{-3} to 10^{4} Ωcm (or more). Electric conduction is done by electrons and holes or preferentially by one or the other type of carrier. A semiconductor can be either pure, in which case it is said to be "intrinsic", or doped with impurities (which make it possible to control its resistivity), in which case it is said to be "extrinsic". If we take, for example, reasonably pure silicon and add one atom of boron or phosphorus to it for 105 atoms of silicon, its resistivity goes from 10^{3} to around 10^{-2} Ωcm.

Combining gallium (atomic number 31) and nitrogen (atomic number 7), gallium nitride (GaN) is a comprehensive bandgap semiconductor material with a rigid, hexagonal crystal structure. GaN was chosen because, since the 1990s, it has been used commonly in light-emitting diodes (LED). Gallium nitride gives off a blue light used for disc-reading in Blu-ray. Additionally, gallium nitride is used in semiconductor power devices, RF components, lasers, and photonics. In the future, we will see GaN in sensor technology.

I.11. Thin films importance

Because of their uses, thin films have become very important in our lives. Thin films are used in many domains, especially in micro and nanotechnology.

One of the most critical applications of thin films is in photovoltaic devices and other solar cells. They protect objects by improving their mechanical properties, resistance to wear and corrosion, or by serving as a thermal barrier. These are, for example, chromium plating, which modifies the optical

properties of objects. In particular, decorative coatings (e.g., gilding) or coatings modifying the reflective power of surfaces (anti-reflective glass or mirrors) should be mentioned.

Thin films can be used to obtain information about the properties of matter because specific measurements can be made more conveniently using thin films.

One of the fields where thin films are not only helpful but also constitute critical manufacturing technology is the semiconductor industry.

So, these are some of the essential things about thin films, which have many roles in technology development.

I.12. Conclusion

In this chapter, we presented general notions on thin films and have seen the role of thin films, their applications, and some of the deposition techniques. We also talked about their proprieties.

Finally, we talked a little about the types of materials (semiconductors, conductors, and insulators), and we also talked about the importance of thin films.

So, in conclusion, the role thin films play in our lives is endless as many more inventions are being made to study thin films. Thin film technology has been used so far from the textile or fabric industry to the gadgets, utensils, vehicles, tools, construction (roads), medical examinations, decoration, etc., all of which are very useful in our everyday life.

Thin-film technologies have played a vital role in making life easier for everybody.

Chapter II

Deposition by electrical discharge

II.1. Introduction

We discussed CVD and PVD's two thin-film deposition methods in the first chapter. So, in this chapter, we will talk about and explain the deposition by an electrical discharge, which is the PVD process.

In physical vapor deposition (PVD) processes, atoms or molecules of material are vaporized from a solid or liquid source, transported in the form of vapor through a vacuum or low-pressure gaseous environment, and condensed on a substrate. [24]

This method, which includes several parts, is the most widely used. The critical part is sputtering, which we employed in our simulation.

II.2. The Physical Vapor Deposition (PVD)

Physical deposition methods are usually referred to as physical vapor deposition methods (PVD) because the process entails vapor generation.

PVD consists of removing growth species from a source or target material via evaporation. Then this vapor is transported to the substrate surface, and eventually, it solidifies on the surface, forming the film. The evaporation is generally carried out under a reduced pressure chamber to avoid impurities in the film formation, which is produced due to collisions between vapor particles and residual gas particles in their displacement from the source to the substrate surface.

PVD techniques are known to offer several advantages, including the deposition of almost any material, high reproducibility of film properties, the use of a large range of substrate materials, the possibility of tailoring the film properties through modification of deposition parameters in single element deposition; and obtaining films with high purity. On the other hand, among the main disadvantages are the use of sophisticated and costly monitoring systems to control the deposition rate and film thickness and the mismatch between the composition of the deposited film and the composition of the evaporator in the case of alloys and compounds. PVD techniques can be classified according to the method employed in vapor generation.

The most common PVD techniques are vacuum-based evaporation and its heating versions, sputtering, laser ablation (PLA), cluster beam, and ion pattering, of which only the most important will be described in detail in this chapter. [25-26].

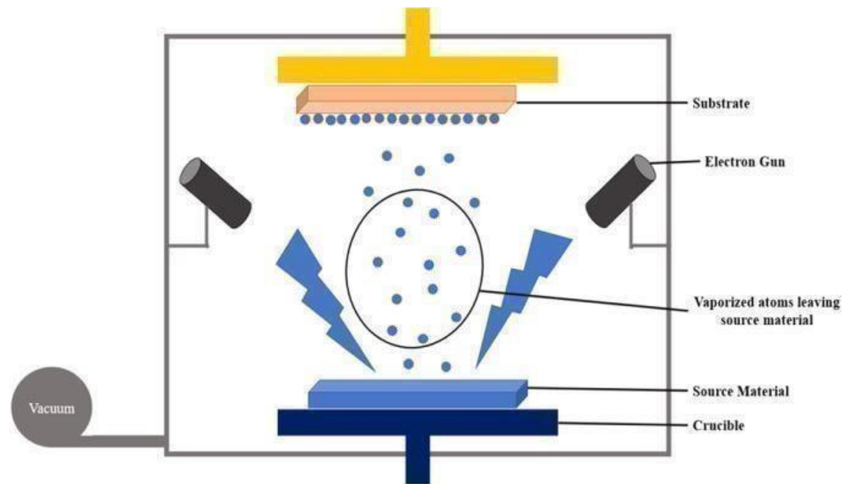


Figure II.01: Schematic of physical vapor deposition process

II.3. Advantages and Disadvantages of the PVD process

- Only one of the methods is used to coat surfaces.
- is safer than other methods.
- Also, it can be used on almost any type of inorganic material.
- is used as the deposition method to produce an extremely hard, corrosion-resistant coating.
- Thin films made with PVD have a high-temperature tolerance and superior removal resistance.
- PVD is also considered an environmentally friendly process.
- Have in higher costs, due in part to the intense heating and cooling that is required.
- The process requires complex machines that need skilled operators.
- Also, the rate at which coating PVD operates is relatively slow.
- PVD is also a line-of-sight technique, which it is not ideal for coating a non-visible surface. [27,28]

II.4. PVD applications

PVD technology is very versatile, enabling one to deposit virtually every type of inorganic material, such as metals, alloys, compounds, and mixtures, as well as some organic materials. PVD coating is generally used to improve hardness, wear resistance, and oxidation resistance. So, such coating is used in a wide range of applications such as aerospace, automotive, surgical/ medical, dyes and molds for all material processing, cutting tools, firearms, optics, watches, thin films, and in the textile industry [29,30]. Figure II.02 shows the applications of PVD.

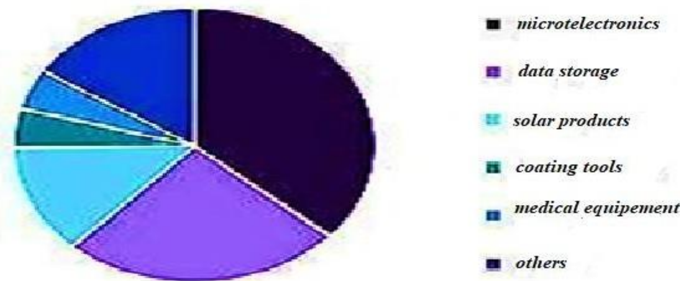


Figure II. 02: applications of Physical vapor deposition

II.5. Physical vapor deposition techniques

There are many techniques in PVD and the most used and important are describing below:

II.5.1. Thermal evaporation

Thermal evaporation is a well-known method for coating a thin film in which the source material evaporates in a vacuum due to high-temperature heating, which facilitates the vapor particles moving and directly reaching a substrate where these vapors again change to a solid state.

In this method, a charge holding boat or resistive coil is used in the form of a powder or solid bar. In order to get the high melting points necessary for metals, the resistive boat/coil is exposed to a large direct current (DC), where the high vacuum (below 10^{-4} Pa) supports the evaporation of the metal andfurther carrying it to the substrate.

This technique is especially applicable for materials with low melting points. A schematic of the thermal evaporation system is exhibited in Fig II.03 [31]

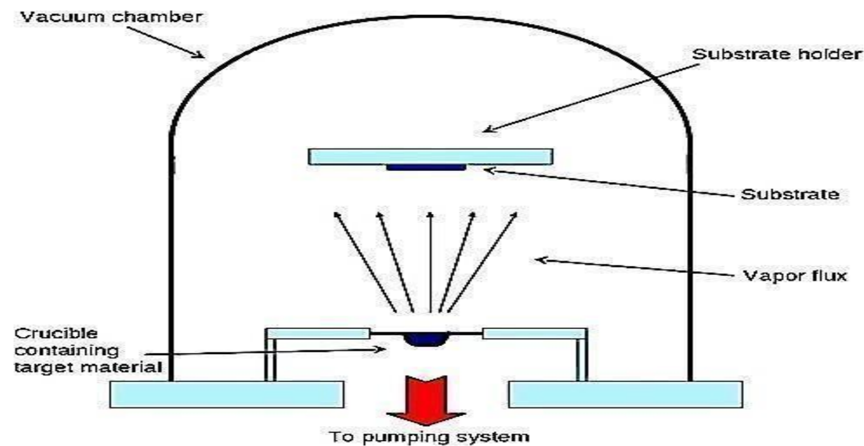


Figure II.03: The phenomenon of thermal evaporation

II.5.2. Ablation Laser

The ablation laser is based on a similar configuration as the previous techniques, i.e., usually an evacuated chamber with a target material to be evaporated. A substrate is placed parallel to the target, where the film condenses. In this case, an additional high-power pulsed laser is placed outside the deposition chamber, which emits the energy to induce the target material's ablation [32].

This technique is broadly employed in depositing alloys, compounds, polymers, semiconductors, and multilayers due to its excellent stoichiometry transfer from the target to the film. Oxide-thin films can also be deposited if oxygen is introduced into the chamber as a background gas.

The irradiation from the laser power, i.e., KrF (248 nm), is focused on the target, producing rapid local heating until reaching the melting point and eventually producing evaporation deposited in the substrate.

The laser ablation process and the quality of the sample are affected by several parameters, including the characteristics of the target material, deposition conditions, laser parameters, and substrate temperature. Although this technique is widely recognized for its diverse and fast applicability, the actual ablation process is yet to be fully understood because the material ejection is not produced solely by a thermal process; a photochemical reaction is likely to be present.

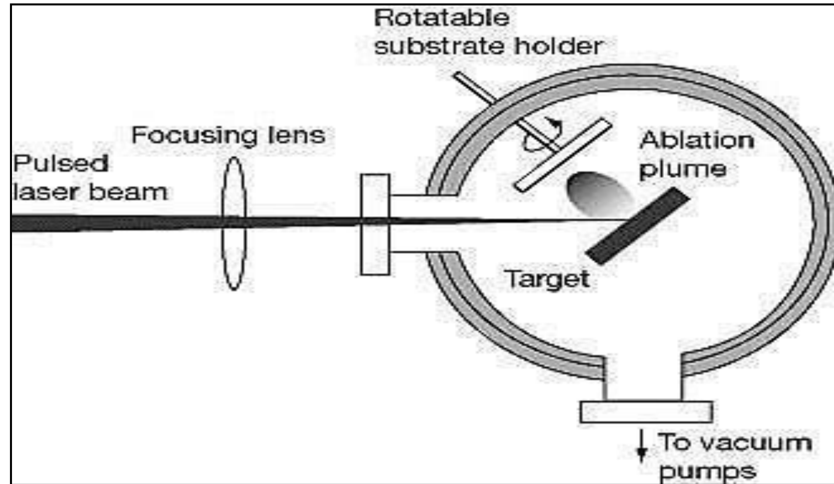


Figure II.04: Schematic diagram of PLD process.

II.5.3. Vacuum evaporation

One of the thin film deposition techniques is vacuum evaporation. Its principle consists in heating the material to be evaporated in a crucible by Joule effect or by bombardment by an electron gun. The evaporation of the material will take place inside the enclosure of the evaporator. Condensation of vapor on a cold substrate leads to the formation of a thin solid layer. [33]

II.5.4. Sputtering

The sputtering technique is used for depositing all materials, whether conductive, semiconducting, or insulating (RF sputtering). In this technique, we can use one target (single-target sputtering) or several targets (multi-target sputtering), which act as the cathode that contains the material or compounds to be deposited. A potential difference is applied between the electrodes, which causes ionization of the inert gas discharge, usually Argon. Some electrons still present will be accelerated and collide with the Argon atoms; thus, Ar+ ions and secondary electrons are created. These secondary electrons will undergo collisions with other atoms of Argon, creating new ions and electrons, creating a plasma. Condensing atoms obtain the deposit from the target, created by its bombardment by the accelerated plasma ions due to the electric discharge [34]. The basic scheme of sputtering is presented in Figure II.05.

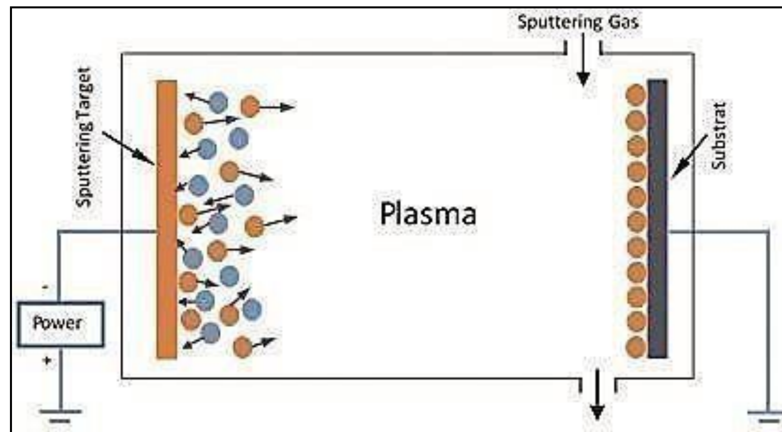


Figure II.05: Schematic diagram of Sputtering

II.5.4.1. Sputtering history

In 1953, HOLLAND and SIDDALL established the experimental conditions for continuous diode sputtering (DC). A hundred years earlier, GROVE and PLUCKER had shown that by establishing a discharge between two conductive electrodes in an enclosure containing a pressurized gas, a deposit corresponding to the constituents of the cathode is formed at the anode.

