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**Efficiency of adjusting deposition parameters on
growth of thin film materials by the application of
electrical discharge**

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Dedication

To my wonderful parent Boudali Sliman and Bachir Bouaidjra Badra, brother Abdellah, sister Zagdani Naziha and dear Rehioui Rania Sarah, I want to express my heartfelt appreciation for your unwavering love, support, and encouragement. each of you has played an invaluable role in my journey, and I am forever grateful for the memories we have created together.

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Thank you for believing in me and being by my side through thick and thin. With all my love.

[Halima Farah].



Dedication

This study is dedicated to my beloved parents, who have been our inspiration and guidance and strengthened us when we thought of giving up. They continually provide their moral, spiritual, emotional, and financial support.

Special dedication to my dear father boumaza benouda, who left us 13 years ago and could not see my work. May Allah rest his soul, for my dear mother benameur hadja , who always pushed and motivated me in my studies and to my beloved sisters boumaza kenza and boumaza fatiha And My little nephew Adem

Thank you for believing in me and being by my side through thick and thin. With all my love.

[BOUMAZA AMINA].

List of Abrogation

MBE :molecule beam epitaxial

ALD :Atomic layer deposition

PVD: Physical vapor deposition

CVD: Chemical vapor deposition

SRIM : Stop and range of atoms Matter

SIMTRA: Simulation of material transport

TFT: Thin film transistors

ICs: Integrated circuits

MOS: Metal oxide semiconductor

DLC: Diamond-like carbon

SILAR: Successive ionic layer adsorption and reaction

DC : Direct current

RF: Radio_Frequency

TCVP : Thermal chemical vapor deposition

LDM : liquid deposition modeling

FMD : Fused deposition modeling

CBE: Chemical beam epitaxy

AC: Alternative current

TRIM: Transport of Ions in matter

ITO: Indium tin oxide

List of Figures

FIGURE I.1 THIN FILM DEPOSITION PROCESSES	7
FIGURE I.2 SCHEMATIC ILLUSTRATION OF THE PHYSICAL VAPOR DEPOSITION PROCESS.....	8
FIGURE I.3 SHEMATIC OF CVD PROCESS.....	9
FIGURE I.4 THE SCHEMATIC ILLUSTRATION FOR PLASMONIC-METAMATERIAL-BASED GRAPHENE/TIO ₂ /AG THIN FILM.....	11
FIGURE I.5 THE THREE POSSIBLE GROWTH MODES	17
FIGURE I.6 DIAGRAM OF THE NUCLEATION OF LAYERS.....	18
FIGURE I.7 DIAGRAM REPRESENTING COALESCENCE.....	18
FIGURE I.8 GROWTH OF THIN FILMS	19
FIGURE I.9 STEPS OF THIN FILMS	19
FIGURE II.1 SCHEMATIC DRAWING OF TWO CONVENTIONAL PVD PROCESSES: (A) SPUTTERING (B) EVAPORATION.....	31
FIGURE II.2 THE FOUR FUNDAMENTAL STATES OF MATTER	34
FIGURE II.3 VACUUM CHAMBERS FOR THE DEPOSITION OF THIN FILM.	35
FIGURE II.4 THIN-FILM SUBSTRATES FOR MICROELECTRONICS	36
FIGURE II.5 SPUTTERING DEPOSITION	38
FIGURE II.6 A SCHEMATIC DRAWING OF THE BASIC MECHANISM OF SPUTTERING	39
FIGURE II.7 DIAGRAM OF THE DC MAGNETRON SPUTTERING PROCESS	40
FIGURE II.8 RF SPUTTERING PROCESSES	41
FIGURE II.9 SCHEMATICS OF REACTIVE SPUTTERING SYSTEM FOR COATING DEPOSITION.	42
FIGURE II.10 WORKING PRINCIPLE OF TRIODE-SPUTTERING DEPOSITION PROCESS.	43
FIGURE II.11 SCHEMATIC REPRESENTATION OF THE DIODE AND MAGNETRON SYSTEM.....	44
FIGURE II.12 PRINCIPLE OF MAGNETRON SPUTTERING	44
FIGURE III.1 MONTE CARLO PRINCIPAL DIAGRAM	47
FIGURE III.2 SRIM-2008 SOFTWARE INTERFACE.	52
FIGURE III.3 SIMTRA SOFTWARE INTERFACE, VERSION V2.1.1.RC.....	54

List of Figures

FIGURE III.4 SPUTTERING YIELD AS A FUNCTION OF ENERGY FOR MATERIALS (CU-SI-IN2O3) BOMBARDED BY ARGON.	60
FIGURE III.5 SPUTTERING YIELD AS A FUNCTION OF ENERGY FOR MATERIALS (CU-SI-IN2O3) BOMBARDED BY XENON.....	61
FIGURE III.6 DEPENDING ON THE PRESSURE IN THE CHAMBER, THE ENERGY DISTRIBUTION OF: A) CU, B) SIO2, C) GAN, ARRIVES AT THE SUBSTRATE LEVELS AND IS BOMBARDED BY AR ION BEAM.	64
FIGURE III.7 DEPENDING ON THE PRESSURE IN THE CHAMBER, THE ENERGY DISTRIBUTION OF: (CU, SIO2, GAN) ARRIVES AT THE SUBSTRATE LEVELS AND IS BOMBARDED BY XE ION BEAM.....	65
FIGURE III.8 DEPENDING ON THE TEMPERATURE IN THE CHAMBER, THE ENERGY DISTRIBUTION OF: (CU, SIO2, GAN) ARRIVES AT THE SUBSTRATE LEVELS AND IS BOMBARDED BY AR ION BEAM.....	67
FIGURE III.9 DEPENDING ON THE TEMPERATURE IN THE CHAMBER, THE ENERGY DISTRIBUTION OF: (CU, SI ,IN2O3) ARRIVES AT THE SUBSTRATE LEVELS AND IS BOMBARDED BY XE ION BEAM.....	68
FIGURE III.10 DEPENDING ON THE DISTANCE IN THE CHAMBER, THE ENERGY DISTRIBUTION OF: (CU,SI ,IN2O3) ARRIVES AT THE SUBSTRATE LEVELS AND IS BOMBARDED BY AR ION BEAM.....	70
FIGURE III.11 DEPENDING ON THE TEMPERATURE IN THE CHAMBER, THE ENERGY DISTRIBUTION OF: (CU,SIO2 ,GAN) ARRIVES AT THE SUBSTRATE LEVELS AND IS BOMBARDED BY XE ION BEAM.....	71

List of tables

TABLE III.1 INPUT AND OUTPUT PARAMETERS OF TRIM.	53
TABLE III.2 SIMULATION AND THEORETICAL RESULTS OF SPUTTERING YIELD	58
TABLE III.3 SPUTTERING YIELD FOR 1,5 KEV OF THE ENERGY OF THE BOMBARDMENT IONS (AR AND XE) AS A FUNCTION OF VARIOUS INCIDENCE ANGLES OF SI, IN ₂ O ₃ AND CU MATERIALS	62
TABLE III.4 TOTAL NUMBER OF ATOMS SPRAYED ON THE SUBSTRATE DEPENDING TO THE PRESSURE	66
TABLE III.05 TOTAL NUMBER OF ATOMS SPRAYED ON THE SUBSTRATE DEPENDING TO THE TEMPERATURE.....	69
TABLE III.6 TOTAL NUMBER OF ATOMS SPRAYED ON THE SUBSTRATE DEPENDING TO THE DISTANCE	72

Contents

Content

General Introduction	11
Chapter 01	3
<u>Generality of thin films.....</u>	<u>3</u>
I.1. Introduction	4
I.2. The history of thin films	4
I.3. Thin film deposition today.....	5
I.4. Definition of thin film.....	6
I.5. Typical deposition methods of thin films.....	6
I.6. Application of thin films.....	12
I.7. Properties of thin films	16
I.8. Mechanism of thin film formation	17
I.9. Steps of thin film deposition process	19
I.10. Interest and Characterization techniques.....	22
I.11. Types of electrical materials	22
I.12. Thin film Challenges and future prospects.....	25
I.13. Importance of thin films	26
I.14. Conclusion.....	27
Chapter 02.....	28
<u>Sputtering process</u>	<u>28</u>
II.1 Introduction	29
II.2 Brief history of PVD	29
II.3 PVD Definition.....	30
II.4 Steps of PVD.....	32
II.5 The components of PVD	33
II.5.1. Vacuum	33
II.5.2. Plasma	33
II.5.3 Vacuum chamber.....	34
II.6 Sputtering history and application	37
II.7 Sputtering definition.....	37
II.8 Mechanism of sputtering.....	38
II.9 Types of sputtering	39
II.10 Advantages of sputtering	45
II.11 Disadvantages of sputtering	46
II.12 conclusion	46
Chapter 03.....	47
<u>Results and Discussions.....</u>	<u>47</u>
III.1 Introduction	48
III.2 Monte Carlo Simulation	48
III.3 History of Monte Carlo	49
III.4 The principle of the Monte Carlo method.....	49
III.5 Advantages and disadvantages of the Monte Carlo method.....	50
III.6 SRIM software.....	51
III.7 SIMTRA Software	53
III.8 Modeling of sputtering yield.....	54
III.9 comparison between modulization and SRIM calculation	56
III.10 Materials used in the simulation	57

Contents

III.12 Conclusion.....	62
III.13 Simulation of Metal transfer (SIMTRA).....	62
III.10 Conclusion.....	72
General Conclusion	73
abstract.....	81

General Introduction

General Introduction

A thin film refers to a layer or multiple layers of material with a thickness ranging from nanometres (referred to as monolayers) to several micrometres. It is known as a multilayer structure when multiple thin films are stacked together. Thin films are deposited onto a substrate for various purposes, including substrate protection, altering its visual appearance for decorative purposes, modifying the substrate's optical or electrical properties, and more.

The process of thin film deposition holds significant importance in numerous applications. It involves applying a thin layer of any substance onto a surface, be it a substrate or already deposited layers. Depending on the process's dominant physical or chemical nature, deposition techniques can be broadly categorized into two groups. This thesis will discuss the most widely used techniques in this field.

The applications of thin films in our daily lives are indisputable, with a simple example being the mirrors we utilize daily to observe our reflections. These mirrors typically consist of a sheet of glass coated with a thin film of metals like aluminium or silver, achieved through deposition techniques such as spray coating or sputtering to create a reflective surface. The advancements in thin film deposition techniques during the 20th century have led to significant technological breakthroughs in various domains, including optical coatings (e.g., anti-reflective coatings), electronic semiconductor devices, hard coatings on cutting tools, magnetic recording media, integrated passive devices, LEDs, and both energy generation (e.g., thin film solar cells) and storage (thin film batteries). [1]

The primary methods for thin film development are PVD (Physical Vapor Deposition) and CVD (Chemical Vapor Deposition). Physical deposition methods are predominantly utilized in research settings, while chemical methods find industrial applications due to their higher yields, superior film quality, and ability to achieve selective deposition. In our work, we will employ sputtering deposition, a technique that enables the deposition of thin films.