The GROVE experiments have given rise to numerous works to explain this phenomenon. Two mechanisms have been proposed:

1- Transfer of movement quantities: Proposed by STARK in 1908. The phenomenon results from a momentum transfer between the incident ion and one of the atoms of the crystal lattice.

2- Local rise in temperature: VON-HIPPEL explains this phenomenon as a transfer of energy from incident ions on a small hemispherical surface which causes local volatilization.

In 1950, WEHNER decided in favor of the first hypothesis. He studied sputtering on a single crystal and observed that sputtering efficiency is sensitive to crystal orientation. WEHNER had difficulty depositing insulators, so he proposed to apply an RF voltage instead of a DC one. this proposal was put into practice in 1962 by ANDERSON and by DAVIDSE and MAISSEL, in 1965, defined the conditions for producing thin layers. Today, there are several variations of these two DC and RF (Radio Frequency) techniques: RF magnetron, triode, bias sputtering, and ion plating. [35]

II.5.4.2. Types of sputtering

II.5.4.2.1. DC Diode Sputtering

DC or Direct Current Sputtering is a thin film Physical Vapor Deposition (PVD) Coating technique where a target material to be used as the coating is bombarded with ionized gas molecules, causing atoms to be “sputtered” off into the plasma. These vaporized atoms are then deposited when they condense as a thin film on the substrate to be coated.

DC Sputtering is the most basic and inexpensive type of sputtering for PVD metal deposition and electrically conductive target coating materials. Two significant advantages of DC as

a power source for this process is that it is easy to control and a low-cost option if a metal deposition for coating is applied. [36].

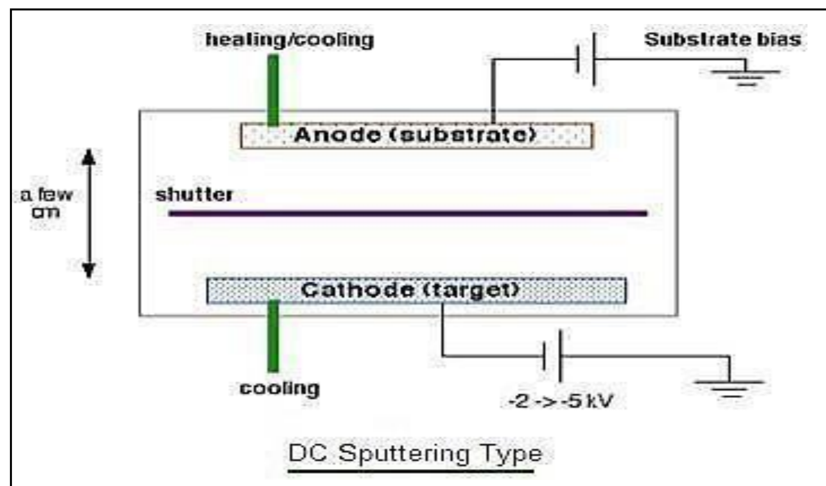


Figure II.06: The fundamental components of a DC sputtering system

II.5.4.2.2. Radiofrequency (RF) sputtering

In radiofrequency diode sputtering, the direct electric field is replaced by an alternating electric field. During the negative alternation, the cathode attracts the ions which spray it, charging it positively. During the positive alternation, it attracts the electrons that discharge it. It is, therefore, possible to spray conductive or dielectric materials.

The ionization of the sputtering gas is low, and as a result, the discharge current and the film growth rate (proportional to the sputtering rate) are also shallow. The deposition rate is considerably lower than that of films evaporated under a vacuum. For this reason, cathodic diode sputtering is little used for the industrial production of thin films. [37].

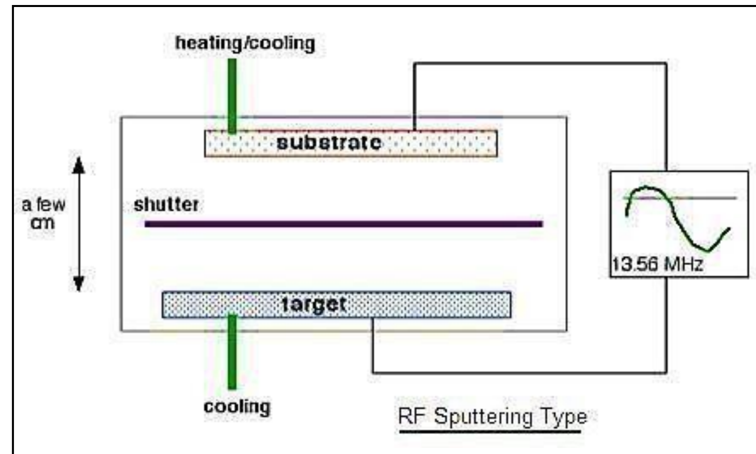


Figure II.07: The fundamental components of a RF sputtering system.

II.5.4.2.3. Magnetron sputtering

Magnetron sputtering is a high-rate vacuum coating technique for depositing metals, alloys, and compounds onto a wide range of materials with thicknesses up to millimeters. It exhibits several significant advantages over other vacuum coating techniques. This property led to the development of many commercial applications, from microelectronic fabrication to simple decorative coatings. There are various advantages of magnetron sputtering, such as:

- high deposition rates.
- ease of sputtering any metal, alloy, or compound.
- high-purity films.
- extremely high adhesion of films.
- excellent coverage of steps and minor features.
- The ability to coat heat-sensitive substrates.

- excellent uniformity on large-area substrates, for example, architectural glass. [38]

Magnetron sputtering is another route to the deposition of thin films on a substrate. This approach's procedure is based on forming a ring-shaped glow plasma (generally confined around the target by a magnet) beyond the cathode surface because of the collision of electrons with the available gas molecule. Resultant ions accelerated toward the cathode and bombarded its surface so that particles were released from it.

In conclusion, ejected particles from the target were deposited in a film on the substrate. Some other particles were disturbed in the path and deposited inside the working chamber. [35].

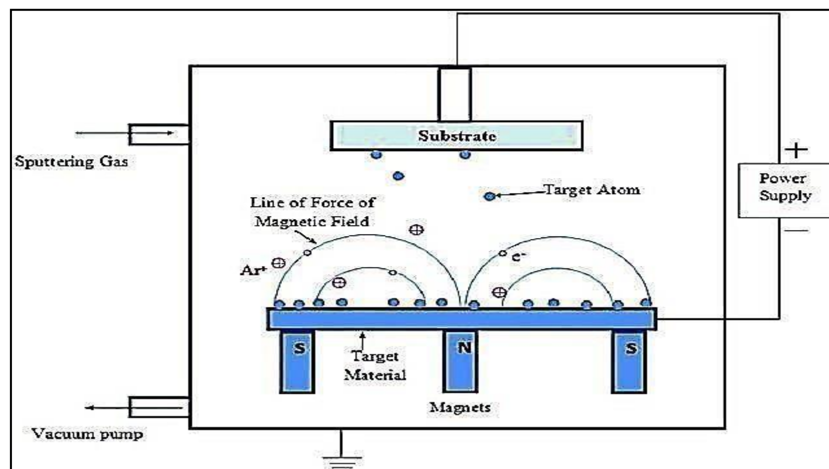


Figure II.08: Working principle of magnetron-sputtering depositionprocess.

II.5.4.2.4. Ion-beam sputtering

The ion beam sputtering (IBS) system is used in the present experiment as shown in Fig II.09. The chamber was pumped down to 8×10^{-7} Torr prior to the deposition using the cry pump.

The ion source is the hot- cathode type with an effective beam diameter of 30 mm. Argon gas was supplied into the ion source and the pressure in the sputtering chamber was set at 1.6×10^{-4}, Torr,during operation. The target was designed for FGM technology.

Other operation conditions of IBS system are as follow: Ion energy 1.2 keV and current density 0.4 mA/cm^2. The deposition rate of Nb/M0 under those condition was about 17.0 Å/ min. [39]

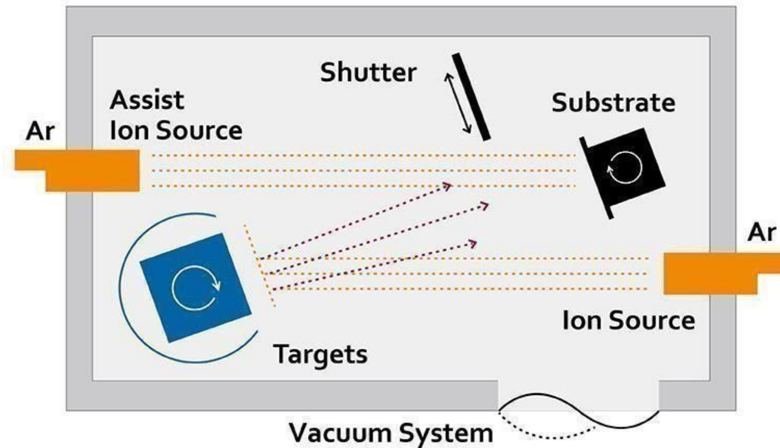


Figure II.09: Schematic diagram of ion beam sputtering system.

II.5.4.2.5. Triode-sputtering

A triode-sputtering deposition involves using a different heated filament to increase the electron density in plasma by thermionic emission, as depicted in Fig II.10.

The use of triode increases the ionization efficiency of plasma to generate intense sputtering discharges, enabling higher discharge rates even at lower target voltages and pressures than conventional PVD-sputtering processes using DC. Sometimes, filament reacts with the working gas and produces scaling that tends to erode filament rapidly during deposition, thus lowering the sputter rate. Although this process is used for thick coating, maintaining uniformity of coating is difficult due to the lack of an electron path guiding mechanism to confine the plasma. [40]

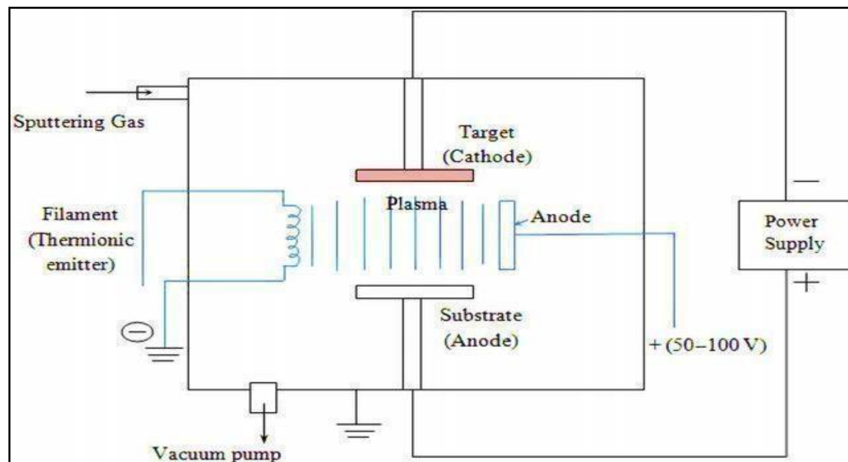


Figure. II.10: Working principle of triode-sputtering deposition process.

II.5.4.3. Advantages of sputtering

The vital advantage of sputter deposition is that even materials with very high melting points are easily sputtered. In contrast, evaporation of these materials in a resistance evaporator or Knudsen cell is problematic or impossible. Sputter-deposited films have a composition close to that of the source material. The difference is due to different elements spreading differently because of their different masses (light elements are deflected more easily by the gas), but this difference is constant. Sputtered films typically have better adhesion to the substrate than evaporated films. The target contains maintenance-free material, making the technique suited for ultrahigh vacuum applications. Sputtering sources contain no hot parts (to avoid heating, they are typically water-cooled) and are compatible with reactive gases such as oxygen. Sputtering can be performed top-down, while evaporation must be performed bottom-up. Advanced processes such as epitaxial growth are possible.

II.5.4.4. Disadvantages of sputtering

Some disadvantages of the sputtering process are that the process is more challenging to combine with a lift-off for structuring the film because the diffuse transport, characteristic of sputtering, makes a complete shadow impossible. Thus, one cannot fully restrict where the atoms go, leading to contamination problems. Also, active control for film-by-film growth is difficult compared to pulsed laser deposition, and inert sputtering gases are built into the growing film as impurities. Pulsed laser deposition is a variant of the sputtering technique in which a laser beam is used for sputtering. The role of the sputtered atoms and sputtered ions and the background gas is thoroughly investigated during the pulsed laser deposition process. [41, 42].

II.5.4.5. Application of sputtering targets

Many products commonly used today have a coating created through sputtering materials. These coatings include:

— **Glass coating**

- Sputter coater targets produce low-radiation coated glass (Low-E glass).

- Low-E glass is commonly used in construction because it can save energy, control light, and improve aesthetics.

— **Optical coating**

- Optical coatings are used mainly in sunglasses, eyeglasses, vehicle headlights, mirrors, windows, and optical filters for laser technology.

— **Solar cell coating**

- With demand for renewable energy on the rise, the third-generation thin-film solar cells are prepared using sputter coating technology.
- The Cadmium telluride sputtering target (CIGS target) has a large solar market share.

— **Semiconductors**

- Most modern-day electronics incorporate essential components produced with tantalum sputtering targets. [43]

II.6. General information on Monte-Carlo method

In preparation for the last chapter, which includes simulation, which depends a lot on the Monte Carlo method, we will talk about this method and explain it a little below:

II.6.1. Monte-Carlo method

Monte Carlo methods are a class of approximate inference techniques that allow for the mathematical modeling of systems with many states and/or those influenced by random events to be modeled. Based on numeric sampling, Monte Carlo methods can assist in developing probabilistic models.

To create a Monte Carlo model for a system, representative samples of the processes that typically occur within that system are simulated. Due to the random nature of some of the components of these processes, each outcome could be unique. Probability density functions are employed to model the various stochastic processes within the more robust system.

Multiple instances of the modeled process must be observed to capture enough data to effectively model a probabilistic representative distribution to build a comprehensive system model.

Data can be generated for deep learning applications where the ground truth of interest can be more precisely determined while retaining the ability to generate large datasets critical for training high-accuracy models using deep learning. [44].

II.6.2. Historical of the Monte-Carlo method

The Monte Carlo method, as it is understood today, was born in Los Alamos in the 1940s when physicists working on particle transport problems began solving them using something which they termed the Monte Carlo method. (Although earlier examples of Monte Carlo techniques exist, the cost of carrying out the experiments rendered them largely impractical and of only specialist interest.) The precise origin of the name varies from one account to another, but there is general agreement that it stems from its relationship with the games of chance played in the casinos of Monte Carlo.

The first revolutionary step introduced at this time was using (pseudo) random number generators in place of physical experiments to perform the calculation.

The second was realizing that it is unnecessary to use collections of independent random variables of known distribution; this concept led to Markov Chain Monte Carlo (MCMC). The physics community has continued to contribute to the development of Monte Carlo methodology, especially Markov Chain Monte Carlo, to the present day.

During the 1980s, the increasing use of Bayesian methods and the associated need to evaluate complex, high-dimensional integrals led to a renewed interest in and development of Markov Chain Monte Carlo methods by the statistics community.; This was the point at which the use of Monte Carlo methods to approximate general integral expressions, particularly expectations concerning complicated probability distributions, became widespread. The increased interest also drove and continues to drive the development of methodology and theory amongst researchers outside of the traditional application domains of Monte Carlo integration. [45].

II.6.3. The importance of the Monte-Carlo method

— **Easy and Efficient**

Monte Carlo algorithms tend to be simple, flexible, and scalable.

When applied to physical systems, Monte Carlo techniques can reduce complex models to a set of primary events and interactions, allowing the possibility to encode model behavior through a set of rules which can be efficiently implemented on a computer. However, this allows much more general models to be implemented and studied on a computer than using analytic methods.

These implementations tend to be highly scalable. For example, the complexity of a simulation program for a machine repair facility would typically not depend on the number of machines or repairers involved.

Finally, Monte Carlo algorithms are eminently parallelizable, mainly when various parts can be run independently.

This allows the parts to be run on different computers and/or processors, significantly reducing the computation time.

— **Randomness as a Strength**

The inherent randomness of the Monte Carlo method is not only essential for the simulation of real-life random systems, but it is also of great benefit over deterministic numerical computation. For example, when employed for randomized optimization, randomness permits stochastic algorithms to escape local optima, naturally enabling better search space exploration. Their deterministic counterparts do not usually share this quality.

— **Insight into Randomness**

The Monte Carlo method has great didactic value as a vehicle for exploring and understanding the behavior of random systems and data.

Indeed, we feel that an essential ingredient for correctly understanding probability and statistics is to carry out random experiments on a computer and observe the outcomes of these experiments—that is, to use Monte Carlo simulation [46].

In addition, modern statistics increasingly rely on computational tools such as resampling and Markov

Chain Monte Carlo to analyze large and/or high dimensional data sets.

- **Theoretical Justification**

There is a vast (and rapidly growing) body of mathematical and statistical knowledge underpinning Monte Carlo techniques, allowing, for example, precise statements on the accuracy of a given Monte Carlo estimator (for example, square-root convergence) or the efficiency of Monte Carlo algorithms.

Much of the current research in Monte Carlo techniques is devoted to finding improved sets of rules and/or encodings of events to boost computational efficiency for complex sampling, estimation, and optimization problems.

II.6.4. Advantages of the Monte-Carlo method

Unlike molecular dynamics simulations, Monte Carlo simulations are free from the restrictions of solving Newton's equations of motion. This freedom allows cleverness in the proposal of moves that generate trial configurations within the statistical mechanic's ensemble of choice. Although these moves may be nontrivial, they can lead to vast speedups of up to 10^{10} or more in sampling equilibrium properties. Specific Monte Carlo moves can also be combined in a simulation allowing the great modeler flexibility in the approach to a specific problem. In addition, Monte Carlo methods are generally easily parallelizable, with some techniques being ideal for use with large CPU clusters.

II.6.5. Disadvantages of the Monte-Carlo method

Because one does not solve Newton's equations of motion, no dynamical information can be gathered from a traditional Monte Carlo simulation. One of the main difficulties of Monte Carlo simulations of proteins in an explicit solvent is the difficulty of conducting large-scale movements. Any move that significantly alters the internal coordinates of the protein without also moving the solvent particles will likely result in considerable overlap of atoms and, thus, the rejection of the trial configuration. Simulations using an implicit solvent do not suffer from these drawbacks, and, therefore, coarse-grained protein models are the most popular systems where Monte Carlo methods are used. [47].

II.7. Conclusion

In this chapter, we talked about precipitation by electric discharge (PVD), which includes several techniques, including old and modern. However, the most important technique is the sputtering, which we explained in detail and discussed its types. Finally, in preparation for the last chapter, we briefly explained the Monte Carlo method.

In the end, we conclude that sputtering is an efficient technique for synthesizing and depositing various thin films on different substrates. During the process, different sputtering parameters are controlled to have an optimum deposition rate and thin films of the required thickness. The optimum thickness will lead to the required specific properties. After a long process of experimentation and research, scientists are now fully aware of the optimum conditions of sputtering parameters' control, which helps industries and labs have thin films with the required electrical and optical properties.

Chapter III
Results and discussion

III.1. Introduction

Developing a functional coating with specific properties in the laboratory is a complicated and time-consuming scientific discipline. However, with the advancement of computer software, it is now possible to devise a bottom-up methodology incorporating the desired characteristics to achieve the working conditions.

This chapter will describe the numerical methodology used in this study. First, the SRIM program is used to calculate the sputtering yield as a function of the energy and incidence angles of the applied gas inside the vacuum chamber. Then, the SIMTRA program determines the energy distribution of the atoms that reach the substrate level.

III.2. The Stopping and range of ions in matter (SRIM)

SRIM is a group of programs that calculate the stopping and range of ions (10 eV - 2 GeV/amu) in matter, including TRIM (the Transport of Ions in Matter), the most comprehensive program. TRIM will calculate the final 3D distribution of the ions and all kinetic phenomena associated with the ion's energy loss: target damage, sputtering, ionization, and phonon production. All target atom cascades in the target are followed in detail.

It can be used for the physics of recoil cascades, the physics of sputtering, the stopping of ions in compounds, and the stopping powers of ions in gases. This includes radiation damage from neutrons, electrons, and photons. [48]

III.3. Three gases used in the simulation

Argon: Because of their high molecular weight, inert gases, specifically argon, are commonly used as sputtering gases because they do not react with the target material or combine with any process gases and produce higher sputtering and deposition rates.

Xenon: is a heavy and extremely rare gas of group 18 (noble gases) that is used under high-pressure in electric arc lamps.

Oxygen: is the most abundant chemical element in the earth's crust. [49]

III.4. Monte-Carlo simulation

The other alternative consists of simulations describing the incident particles trajectory. The evolution of the cascade processes in the target and the ejection mechanism. As an example, binary collision Monte Carlo codes like SRIM are available to simulate the sputtering process and calculate the sputtering yield. This software consists of several modules that calculate the paths of ions in matter. Among these modules, one that has been used is the TRIM (Transport of Ions in Matter) module.

For this study, we set the TRIM module by using “Surface Sputtering/Monolayer Collision steps” included in this software for processing in a precise manner by sputtering a target. [50]

III.5. Operating principle

The simulations are performed by Monte Carlo method within the limits of binary cascades in an amorphous target. The user can define the initial parameters of the target (material, composition, density) and the primary ions (nature, energy and angle of incidence).

The choice of the number of incident particles defines the statistical quality of the simulation. As for any simulation, the increase in the number of particles increases the calculation time. The collisions are treated as two-body systems (BCA approximation: Binary Collision Approximation), i.e., the different shocks are not correlated. After a collision, the atoms can undergo other collisions. This model implicitly assumes that no energy is given to the electrons, and more generally, it ignores any inelastic diffusion. The SRIM calculation is based on several simplifying assumptions. First, the material is considered amorphous, even if the average distance between the atoms corresponds to the interatomic distance of the crystalline material. Therefore, SRIM cannot consider a possible channeling effect, which reduces the probability of having atomic shocks by two orders of magnitude. Moreover, the atoms are considered as immobile (the material is at 0 K) which puts aside the recombination phenomena between, for example, a displaced atom and a vacancy. The calculated rate should therefore be considered as an upper limit of possible damage caused by the analysis beam.

However, studies based on SRIM calculations have shown good correlations between the calculated and measured sputtering yields and the angular distribution of the sputtered atoms. In general, this method performs well when studying the relative influence of an experimental quantity on the system. In the case of our study, we used the TRIM (Transport of Ions in Matter) software, a complete program included in the SRIM-2008 version. TRIM accepts complex composite targets with up to eight layers of different materials. It will calculate the final 3D ion distribution and all the kinetic phenomena associated with the ion energy loss: target damage, sputtering, ionization, and phonon production. [51].

III.6. Sputter yield measurement using the Monte Carlo method

When the energy of the ion is greater than the threshold energy of the solid, it is large enough to eject atoms from the target that go afterward toward the substrate. In this case, a sputter yield (Y)is defined as the average number of atoms ejected from the solid in a vacuum by the impact of primary ions. For example, when a Primary ion ejects one atom of the target on average, we say that Y is equal to one. In general, Y is the ratio of the number of particles emitted to the number of projectiles. [52].

$$Y(E)=\frac{\text{number of atoms emitted}}{\text{number of projectiles}}$$

Sputter yield is a characteristic of the torque between the ion and the target. It depends on many parameters and changes with the energy and the nature of the incident ion. [52]

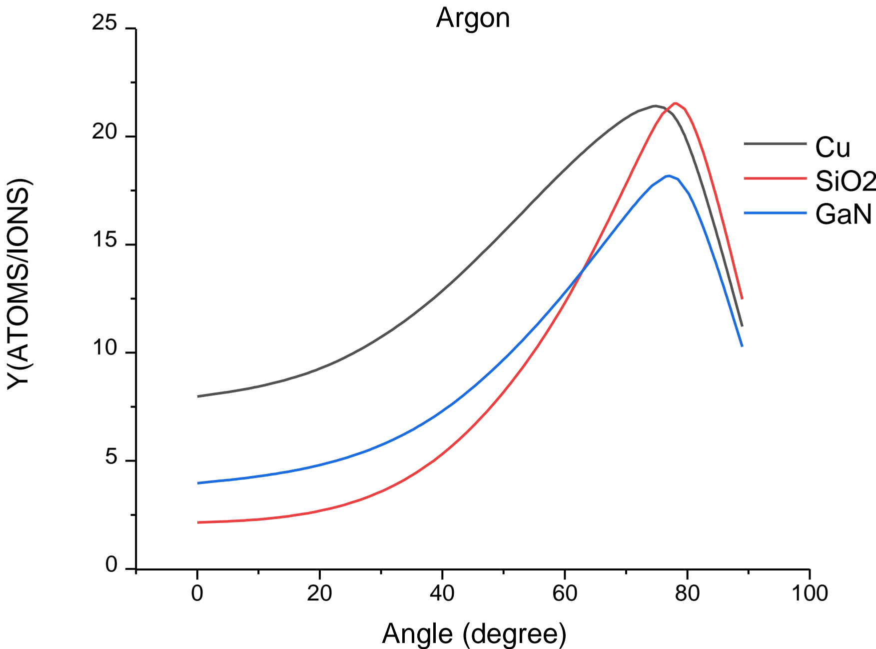
III.7. Variation of the sputtering yield according to the incidence angles and energies of particles

The figures in the next page show the sputtering yield obtained by SRIM simulation for different materials (Cu, SiO_2, and GaN) bombarded by three gases (Argon, Xenon, and Oxygen). Furthermore, we will start with a variation of the sputtering according to the incidence angles.

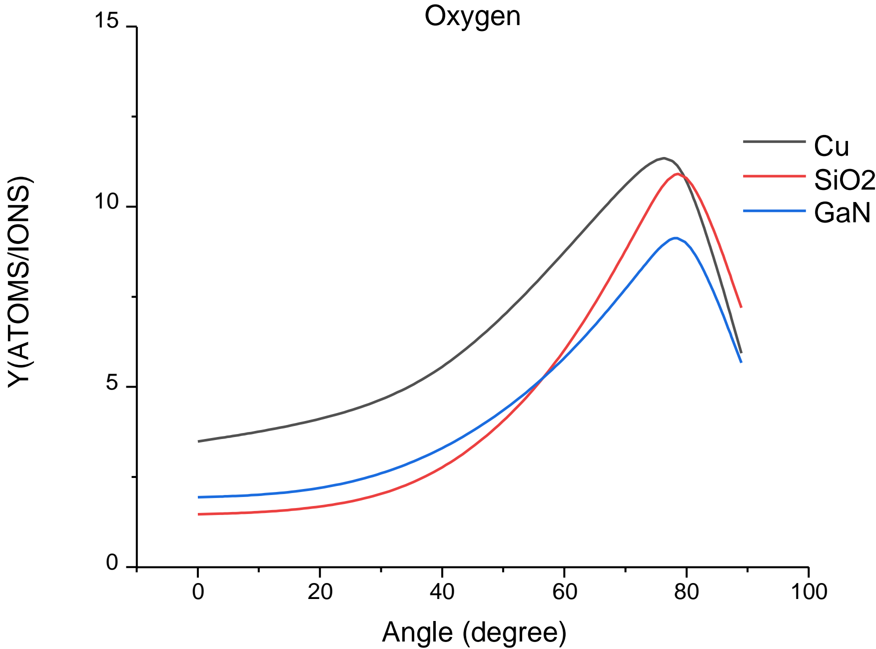
III.8. Sputtering yield as function of incidence angles

in this party we fixed the energy on the value E= 10Kev and changed the value of angle (θ) where θ = [0°,20°,40°,60°,75°,80°,89°]:

a)



b)



c)

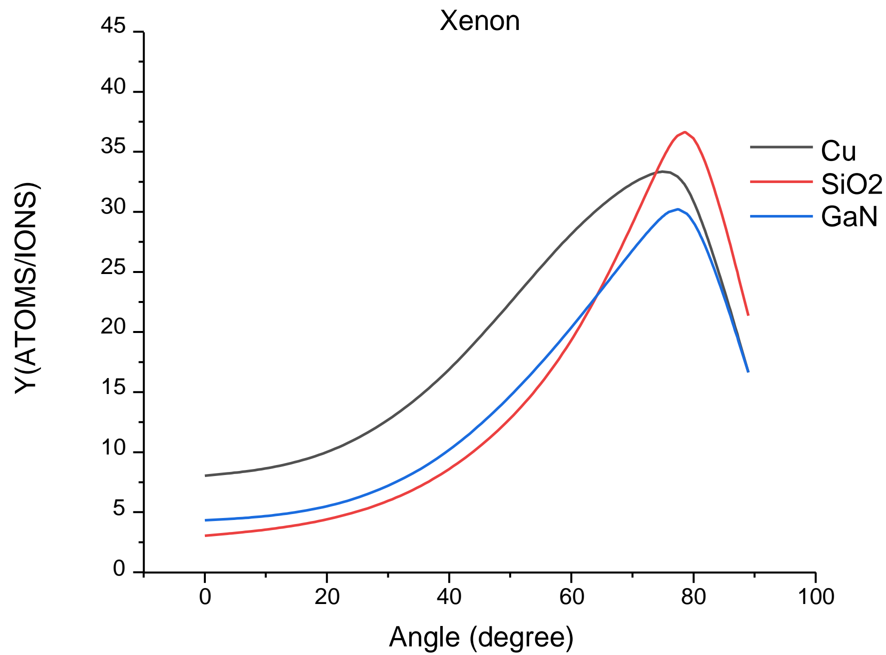


Figure III.01: Sputtering yield as a function of incidence angles for materials (Cu, SiO_2, GaN) bombarded by gasses: a) Ar, b) O_2 c) Xe.