The theoretical calculation of the sputtering yield will be conducted using the Yamamura and Tawara theory, and we have selected the SRIM and SIMTRA software for simulating the bombardment of three noble ionized gases (Ar, Xe) on three different materials (copper (Cu), Indium oxide (In_2O_3), and Silicon (Si)). This study aims to investigate the impact of various parameters such as energy, incident angle, electrode spacing, high pressure, and high temperature on the growth of thin films. We divided our work into three chapters:

General Introduction

The first chapter delves into the fundamental aspects of thin films, including Their definition, fabrication methods, properties, and applications. It explores the unique characteristics of thin films due to their reduced dimensions and their implications for various industries. The chapter aims to establish a solid foundation of knowledge and terminology that will be further expanded upon in subsequent chapters.

In the second chapter, we talk about the deposit of PVD and these various techniques; we based mainly on the technique of sputtering by the electric discharge and these different types and their advantages and disadvantages, and we ended with the presentation of the Monte Carlo simulation.

The last chapter introduces the simulation tools SRIM and SMITRA, which are used to analyse ion-solid interactions and simulate the behaviour of thin films. The chapter explores the calculation of sputter yield by the Yamamura and Tawara models. It compares it with the SRIM simulation result, and we will investigate the behaviour of sputtered atoms and their arrival at the substrate by utilizing SRIM and SMITRA simulations. We aim to understand how different factors, such as energy, pressure, temperature, and distance, affect the number of atoms reaching the substrate and achieving a perfect thin film.

Chapter 01:

Generality about thin films

I.1. Introduction

Thin solid films are fabricated by depositing individual atoms on a substrate. Their thicknesses are typically less than several microns. Historically Bunsen and Grove obtained thin metal films in a vacuum system 1852. Thin films are now widely used for making electronic devices, optical coatings, and decorative parts. Thin films are also necessary for developing novel optical devices, as well as hard coatings and wear-resistant films. By variations in the deposition process and modifications of the film properties during deposition, a range of unusual properties can be obtained which are not possible with bulk materials.[2]

This chapter covers general information about thin film technology. Only over the last four decades have they been used significantly in practical situations. They are used in semiconductor devices, wireless communications, telecommunications, integrated circuits, rectifiers, transistors, solar cells, light-emitting diodes, photoconductors, light crystal displays, magneto-optic memories, audio and video systems, compact discs, electro-optic coatings, memories, multilayer capacitors, flat-panel displays, bright windows, computer chips, magneto-optic discs, lithography, microelectromechanical systems (MEMS), and multifunctional emerging coatings, as well as other emerging cutting technologies. Thin films have been used for over a half-century to make electronic devices, optical coatings, instrument hard coatings, and decorative parts.

I.2. The history of thin films

In the 1960s, thin film transistors (TFT) and integrated circuits (ICs) were extensively studied. These trials were not used in practice due to the drift of the TFT. After the developments of Si-(MOS) (Metal Oxide Semiconductor) IC in the 1970s, thin film materials were used only for passive devices. The actual market of thin films could not be developed like Si-IC. Various new materials were developed in the academic phase, such as diamond-like carbon (DLC) and high-Tc superconductors.

Thin film technology is a well-established material processing technology. However, thin film technology is still being developed daily since it is critical in developing new functional materials such as nanometer materials and/or artificial superlattices in the twenty-first century.[3].

In 1652, the German scientist Otto von Guericke developed the first vacuum system. Two centuries later, William Grove, a Welsh physicist, conducted the first physical sputter deposition experiments using von Guericke's high vacuum method and a DC voltaic pile to deposit iron oxide on a silver substrate.

By the late 19th century, scientists already used sputter-deposited metal films as optical lens coatings. In 1921, Albert Hull presented the magnetron, a vacuum-tube device that brought higher speed and accuracy into film deposition. [4]

I.3. Thin film deposition today

Today, entire industries rely on the ability to deposit pure, atomic-scale thin film onto a variety of substrates. Thin films play a vital part in the following:

- Implants and biosensors
- Thin film batteries
- Optoelectronic application like precision optics and optical filters
- LED display and other consumer electronics
- Photovoltaic cells

Thin film technology continues to evolve and benefit diverse industries. For example, in the coronavirus era, innovative thin film chips enabled the manufacture of no-contact thermometers. Likewise, in recent years, thin film techniques have made the transition to renewable energy more practical and affordable through its usage in photovoltaic solar panel production.

Research continues to perfect deposition technologies and improve thin film performance. This valuable process will continue to be central to industrial, biomedical, and environmental endeavors for decades. [4]

I.4. Definition of thin film

The thin film refers to a layer of material that has a thickness on the order of nanometers to micrometers. Thin films can be deposited onto a substrate using various methods, such as physical vapor deposition, chemical vapor deposition, and sputtering. Thin films have many applications, including electronics, optics, and coatings. They are used in producing electronic devices such as integrated circuits, solar cells, and sensors, as well as in producing anti-reflective coatings for lenses, mirrors, and windows. Thin films can also modify the surface properties of materials, such as improving their hardness, wear resistance, and corrosion resistance.

I.5. Typical deposition methods of thin films

In the present time, thin films can be fabricated in various ways. The techniques can be divided into physical methods and chemical methods. This thesis aims to study thin film's deposition techniques, factors influencing the deposition process, thin film characterization, and its application. They are distinguishing features between physical deposition technique and chemical deposition technique.

Physical deposition techniques include physical vapor deposition, electron beam evaporation, and thermal evaporation techniques. The physical deposition method of the deposition processed physically cannot take place chemical reaction. However, chemical deposition techniques contain just like that of chemical vapor deposition, successive ionic layer adsorption and reaction (SILAR), and chemical bath deposition in chemical deposition techniques which have been used in ultrathin film growth. In addition, a chemical reaction occurs in the chemical deposition method, but the physical deposition method does not occur in a chemical reaction. In the case of chemical deposition techniques is to produce high-quality films.[5]

Typical deposition methods of thin films are shown in Fig.1.1 The deposition methods are composed of the physical vapor deposition (PVD) process and the chemical vapor deposition (CVD) process.

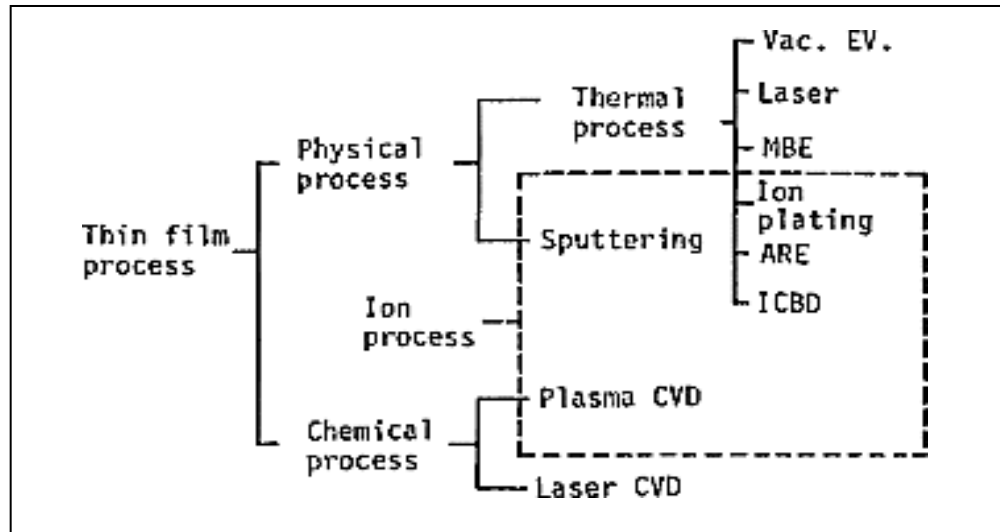


Figure I.1 Thin film deposition processes.[3]

I.5.1. Physical Vapor Deposition (PVD)

Physical vapor deposition (PVD) is a vaporization coating technique that involves material transfer at the atomic level. The process can be described according to the following sequence of steps:

- The material to be deposited is converted into a vapor by physical means (high-temperature vacuum or gaseous plasma),
- The vapor is transported to a region of low pressure from its source to the substrate.
- The vapor undergoes condensation on the substrate to form a thin film..

Typically, PVD processes deposit films with thicknesses ranging from a few nanometers to few microns. However, they can also form multilayer coatings, graded composition deposits, thick deposits, and freestanding structures.

A typical PVD process is shown in Fig. I.2. PVD thin-film technology covers various deposition techniques, including electron-beam or hot-boat evaporation, reactive evaporation, and ion plating. PVD techniques also include processes based on sputtering, whether by plasma or by

an ion beam. PVD is also used to describe the deposition from arc sources that may or may not be filtered. This process can generally be divided into two groups: evaporation and sputtering. Evaporation refers to thin films being deposited by thermal means. In contrast, in the sputtering mode, the atoms or molecules are dislodged from the solid target through the impact of gaseous ions (plasma). Both methods have been further developed into several specific techniques [6].

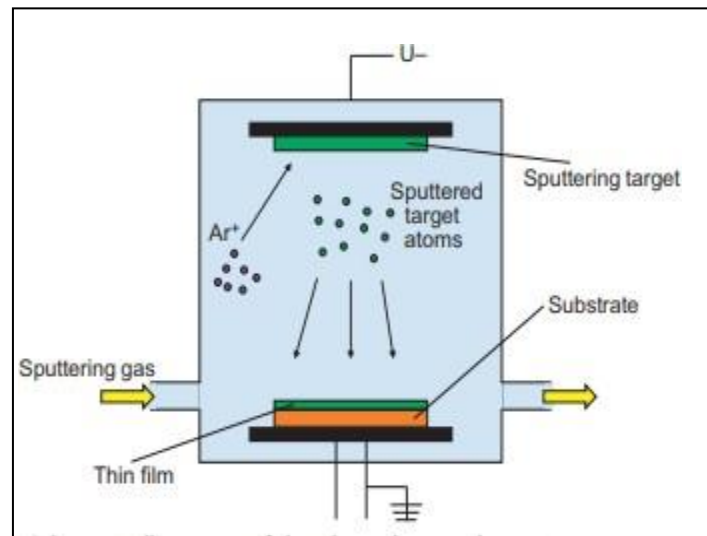


Figure I.2 Schematic illustration of the physical vapor deposition process [6]

1. Sputtering process

Sputtering consists of the bombardment of the target material with energetic particles to dislodge atoms from its surface, which eventually travel through the plasma to condense onto the substrate. Three sputtering techniques are the most employed for thin film growth, including DC, RF, and magnetron diode.[7].