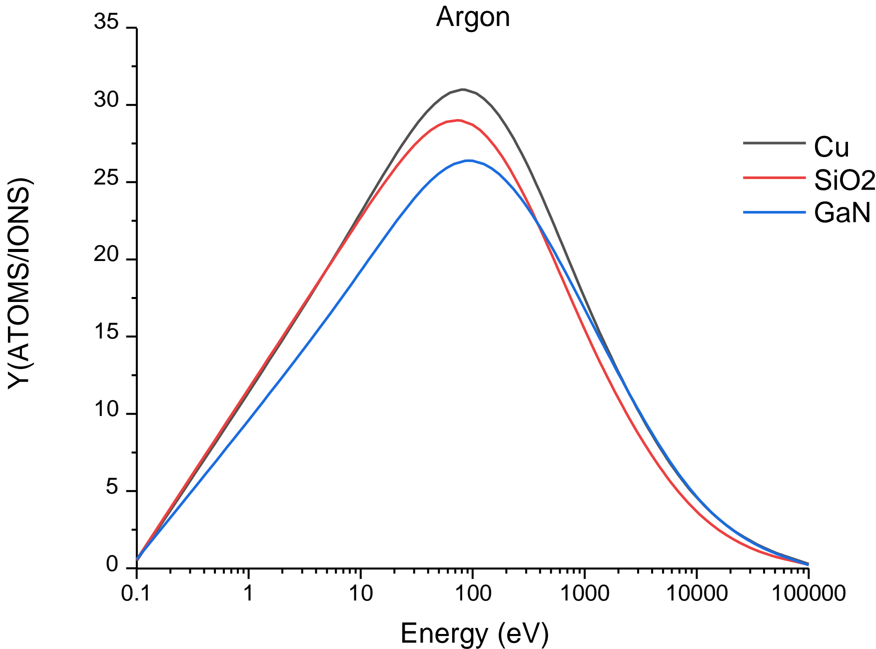
The curves above show the sputtering yield variation as the incidence angles increase with the three different gases (argon, oxygen, and xenon) for each material (Cu, SiO_2, and GaN).

In all cases, the sputtering yield increases as the angle of incidence increases. Before declining, the sputtering yield reaches a maximum incidence angle of approximately 80° for SiO_2 and GaN and approximately 75° for Cu.

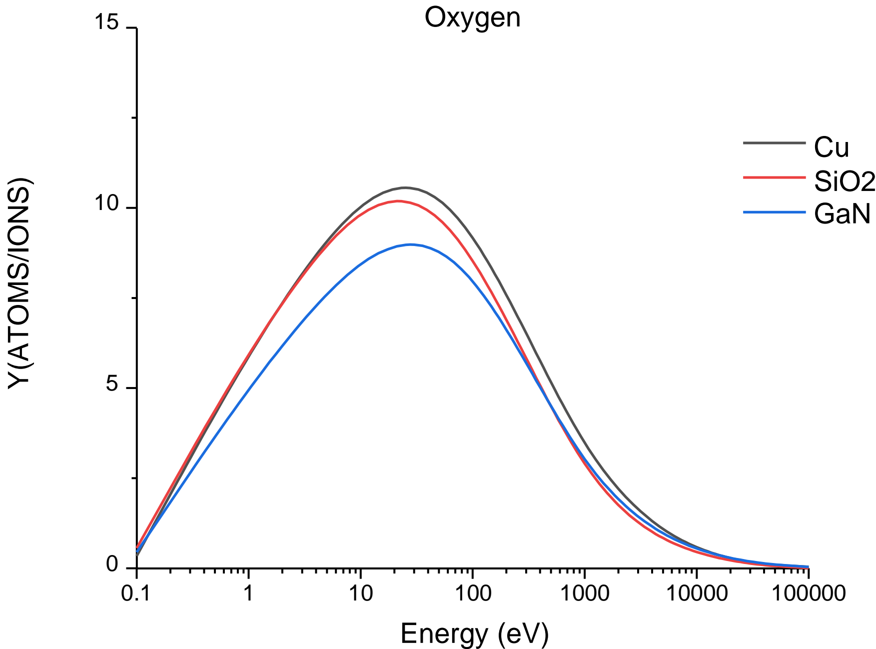
III.9. Sputtering yield as function of the energy

In this part, we chose the optimal incidence angle from the previous calculation and started the energy variation.

a)



b)



c)

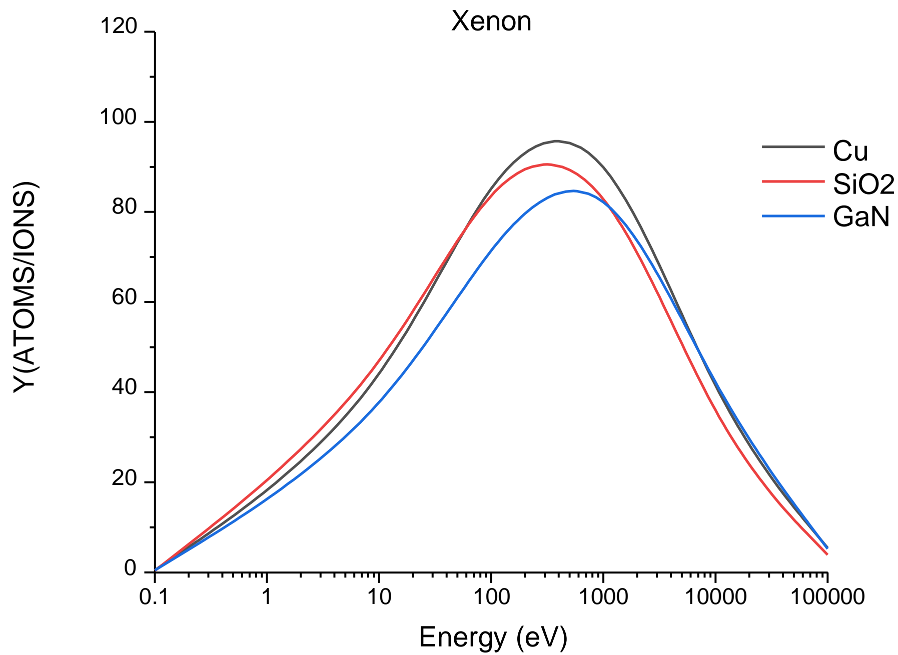


Figure III.02: Sputtering yield as function of incidence energy for materials (Cu, SiO_2, GaN) bombarded by gasses: a) Ar, b) O_2 c) Xe.

The results with the Monte Carlo simulation SRIM of the sputtering yield for the materials (Cu, SiO_2, GaN) bombarded by the gases (Argon, Oxygen, Xenon) are shown in the curves above.

It can be seen that the sputtering yield obtained with xenon (Xe) appears to be relatively high when compared to those obtained with argon (Ar) and oxygen (O_2).

Furthermore, the yield obtained by the energy variation increases to a specific value until it decreases because incident particles enter deeply into the target and, hence, the particles are not removed appropriately.

III.10. Simulation results obtained from the SRIM simulation

The maximum energies and incidence angles for all materials (Cu, SiO_2, GaN) subjected to ion beam bombardment by gasses (Ar, O_2, Xe) are shown in the table below:

		Copper Cu	Silicon dioxide SiO_2	Gallium Nitride GaN
ARGON	E_{max} (KeV)	100	100	100
	θ_{max}(degree)	75°	80°	80°
	Y_{max} (Atoms/ions)	36.66	33.82	30.75
OXYGEN	E_{max} (KeV)	10	10	10
	θ_{max}(degree)	75°	80°	80°
	Y_{max} (Atoms/ions)	11.69	11.59	9.66
XENON	E_{max} (KeV)	1000	1000	1000
	θ_{max}(degree)	75°	80°	80°
	Y_{max} (Atoms/ions)	102.69	93.81	94.83

Table III.01: Energies, angles and maximum efficiency obtained by SRIM

III.11. Conclusion

In the first simulation, we introduced the SRIM, which has recently become the most popular sputtering process, to understand the effect of energy and the incidence angles on the sputtering yield calculation. According to these few results of simulations, we can conclude:

When we apply the perfect incidence angle named θmax and reach a specific energy value named Emax, we will get the best result for the sputtering yield, which is conducted to the maximum value named Ymax. Those values of energy and incidence angle help us obtain a maximum of ejected particles and, hence, a perfect film at the end.

We notice that the obtained angle of bombardment is not the same with the application of the same gas because it changes depending on the strength of the link between the atoms, which is why copper is 75 ° and the other materials 80 °.

III.12. Simulation of Metal transfer (SIMTRA)

SIMTRA (Simulation of Metal Transfer) is a test particle Monte Carlo code developed to simulate the metal flux during magnetron sputtering. Using predefined surfaces, the user can create a geometrical representation of experimental setup, which is visualized by the graphical user interface. The movement of several particles, generated with initial conditions (position, energy, and direction) from a target surface, is tracked until they cross one of the defined surfaces.

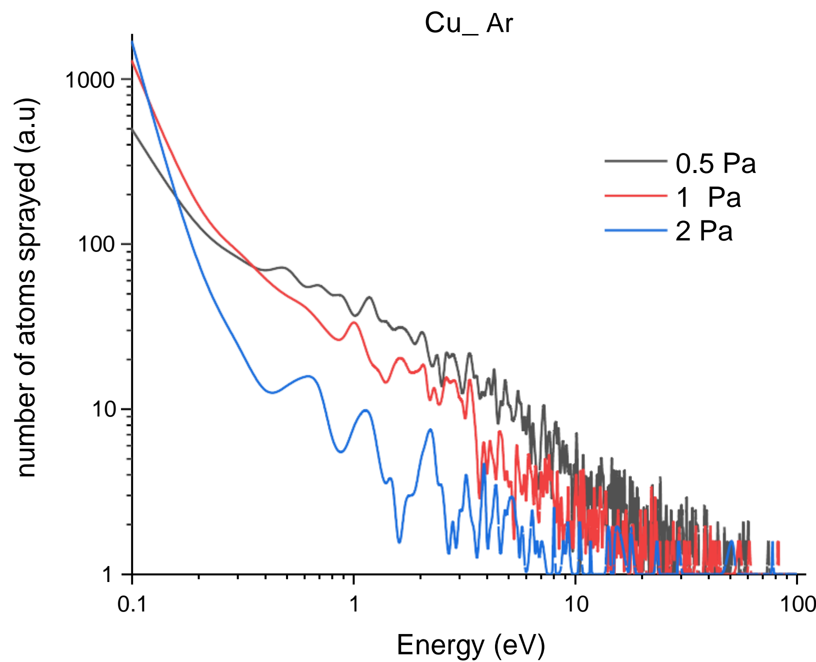
Several options are available to customize the particle generation, and transport through the gas phase, such as custom racetracks, initial energy, angular distributions, in-or exclude gas motion and diffusion, and several interaction potentials. [53]

III.13. The effect of pressure variation on the number of particles arriving in the substrate

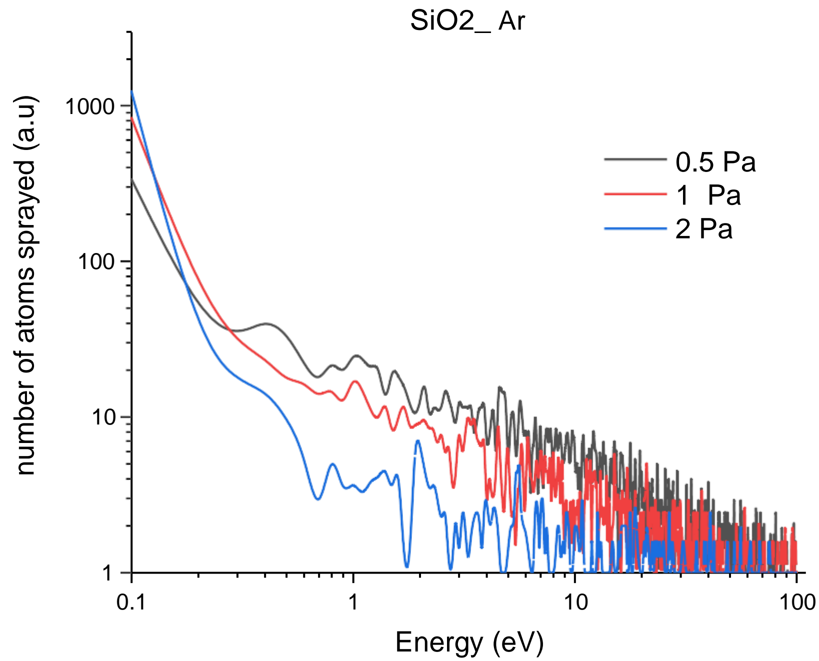
The curves below show the results of the SIMTRA (Simulation of Metal Transfer) simulation. In this first part of the simulation, we fixed the temperature at 300 k and changed the pressure (0.5, 1, 2 Pa), intending to understand the influence of the pressure on the arriving in the substrate atoms with the same gases (Argon, Oxygen, Xenon) and materials (Cu, SiO_2, GaN) that we used in the SRIM simulation.