2. Vacuum chamber

It is among the most popular PVD techniques due to its simplicity in operation and high deposition rate. This technique uses heating sources to evaporate the deposition material onto the substrate surface, where it condenses, forming a thin film within a vacuum chamber. This technique is suitable for depositing elements or compounds at temperatures below 2000 K [4]. According to the

method used to evaporate the target material, this technique can be subdivided into resistance-heated and electron-beam evaporation.

3. Laser ablation

Laser ablation 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 placed parallel to the target where the film condensates, and in this case, an additional high-power pulsed laser placed outside the deposition chamber which emits the energy for inducing the ablation of the target material [7].

I.5.2. Chemical vapor deposition (CVD)

Chemical vapor deposition is a chemical process used to produce high-quality, high-performance solid materials. The process is often used in the semiconductor industry to produce thin films. In a typical chemical vapor deposition, the water (substrate) is exposed to one or more volatile precursors that react and/ or decompose on the substrate surface to produce the desired deposit. Frequently, volatile byproducts are also produced, which are removed by gas flow through the reaction chamber.[6].

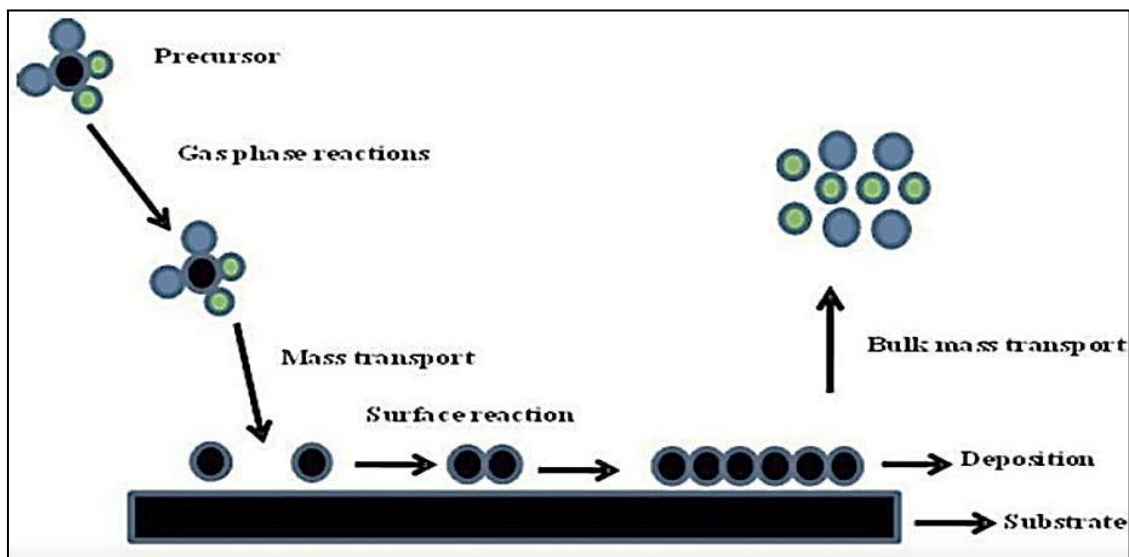


Figure I.3 schematic of CVD process [5]

1. Thermal chemical vapor deposition

Thermal chemical vapor deposition (TCVD) is used for obtaining solid thin films from gaseous materials through the excitation of thermal energy. At high temperatures, the reaction gas is decomposed into active atoms and active groups by thermal energy and a solid film forms on the surface of the high-temperature workpiece. The entire reaction process is in thermal equilibrium and can be divided into three processes: thermal activation, decomposition, and thermal combination [5–7]. The reaction can be carried out under normal pressure or a low vacuum of about 100 Pa. TCVD is widely used and forms the basis for other deposition technologies that use gaseous material sources. We introduce the characteristics of TCVD based on the TiN film deposition.[8].

2. Atomic layer deposition (ALD)

Atomic layer deposition (ALD) is among the most resembling techniques to CVD since they share several features with just minor differences. Like CVD, a volatile precursor is used in ALD as the source to perform deposition. However, in contrast to the simultaneous introduction of precursors and reactants to the chamber in CVD, each precursor and reactant is entered in sequence in ALD. This gives the opportunity to precisely control the deposition properties as well as to tune the thickness in the atomic range [9].

3. Sol-gel process

The sol-gel process describes forming of a network of oxide layers through the condensation reaction of silane alkoxides and some metal precursors in the liquid phase. Sol-gel is usually made in two ways. The inorganic process involves developing a network through the formation of sol suspensions of oxides and suspension of sol in the liquid phase. However, the most used method is the organic process, which usually begins with alkoxides or metalloids monomer precursors in organic solvents. The recent approach takes the gain of producing a hybrid material that combines the behavior of both the organic and inorganic processes. The sol-gel formation generally takes place in four stages, i.e., hydrolysis, condensation, followed polymerization, and particle formation agglomeration, which spreads throughout the liquid medium and leads to

coagulation by gelation. After the hydrolysis reaction, condensation reactions co-occur and are followed by steps to form alcohol and water as by-products [10].

4. Spin coating

The spin-coating technique is used to prepare uniform thin films in the micrometer to nanometer thickness range. The substrate is mounted on a chuck that rotates the sample, and the centrifugal force radiates the liquid outward. Viscous force and surface tension are the leading causes of flat deposition on the surface. Finally, the thin film is formed by the evaporation. The spin coating consists of several stages: fluid dispense, spin-up, stable fluid outflow, spin-off, and evaporation.

The advantages of spin coating are to produce excellent, thin, and uniform coating, while the disadvantage is the difficulty with large area samples [11].

5. Spray pyrolysis

Spray pyrolysis is an essential technique in depositing a thin film on the dielectric matrix by spraying a precursor solution on a heated surface. Pham et al. (2010) synthesized a chemical-converted graphene film by a fast, low-cost, and simple process using spray deposition of GO–hydrazine dispersion. Chandra et al. (2014) used a simple spray pyrolysis technique to synthesize plasmonic-metamaterial-based graphene/TiO₂/Ag with low resistivity (resistivity~ $2.4 \times 10^2 \Omega\text{-cm}$) and as shown in Figure 1.4. [12].

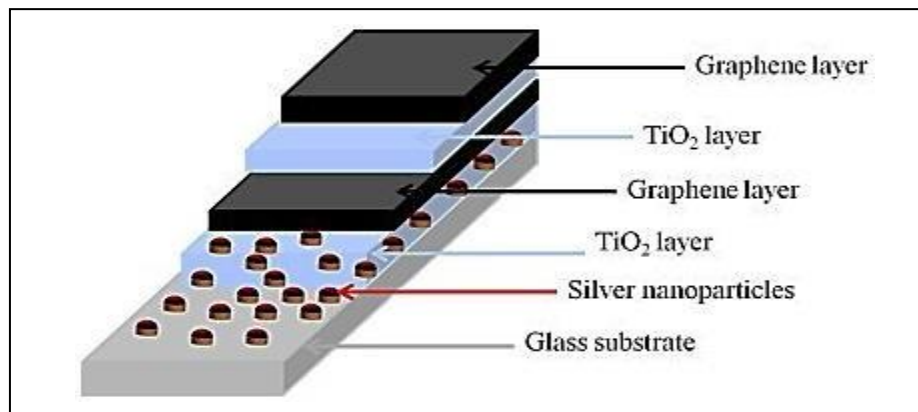


Figure 1.4. Schematic for plasmonic-metamaterial-based graphene/TiO₂/Ag thin film.[12]

I.6 Application of thin films

I.6.1 Magnetic thin film application

Magnetic thin films are essential for many devices, including electronics, data storage, radio-frequency identification, microwave devices, displays, circuit boards, and optoelectronics. Beyond that, they are critical for fabricating wearable electronics, including biomedical sensors.

Magnetic films are ideal for those industries due to their lightweight, portable size, flexible substrates, and biocompatibility. These properties make them highly suitable for photonic, spintronic, and recording devices. Sensors containing magnetic films that use a flexible substrate (instead of a flat substrate) during deposition may even detect the magnetic field of living organisms. [13].

I.6.2 Optical Thin Films

Optical thin films have firm roots in today's modern technologies. Standard applications include optical coatings and optoelectronics, which have impressive uses. For example, manufacturers can create optoelectronic thin-film chips (semiconductors) using molecular beam epitaxy. MBE involves depositing a single atom onto the substrate to create epitaxial films.

A high vacuum environment is necessary to fabricate optical coatings with numerous uses, including lenses (i.e., glasses, telescopes) and mirrors. The coating itself affects how the optics reflect and convey light; for example, we can create anti-reflective coatings or the opposite, highly reflective coatings. [14].

I.6.3 Polymer Thin Film Applications

Applications for polymer thin films range from solar cells and electronics to healthcare and memory chips. Advancements in chemical deposition methods (CVD) allow greater control over polymer film coatings, including coating thickness and conformity. Specific chemical reactions allow for solvent-free fabrication, eliminating the risk of adverse reactions to human tissue. [15]

Now, there are “smart membranes,” which change permeability or selectivity based on environmental stimuli, like low temperatures, external pressures, or pH changes. These polymer thin film coatings have many biomedical applications, including medications delivery systems, tissue engineering, and biosensor creation [16].

I.6.4 Thin-Film Battery Applications

Now, thin-film batteries are the superior choice over lithium-ion. They are thinner, lighter, and denser without sacrificing voltage or current. Their narrower proportions are ideal for use in complex electronics, like ultra-thin laptops. Another application for thin-film batteries is in the healthcare industry, where they power implantable medical devices. [13].

I.6.5 Thin-Film Coating Applications

Thin-film coatings provide many practical uses in various industries and technologies. During deposition, manufacturers use coating techniques to improve the chemical and mechanical properties of target materials. Common examples include anti-reflective coatings, anti-ultraviolet or infrared coatings, anti-scratch coatings, and lens polarisation.[16]

Additional uses for film coatings include:

- **Anti-corrosion coatings:** Reduce rust and degradation in pipes, engine parts, bearings, etc.
- **Hard coatings:** Increase the durability of cutting tools while reducing friction
- **Architectural glazing:** Improve energy efficiency and lower utility costs in offices and skyscrapers.