- **Argon**

a)



b)



c)

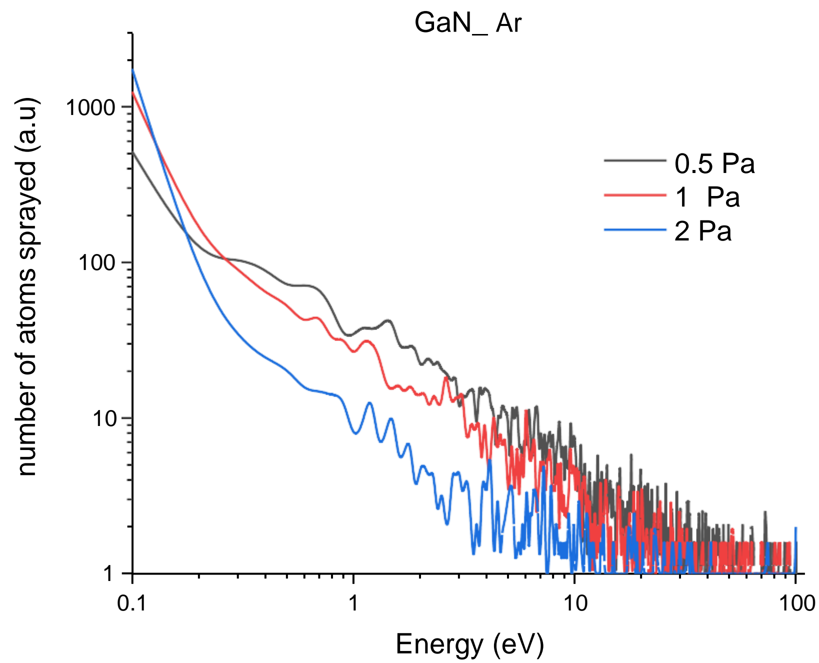
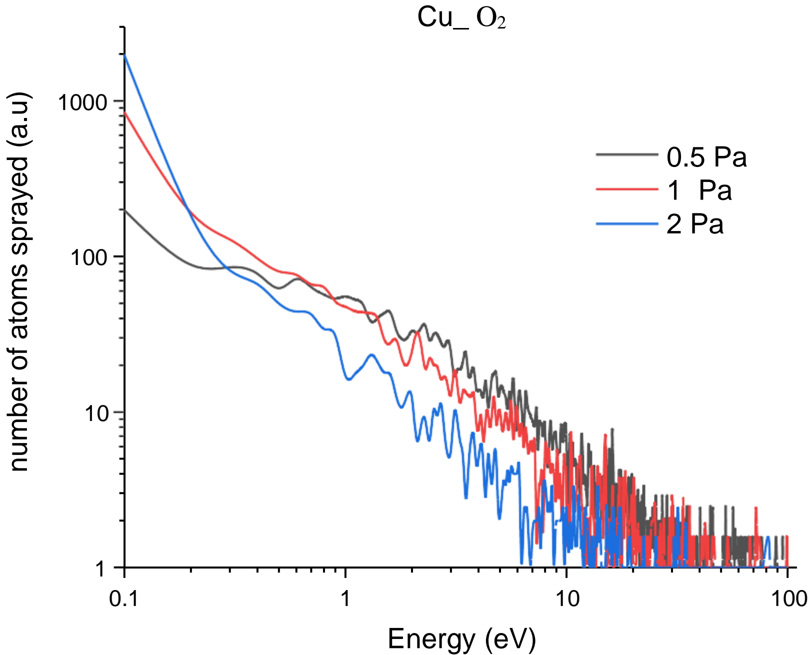


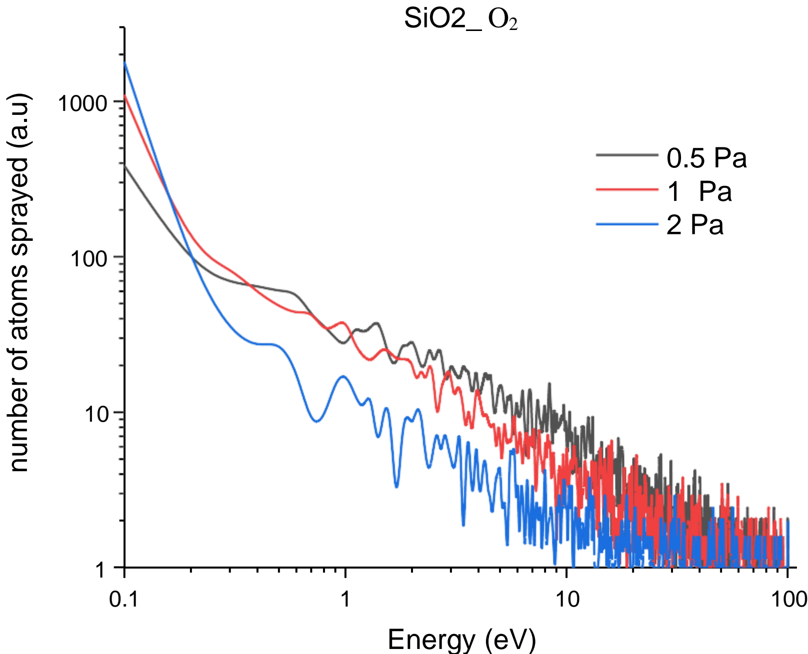
Figure III.03: Depending on the pressure in the chamber, the energy distribution of: a) Cu,b)SiO_2 ,c) GaN, arrives at the substrate levels and is bombarded by Ar ion beam.

- **Oxygen**

a)



b)



c)

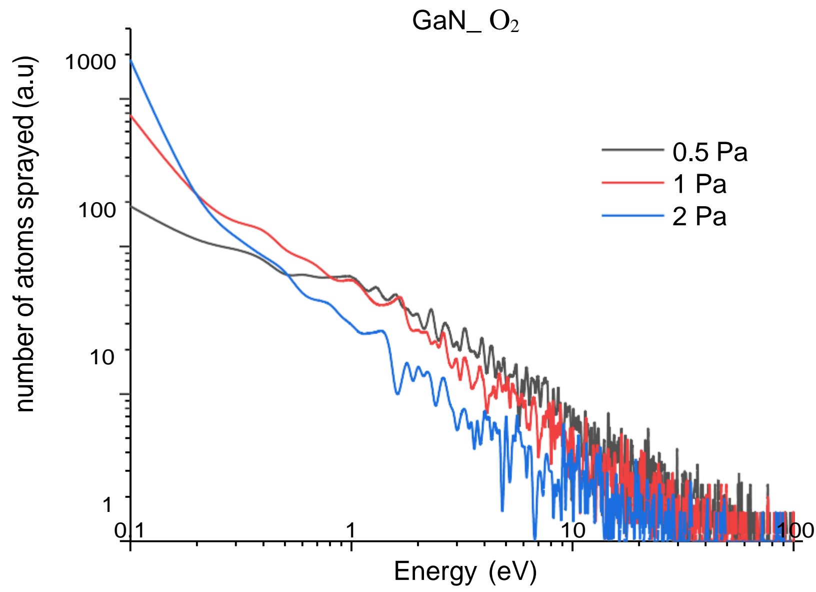
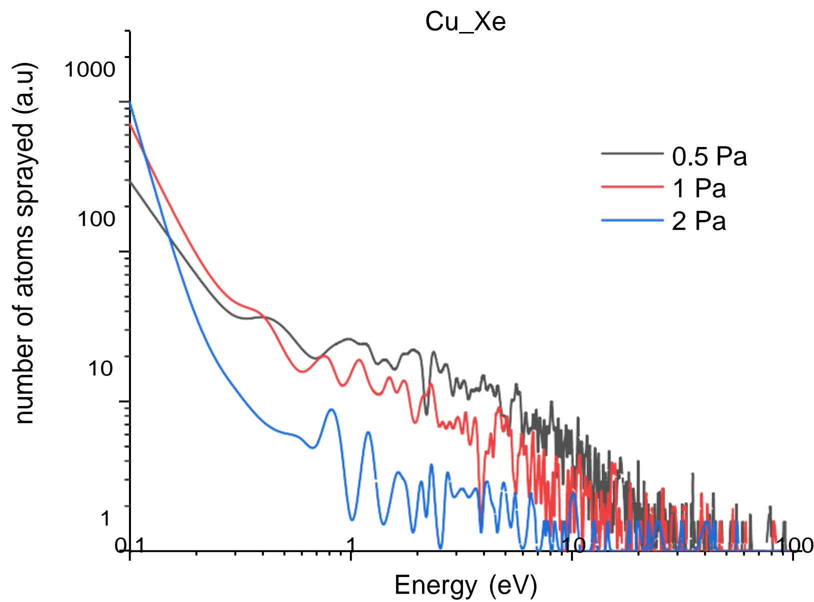


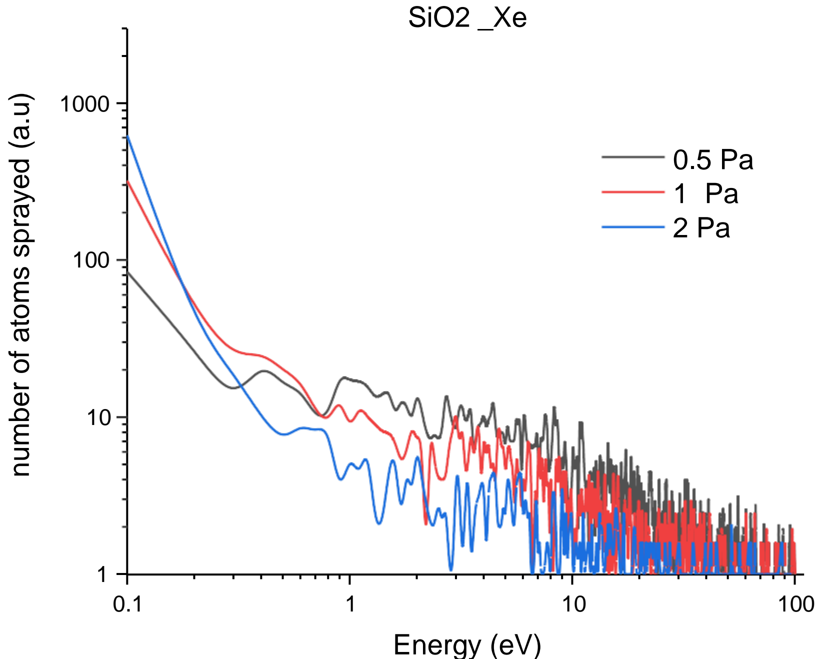
Figure III.04: Depending on the pressure in the chamber, the energy distribution of: a) Cu ,b) SiO_2 ,c) GaN, arrives at the substrate levels and is bombarded by an O_2 ion beam.

- **Xenon**

a)



b)



c)

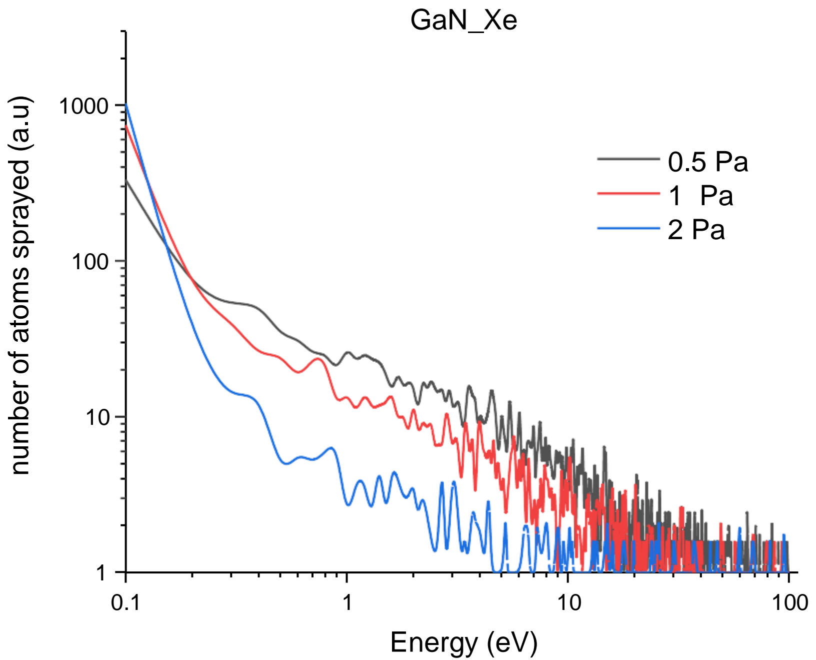


Figure III.05: Depending on the pressure in the chamber, the energy distribution of: a) Cu,b) SiO_2 ,c) GaN, arrives at the substrate levels and is bombarded by an Xe ion beam.

III.14. The number of atoms arriving on the substrate depends on the applied pressure.

		Copper Cu	Silicon dioxide SiO_2	Gallium Nitride GaN
ARGON	0.5 Pa	3100	3316	3483
	1 Pa	2985	2819	3332
	2 Pa	2283	2234	2677
OXYGEN	0.5 Pa	3013	3293	3245
	1 Pa	2974	3084	3207
	2 Pa	2895	2400	3185
XENON	0.5 Pa	3312	3738	3707
	1 Pa	2992	3189	3288
	2 Pa	2435	2623	2684

Table III. 02: total number of atoms sprayed on the substrate depending to the pressure

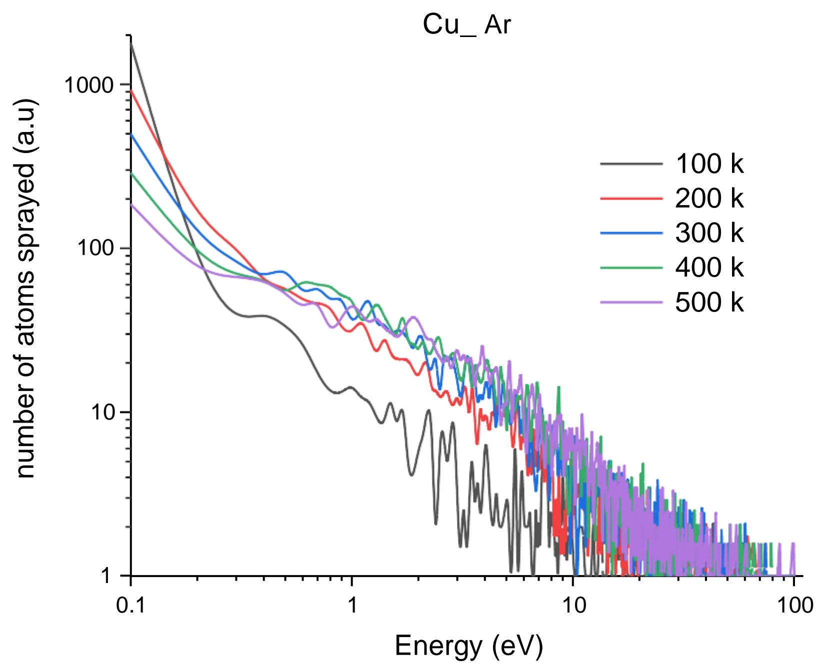
We can see from the curves and table above extracted from the simulation that the number of atoms reaching the substrate level is significant with the application of pressure of around 0.5 Pa. As the pressure rises, it will affect the process, and the number of atoms will dramatically decrease.

III.15. The effect of temperature variation on the number of particles arriving at the substrate

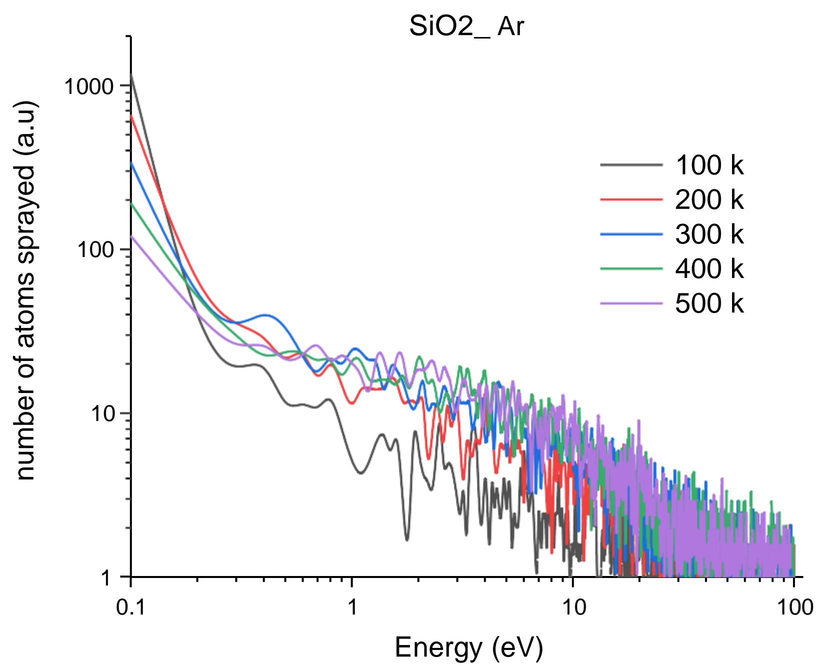
In this second part of the simulation, we fixed the pressure at 0.5 Pa (shown in the previous simulation as an good value), and we varied the temperature (100, 200, 300, 400, and 500 ° k) to know the effect of the temperature on the transportation of the ejected particles with the use of the same materials and gases.

- **Argon**

a)



b)



c)

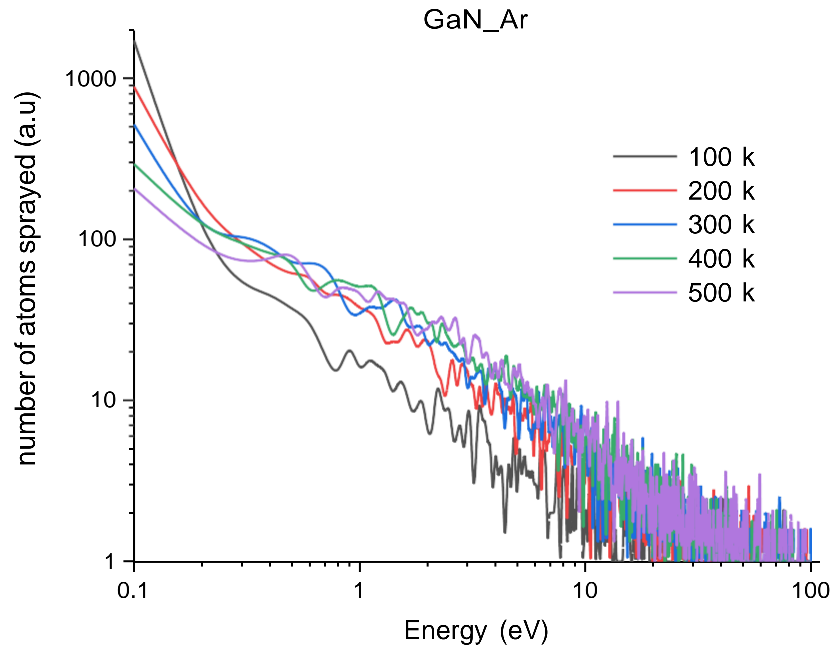
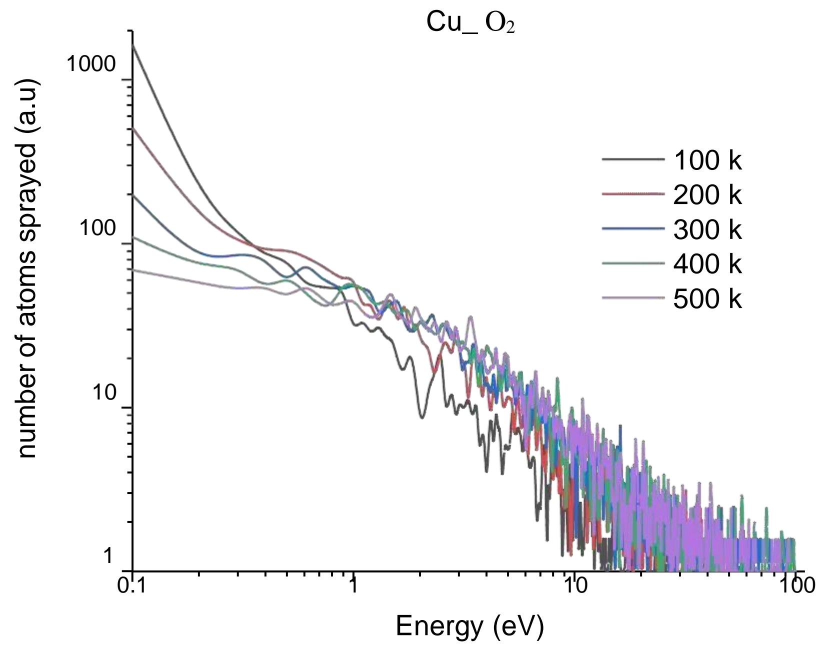


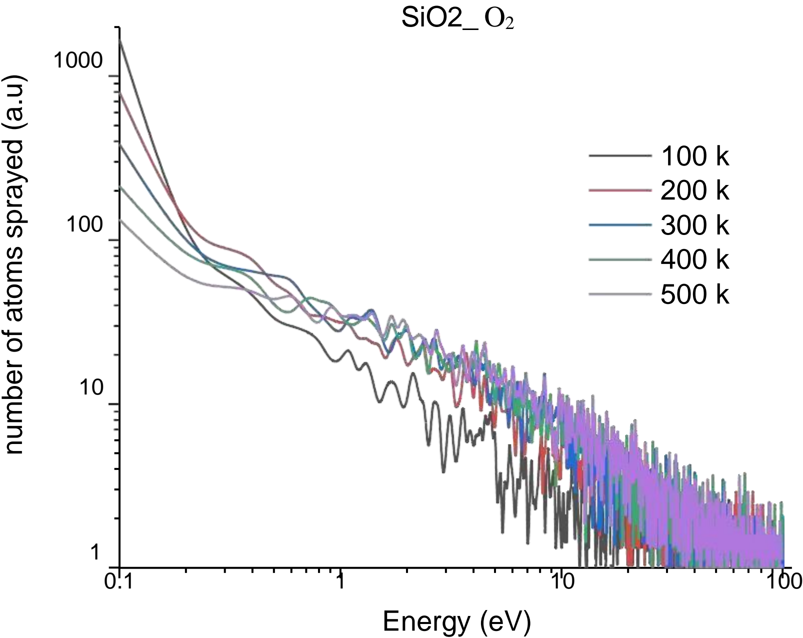
Figure III.06: Depending on the temperature in the chamber, the energy distribution of : a) Cu , b) SiO_2 ,c) GaN, arrives at the substrate levels and is bombarded by an Ar ion beam.

- **Oxygen**

a)



b)



c)

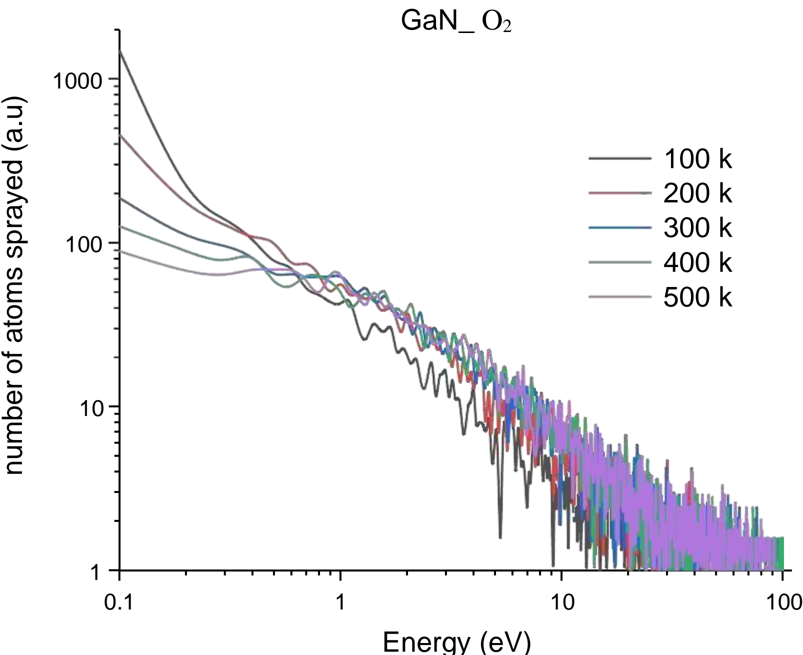
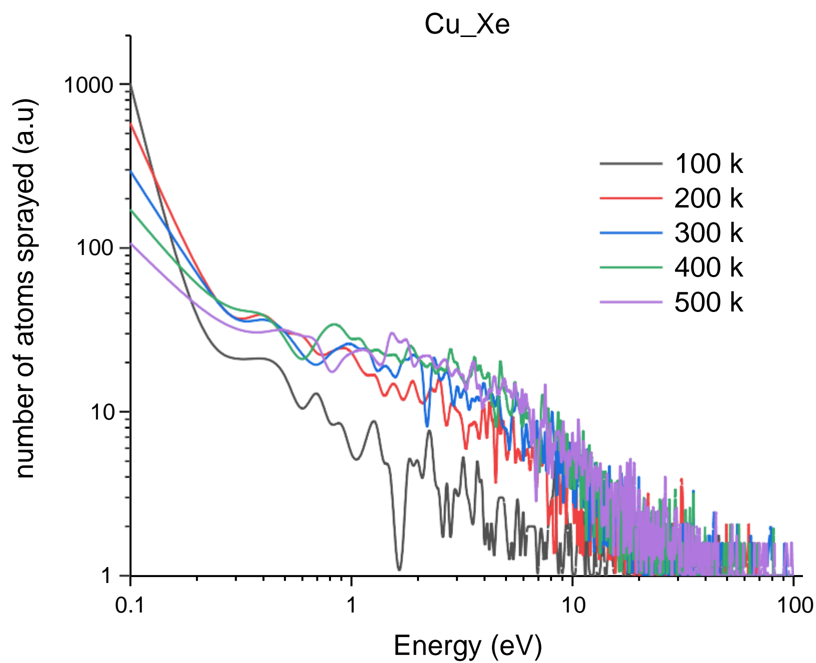


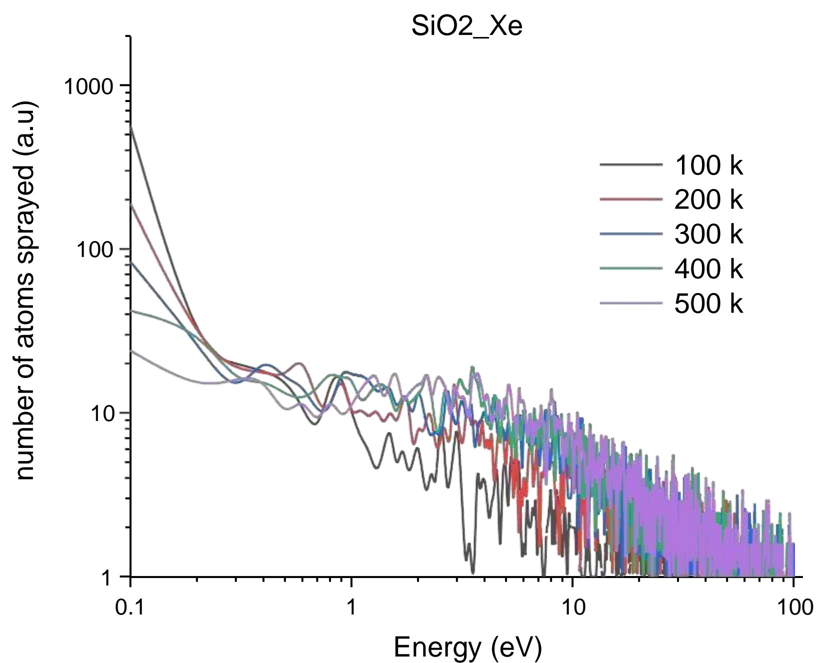
Figure III.07: Depending on the temperature in the chamber, the energy distribution of : a) Cu , b) SiO_2 ,c) GaN, arrives at the substrate levels and is bombarded by an O_2 ion beam.