I.6.6 Thin-Film Solar Cells Applications

Thin-film solar cells are invaluable to the solar energy sector, providing clean, low-cost energy generation. The two primary technologies are thermal energy and photovoltaic systems. At

first, solar cell technology used amorphous silicon thin films. However, the standard is copper indium gallium selenide, which has excellent stability and higher efficiency (around 23%).

Thin-film solar cells are also prevalent in the solar energy sector because their absorber layer has a high absorption coefficient. That allows for a considerable reduction in cost and material thickness while increasing conversion efficiency. [16].

I.6.7 Zinc Oxide-Based Thin-Film Applications

ZnO thin film applications (zinc oxide) are commonplace in several industries, including thermal, optical, magnetic, and electrical industry. However, primary uses of ZnO thin films include semiconductor devices and coatings. ZnO films are also suitable for these applications:

- Displays
- Solar cells
- LED
- OLED
- Gas sensors
- Lasers
- Biosensors
- Photodetectors

ZnO is also physically and chemically stable, readily available, inexpensive, and has excellent conductivity. For those reasons, it's a popular alternative to other materials in the thin film sector, like indium tin oxide or gallium nitride. [17].

I.6.8 Thin Film Resistor Applications

Thin-film resistors are widespread in modern technology and crucial among thin-film applications. Its applications range from radio receivers and circuit boards to computers and radiofrequency devices. Additional applications include monitors, wireless routers, Bluetooth modules, cell phone receivers, and invaluable electronics.

For example, due to their high resistivity, nickel-chromium alloy-embedded resistors are vital for manufacturing smaller, thinner electronic devices. Researchers discovered that embedding these resistors into a printed wiring board improves electrical performance and reliability while increasing device functionality. They can also enhance temperature stability by infusing the alloy with small amounts of aluminum and silicon [18].

I.6.9 Thin film 3D printing application

3D printing is a fabrication technology that creates a three-dimensional object from a digital model. This technology has evolved very rapidly in recent years and has shifted apart from its traditional application fields.

The difference among printer types is based on cost, spatial resolution, and materials. Interestingly, the liquid deposition modeling (LDM) method which creates the laid down successive material layers directly from a liquid/paste has emerged as a versatile and cost effective technique to overcome the limits imposed by the fused deposition modeling (FMD).

The system allows functional, end-use materials such as TiO₂ and other conductive pastes to fabricate thin films for optoelectronic applications. The deposition mechanism is based on a mechanic or a pneumatic system in which the pressure will push forward the materials through the extruder. Thus. With proper pressure force and moving speed, it is possible to accurately control the flow of materials and the retraction to interrupt deposition. By this method, the production of freeform structure could be achieved by using a computer-controlled extruder moving along the x,y and z axes. For example, a direct deposition of conductive polymer-based 3D microstructures was printed by a low-cost LDM 3D printing system .[19].

I.6.10 Thin film semiconductors applications

Semiconductor materials are defined as materials in a solid form whose conductivity has a value between conductors and insulators. Semiconductor materials play an essential role in the advances in the modern electronics industry in the twenty-first century and the industrial applications of many electronic devices. These materials include many materials, such as silicon,

gallium arsenide, germanium, cadmium sulfide, and cadmium telluride, which are widely used today. From the first silicon integrated circuits produced in semiconductor technology, high-tech microprocessors, solar cells, and many other electronic devices have developed rapidly.

Today, semiconductor thin films are generally produced in one or more thin layers. Typical applications of such structures include many electronic materials such as transistors, sensors, and photovoltaic devices. The structural, chemical, and physical properties of semiconductor thin films are directly related to the production technique, and their thickness ranges from a few nanometers to hundreds of micrometers [20].

I.7 Properties of thin films

I.7.1 Optical properties

Optical experiments provide a good way of examining the properties of semiconductors. Particularly measuring the absorption coefficient for various energies gives information about the band gaps of the material. Knowledge of these band gaps is essential for understanding the electrical properties of a semiconductor and is, therefore, of great practical interest [21].

I.7.2 Mechanical properties

The mechanical properties of thin films on substrates are described and studied. It is shown that enormous stresses may be present in the thin films comprising integrated circuits and magnetic disks and that these stresses can cause deformation and fracture. The approaches that have proven helpful in the study of bulk structural materials can be used to understand the mechanical behavior of thin film materials. Understanding the mechanical properties of thin films on substrates requires an understanding of the stresses in thin film structures as well as a knowledge of the mechanisms by which thin films deform. The fundamentals of these processes are reviewed.

The experimental study of the mechanical properties of thin films requires developing and using nontraditional mechanical testing techniques. Some of the techniques that have been developed recently.[22]

I.7.3. Electrical properties

Three types of electron materials exist metal, semiconductor, and dielectric. Electrical transport nature is different for 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 imperfect level of the layer are the most significant parameters that define the type, mechanism, and stability of the electrical transport [23].