- **Xenon**

a)



b)



c)

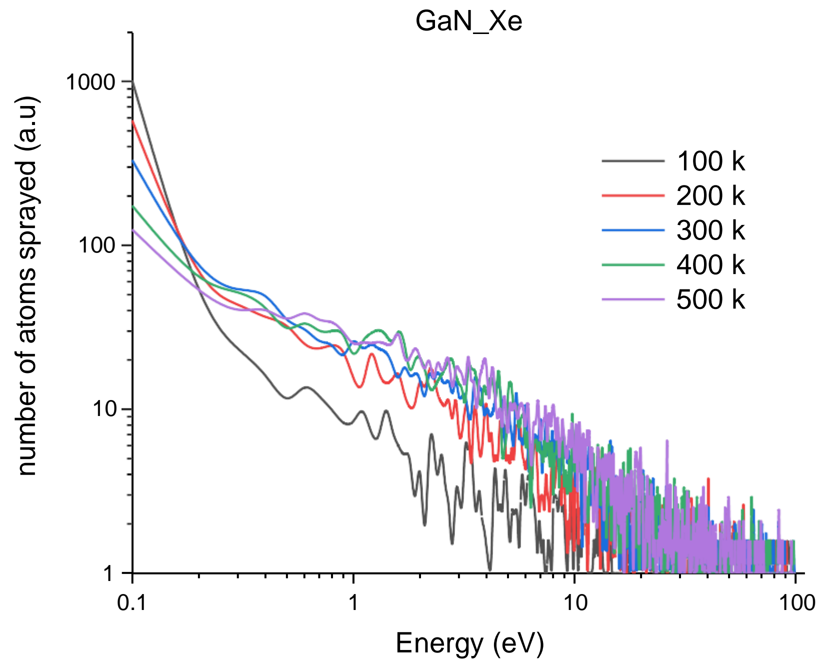


Figure III.08: Depending on the temperature in the chamber, the energy distribution of: a) Cu , b) SiO_2 , c) GaN, arrives at the substrate levels and is bombarded by an Xe ion beam.

III.16. The number of atoms sprayed on the substrate according to the temperature

		Copper Cu	Silicon dioxide SiO_2	Gallium Nitride GaN
ARGON	100 k	2767	2542	3113
	300 k	3100	3316	3483
	500 k	3120	3455	3676
OXYGEN	100 k	2203	2522	2697
	300 k	2225	2993	2772
	500 k	2547	3135	3445
XENON	100 k	2810	2978	3171
	300 k	3312	3438	3707
	500 k	3478	3602	3960

Table III. 03: total number of atoms sprayed on the substrate depending to the temperature.

We can see from the curves and the table above that the number of particles reaching the substrate at 100° k is few compared to other temperatures (200°,300°,400°,500° k), as the temperature rises so the number of particles reaching the substrate increases.

The curves show that as the temperature rises, many of the particles reach the substrate with high energy, which will affect the morphology of the substrate.

The effect of temperature on the bonding of the target atoms weakens that bond and makes it easier to break when we bombard them with one of the gases, resulting in an increase in the number of particles reaching the substrate.

III.17. 3D visualization of the ejected atoms reaching the substrate level.

The figures below demonstrate the impact of the applied temperature on the thin film morphology with the application of argon as the vacuum chamber gas and three materials (Cu, SiO_2, and GaN) as targets.

- **Copper (Cu)**

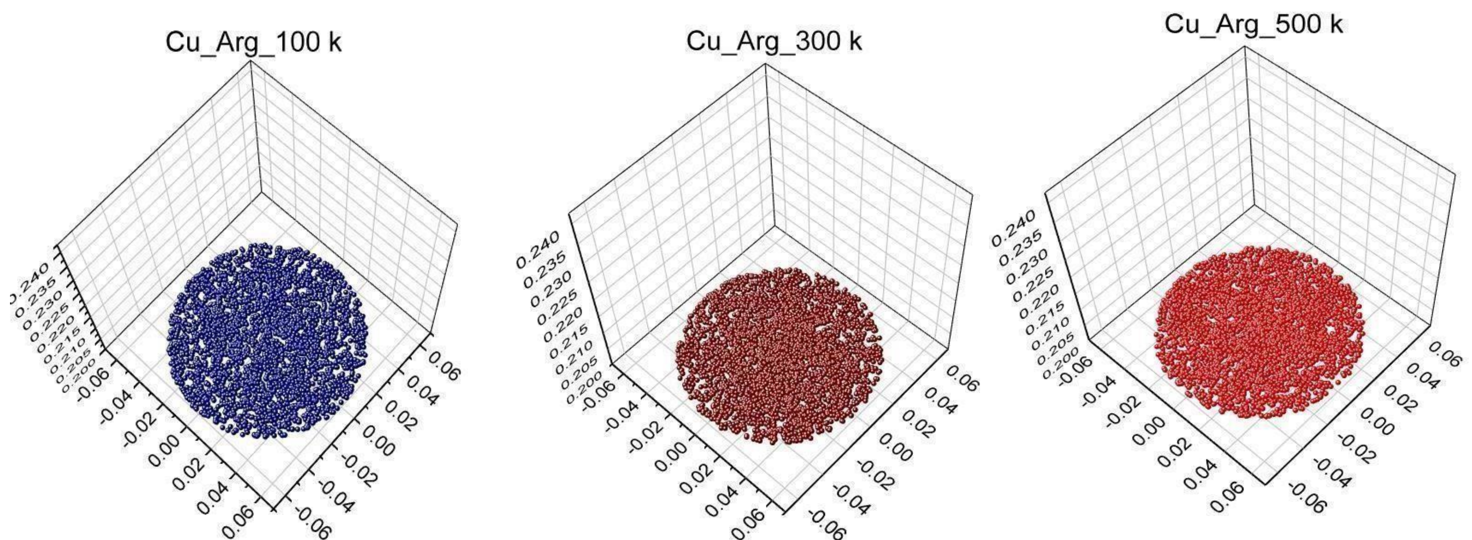


Figure III.09: The location of Cu atoms bombarded with Ar on the substrate according on the variation of temperature of the chambre.

- **Silicon dioxide (SiO_2)**

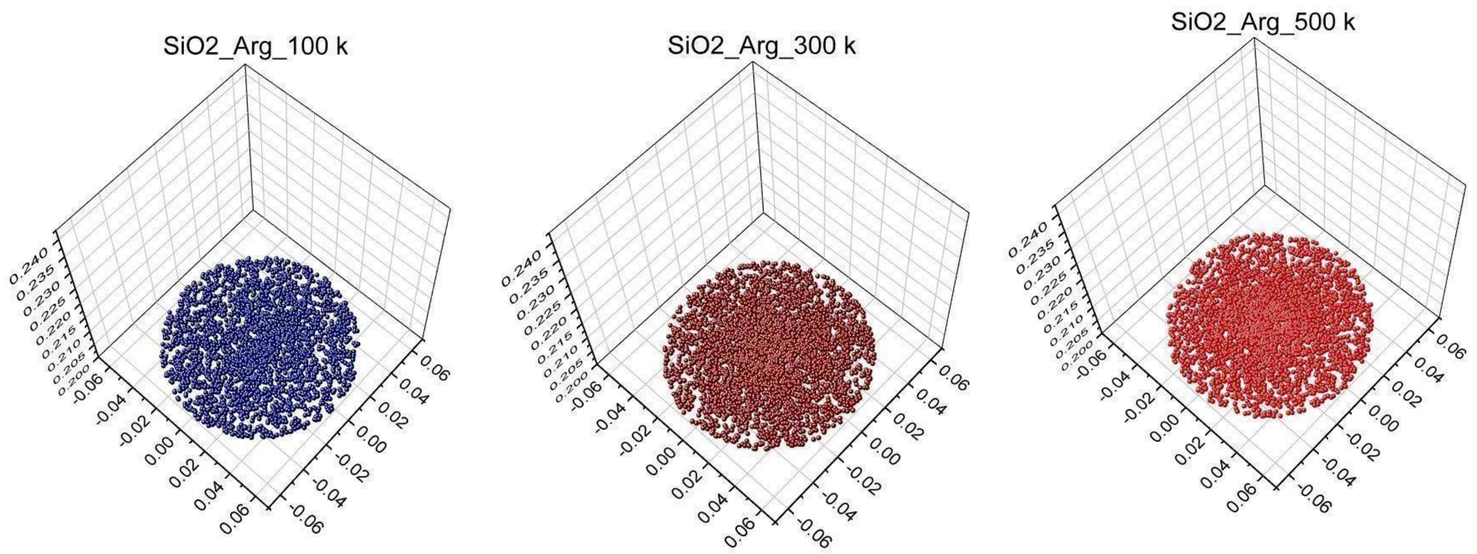


Figure III.10: The location of SiO_2 atoms bombarded with Argon on the substrate according on the variation of temperature of the chambre.

- **Gallium Nitride (GaN)**

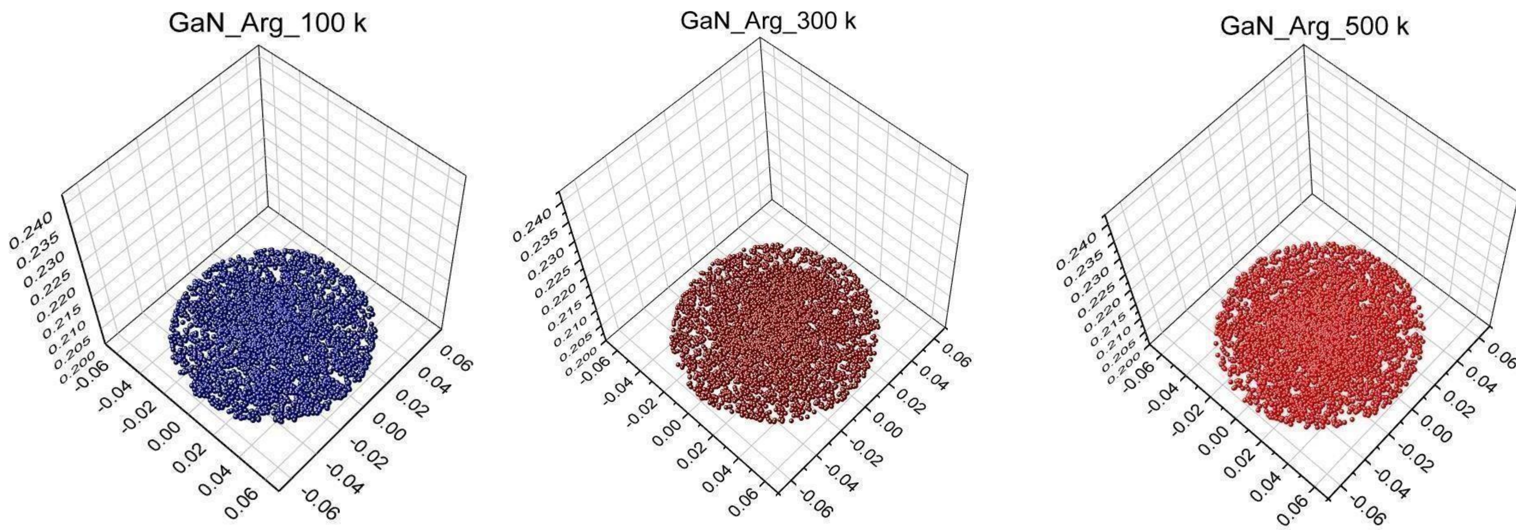


Figure III.11: The location of GaN atoms bombarded with Argon on the substrate according on the variation of temperature of the chambre.

From the results extracted from this part of simulation (3D visualization of the ejected atoms reaching the substrate level) we can see that, the number of atoms reaching the substrate level is significant with the application of temperature of around 500° k compared to 100° k and 300° k, this is confirmation for the previous part.

So, the number of atoms ejected that land on the substrate level increases, and their location on the substrate constructs a perfect thin film shape when the temperature rises.

III.18. Conclusion

Based on the results obtained from the SIMTRA simulation of the variation in pressure and temperature and their effects on the sputtering process and thin film quality, we can conclude that the number of atoms ejected from the target increases with a decrease in pressure and an increase in temperature because the bond between the atoms weakens. It becomes easy to crack, but the materials and gas have limits to withstand high pressure and even high temperatures, so if we exceed that value, the materials or gas will burn due to high heat or deteriorate due to high pressure.

General Conclusion

General Conclusion

With the development of nanotechnology, interest in the research and production of thin materials (semiconductors, conductors or insulators) that are efficient and inexpensive is increasing day by day. The microstructures of these films are the object of our interest to serve the industry by taking into account the different parameters that influence the morphology of these films.

The sputtering deposition technique aims to produce high-quality coated film with desirable properties for diverse applications in instruments and devices.

The interest of this work is the deposition of thin layers by sputtering of semiconductors (gallium nitride) and conductor (copper) and silicon dioxide as an insulator. to study the phenomenon from the start, simulations with Monte Carlo methods (SRIM and SIMTRA) were used to calculate the sputtered yield Y according to the nature of the gas and the materials used, the energies and the angles of incidence sconces; as well as the number of particles sprayed arriving at the substrate and their energies as a function of temperature and pressure, very important parameters in optimizing the yield of the thin layers deposited.

The results obtained by the SRIM simulation show:

1. By varying the energies of the plasma ions, the maximum sputtering yield for the ejected particles from the materials (Cu, SiO_2, and GaN) is achieved (with different values) at an angle of incidence of approximately around 80 and 75 degrees. The figures look almost the same. They start with low yield values initially due to the ion energy threshold that has not yet been reached and after a maximum decrease due to penetration or the target's exhaustion.
2. From these results, it can be seen that the yield inferred from the xenon (Xe) ions is quite large compared to Argon (Ar), Oxygen (O_2), but as the xenon gas is very expensive and rare, sputtering for oxygen is very low, the Argon gas is the dominant gas.

The results obtained by the SIMTRA simulation show that:

1. The maximum number of atoms arriving at the substrate with low energies ensures, in the end, uniform film deposition and contributes to the creation of thin films with the desired morphology.
2. When bombarded by the different gas ion beam, many atoms can be reached on the substrate.

3. High pressure leads to a decrease in the number of atoms arrived on the substrate, the wrong chose of this parameter will affect the thin film morphology.
4. High temperature leads to an increase in the number of atoms arrived on the substrate, but also wrong chose of this parameter will affect on the target and the thin film morphology and also will affect on the substrate.

Moreover, our study finally showed its effectiveness and its contribution to the development in the various industries using the thin layer for the realization of many tools essential to our daily life.

Bibliographic references

References :

[1] A. Bouazza and A. Settaouti, ‘’Etude et simulation de l’influence de divers paramètressur le processus de pulvérisation d’atomes dans un plasma’’, doctoral thesis, université USTO-Oran 2017

[2] Abdelkader Bouazza and Youcef Belhadji, Salah Eddine Chouaib Refas, ‘3D sputtering simulations of the CZTS, Si and CIGS thin films using Monte-Carlo method ‘’ , October,2021

[3]L. Baghriche,” élaboration et caractérisation des couche minces d’oxyde de zinc et sulfure de zinc preparess par spray ultrasonique”,doctoral thesis, Fereres Mentouri university,2015

[4] Dr. Samira Naghdi,” Thin-films: definition, deposition techniques, and applications” webinar: Bu-Ali Sina University, February 22, 2021.

[5] Jack J. VanGemert,” The Development of a thin film sputter deposition system using a novel hidden anode ion source and motion control”, master thesis , Colorado University,2020

[6]S. Hariech, ” Elaboration et caractérisation des couches minces de sulfure de cadmium (CdS) préparées par bain chimique (CBD) ” magister’s memory, University Mentouri- Constantine ,2009.

[7] Anuja.E,” Preparation and effect of complexing agents on fecus2 and zncus2 thin films by chemical bath deposition method for photo response applications”, Anna University,2019.

[8] Chen, Wei ; Zhong, Jialin; Li, Junzi; Saxena, Nitin; Kreuzer, Lucas P.; Liu, Haochen; Song, Lin; Su, Bo; Yang, Dan; Wang, Kun; Schlipf, Johannes (2 May 2019). "Structure and Charge Carrier Dynamics in Colloidal PbS Quantum Dot Solids". The Journal of Physical Chemistry Letters.

[9] Zou, Yuqin; Guo, Renjun; Buyruk, Ali; Chen, Wei; Xiao, Tianxiao; Yin, Shanshan; Jiang, Xinyu; Kreuzer, Lucas P.; Mu, Cheng; Ameri, Tayebeh; Schwartzkopf, Matthias (25 November 2020). "Sodium Dodecylbenzene Sulfonate Interface Modification of Methylammonium Lead Iodide for Surface Passivation of Perovskite Solar Cells". ACS Applied Materials & Interfaces.

[10] Chen, Wei; Guo, Renjun; Tang, Haodong; Wienhold, Kerstin S.; Li, Nian; Jiang, Zhengyan; Tang, Jun; Jiang, Xinyu; Kreuzer, Lucas P.; Liu, Haochen; Schwartzkopf, Matthias (2021). "Operando structure degradation study of PbS quantum dot solar cells". Energy & Environmental Science.

[11] Salah Yahaoui, ” L’effet de la molarité des différentes sources d’étain sur les propriétés des couches minces d’oxyde d’étain SnO2 élaborées par Spray Ultrasonique”, magister’s memory, Université Mohamed Khider – Biskra, 2014.

[12] Lamri Sabah, ”Elaboration et Caractérisation des Couches Minces de ZnO Dopées par l’Indium”, magister’s memory in Physics, Université Mohamed Khider – Biskra, 2012

[13] S. Guitouni,‘’Corrélation entre les propriétés thermo physiques des gouttelettes et les propriétés des couches minces déposées par le procédé spray’’, magister’s memory, Université de Constantine, 2010.

[14] Stergios Logothetidis,” Nanostructured Materials and Their Applications” p,105, 2012.

[15] Hartmut Frey and Hamid R. Khan,”Handbook of Thin Film Technology”. (Berlin, Heidelberg: Springer Berlin/Heidelberg, Berlin, Heidelberg), 2015.

[16] Hans K. Pulker, (Berlin, Heidelberg: Springer Berlin Heidelberg: Berlin, Heidelberg), pp 353-369.

[17] John R. Arthur,” In Specimen Handling, Preparation, and Treatments in Surface Characterization”, ed. Alvin W. Czanderna, Powell Cedric J., Madey Theodore E., Hercules David M. and Yates John T. (Springer US: Boston, MA, 1998), pp. 239-293.

[18] Saba Farooq, Zainab Ngaini, Sana Farooq, “Chapter 2- Manufacturing and design of smart polymer composites “in Smart Polymer Nanocomposites, 2021

[19] Fatima Khelfaoui, “Etude du mécanisme de croissance des couches a-Si :H élaborées par pulvérisation cathodique : interaction plasma-substrat”, doctoral thésis,2014.

[20] J. Tranchant, “ Etude de couches minces déposées par pulvérisation magnétron post-ionisée pour l’ingénierie de contraintes – cas du mocr et de nano-canaux de carbone “, doctoral thesis, université de Nantes, 2007.

[21] Habiba Benamra, “ L’effet de la température du substrat et de la molarité sur les propriétés des couches minces de sulfure de zinc déposées par spray ultrasonique“ , magister’s memory, Université Mohamed Kheider-Biskra ,2013.

[22] M. C. Rao, M. S. Shekhawat, “A brief survey on basic properties of thin films for device application “,2013

[23] Alain Chovet, Pascal Masson“cours de : physique des semi- conducteurs “, Ecole polytechnique Universitaire de Marseille,2004/2005.

[24] Donald M. Mattox in “Handbook of Physical Vapor Deposition (PVD) Processing “, ISBN 0-8155-1422-0, Noyes Publications, Westwood, NJ (1998)

[25] K. L. Choy, “Chemical vapor deposition of coatings, Progress in Materials Science“, vol. 48,57-170 ,2003.

[26] Klaus-Hermann Dahmen, in “Encyclopedia of Physical Science and Technology (Third Edition) “, 2003.

[27] B. Smith, “The difference between physical vapor deposition and chemical vapor deposition“,2018.

[28]N.Selvakumar, H.C.Barshilia, “ Review of physical vapor deposited PVD spectrally selective coatings for mid-and high temperature solar thermal applications“,2012

[29] D. Mattox, “Hand book of physical vapor deposition processing “,2010, p.29.

[30] Tahir Iqbal Awan,Almas Bashir,Aqsa Tehseen , ‘‘ Chapter 3 - Interfaces and surfaces ‘‘ ,in Chemistry of Nanomaterials, 2020

[31] Z. Liu, “chapter 4: Management and Control of Corrosion “, in Shreir's Corrosion, 2010.

[32] K. Ouali, ‘’Etude des propriétés structurales et électriques des couches minces de FexCo1-x (x massif = 0, 0.25, 0.5, 0.75 et 1) élaborées par évaporation sous vide’’, université de M’sila, mémoire de master, (2014).

[33] Mustapha Zaghrioui,“ Synthèse par pulvérisation et caractérisation de couches minces de $NdNiO_3$ .Etude de la transition metal-isolait par spectrometrie Raman’’, doctoral thesis,2000

[34] Abdelkader Bouazza and Abderrahmane Settaouti, “Understanding the contribution of energy and angular distribution in the morphology of thin films using Monte Carlo simulation “, 2018

[35] Matt Hughes - President - Semicore Equipment,’’ what is DC sputtering? “, SEMICORE Equipment, 2016

[36] S. Audisio, M. Caillet, A. Galerie & H. Mazielle, ‘’Revêtement et traitements desurface, Fonctionnalités, durabilité, procèes’’, Engineering techniques, 1999.

[37] Ioan Valentin Tudose, Florin Comanescu, Petronela Pascariu, Stefan Bucur, Laurentiu Rusen, Felicia Iacomi, Emmanue Koudoumas, Mirela Petruta Suchea in ‘’ Chapter 2 - Chemical and physical methods for multifunctional nanostructured interface fabrication’’, 2019

[38] Mitsuo Iwase, Yoshihiko Hirai, in ‘’Functionally Graded Materials’’ , 1997.

[39] Neelesh K. Jain ,Mayur S. Sawant ,Sagar H. Nikam ,Suyog Jhavar in" Metal Deposition: Plasma-Based Processes" Department of Mechanical Engineering, Indian Institute of technology Indore, Indore, India, 2017

[40] Mohammad Reza Rashidian Vaziri, “Microscopic description of the thermalization process during pulsed laser deposition of aluminium in the presence of argon background gas”, Journal of Physics D Applied Physics. 2010.

References

[41] Mohammad Reza Rashidian Vaziri in, "Monte Carlo simulation of the subsurface growth mode during pulsed laser deposition". Journal of Applied Physics. 2011.

[42] Julissa Green in ‘’ What Are the Applications of Sputtering Targets?’’ website Stanford Advanced Materials, 31 july 2019

[43] Navid Mavaddat,Selam Ahderom, Valentina Tiporlini, Kamal Alameh ,in Deep Learning Techniques for Biomedical and Health Informatics, 2020 (Simulation of biomedical signals and images using Monte Carlo methods for training of deep learning networks).

[44] A.M. Johansen, in International Encyclopedia of Education (Third Edition), 2010.

[45] Julien I.E. Hoffman, in Basic Biostatistics for Medical and Biomedical Practitioners (Second Edition), 2019.

[46] D. P. Kroese and J. C. C. Chan. Statistical Modeling and Computation. Springer, New York, 2014.

[47] Hu, J., Ma, A., and Dinner, A. R. Monte Carlo simulations of biomolecules: The MC modulein Charmm. J. Comput. Chem. 27, 203–216, 2006.

[48] J. F. Ziegler, J. P. Biersack and U. Littmark, in" The Stopping and Range of Ions in Solids", Pergamon Press, New York, 1985.

[49] Technology note, ‘’Magetron sputtering’’ in Materials Science, INC. Vacuum & thin films.2014.

[50] Abdelkader Bouazza and Abderrahmane Settaouti in,’’ Study and simulation of the sputtering process of material layers in plasma’’, 2016

[51] Ahcene SIAD in "Etude numérique et expérimentale de la croissance de couches minces déposées par pulvérisation réactive ", Doctoral Thésis, 25 november 2016.

[52] Understanding the contribution of energy and angular distribution in the morphology of thin films using Monte Carlo simulation Abdelkader Bouazza and Abderrahmane Settaouti. DOI: 10.1515/mcma- 2016-, Received January 15, 2018; accepted ... 2018

[53] The metal flux from a rotating cylindrical magnetron: a Monte Carlo simulation. K. Van Aeken, S. Mahieu, D. Depla, Journal of Physics D.: Applied Physics 41 (2008) 205307

Abstract

Abstract

Thin films are a qualitative leap in the development and miniaturization of the electronic domain and the production of electronic components; one method used to produce these thin films is the sputtering. Atomic energy and angular distribution are the most effective indicators for improving spraying and thus deposition. The main objective of our work is to see the effects of other factors such as high pressure and high temperature, which have an important effect in the formation of thin films, and we used three gases in our work to see which one gives us a better result, as well as three materials (copper (conductor), silicon dioxide (insulator), gallium nitride (semiconductor)), and we used simulation programs in our work SRIM and SIMTRA.

Résume

Les couches minces constituent un saut qualitatif dans le développement et la miniaturisation du domaine électronique et la production de composants électroniques ; une méthode utilisée pour produire ces couches minces est la technique de pulvérisation cathodique. L'énergie atomique et la distribution angulaire sont les indicateurs les plus efficaces pour améliorer la pulvérisation et donc le dépôt. L'objectif principal de notre travail est de voir les effets d'autres facteurs tels que la haute pression et la haute température, qui ont un effet important dans la formation de couches minces, et nous avons utilisé trois gaz dans notre travail pour voir lequel nous donne un meilleur résultat, ainsi que trois matériaux (cuivre (conducteur), dioxyde de silicium (isolant), nitrure de gallium (semi-conducteur)), et nous avons utilisé des programmes de simulation dans nos travaux SRIM et SIMTRA.

ملخص

تشكل الاغشية الرقيقة نقلة نوعية في تطوير وتصغير الالكترونيات وإنتاج المكونات الإلكترونية؛ إحدى الطرق المستخدمة لإنتاج هذه الطبقات الرقيقة هي تقنية الرش. تعد الطاقة الذرية والتوزيع الزاوي من أكثر المؤشرات فعالية لتحسين الرش وبالتالي الترسب. الهدف الأساسي من عملنا هو رؤية تأثيرات العوامل الأخرى مثل الضغط العالي ودرجة الحرارة المرتفعة والتي لها تأثير قوي في تكوين الأغشية الرقيقة، واستخدمنا في دراستنا ثلاث غازات لنرى أيها يعطينا نتيجة أفضل، بالإضافة إلى ثلاث مواد (نحاس (موصل)، وثاني أكسيد السيليكون (عازل)، ونتريد الغاليوم (أشباه الموصلات))، واستخدمنا برامج محاكاة في عملنا SRIM وSIMTRA.