I.8. Mechanism of thin film formation

The growth process of a thin film can be summarized as follows: crystal nucleation effect, followed by surface diffusion growth and island formation, then the formation of larger islands, and finally, the formation of a continuous film by filling the spaces between these islands. Depending on the thermodynamic parameters of the deposition and substrate surface, the nucleation and island growth steps can be described as being of the following types:

- Of the island type (called Volmer-Weber).
- Of the layer type (called Frank-van der Merwe).
- Of the mixed type (called Stranski-Krastanov).[24]

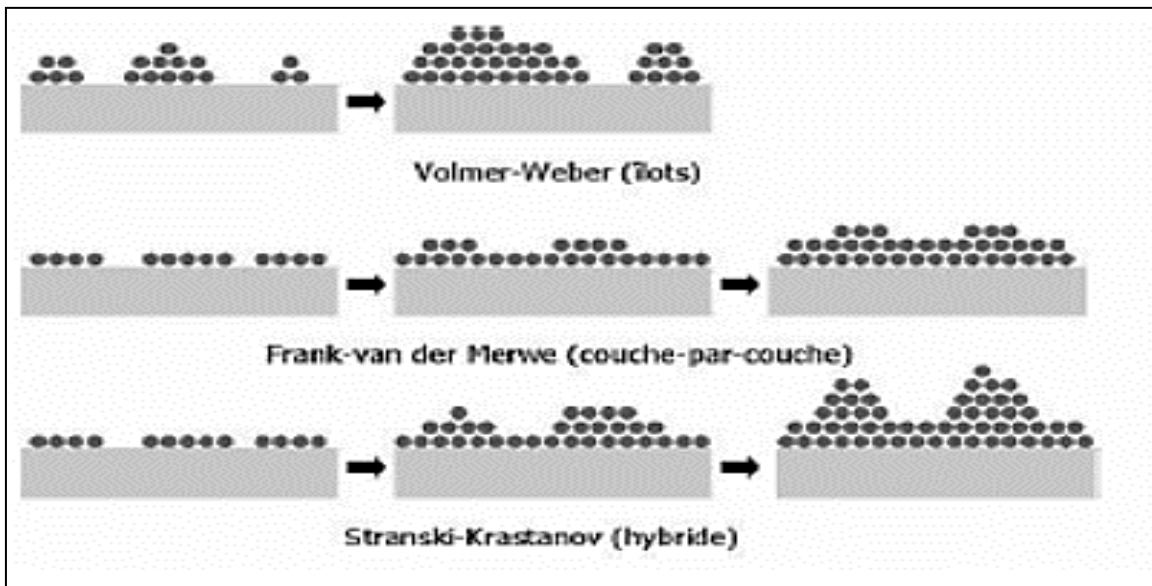


Figure I.5 The three possible growth modes

a) Nucleation

This phenomenon accompanies changes in the state of matter and consists of the appearance, within a given medium, of transformation points from which a new physical or chemical structure develops. The sputtered species arriving on the substrate are not thermodynamically in equilibrium with the substrate and move over its entire surface. In this state, they interact and form "clusters." These "clusters," called nuclei, are unstable and tend to desorb. Under certain deposition conditions, they collide with other adsorbed species and begin to grow. After reaching a critical size, these clusters become thermodynamically stable, and the nucleation barrier is crossed.[26].

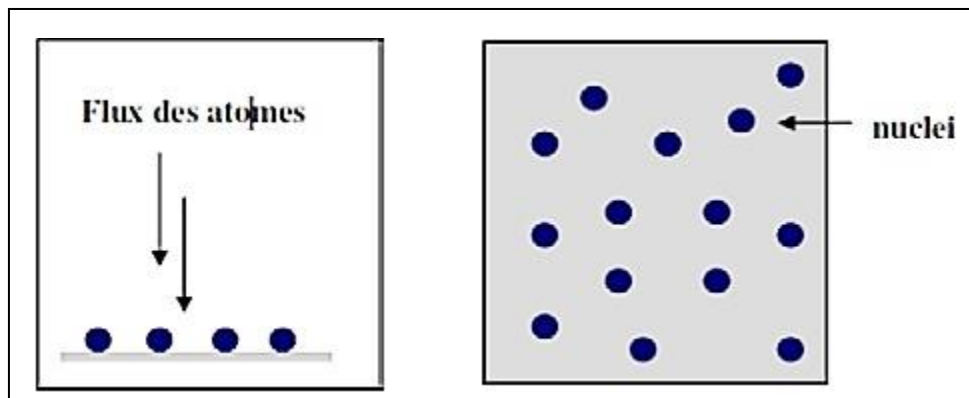


Figure I.6 Diagram of the nucleation of layers[26]

b) The coalescence

The first coalescence step corresponds to the growth of stable islands by absorption of smaller ones by larger ones. This step is distinguished from a second, faster, large-scale coalescence step in which the islands, having reached a critical density, flatten to increase their covering surface and join together. If the probability that all islands on the substrate are of the same orientation is low, coalescence produces a polycrystalline deposit. Otherwise, a thin, single-crystal layer develops.[26].

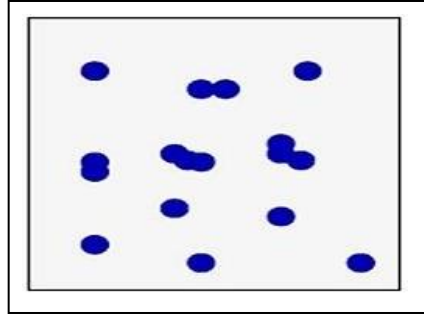


Figure I.7 Diagram representing coalescence.[26]

c) The growth

In this stage, the islands begin to coalesce. The growth of surface mobility of the adsorbed species enhances this tendency to form larger islands. This enhancement is achieved by increasing the substrate temperature. These larger islands further grow, leaving channels and holes on the substrate. The film structure in this stage changes from a type of discontinuous islands to a porous network. A continuous film is formed by filling the channels and holes. [26].

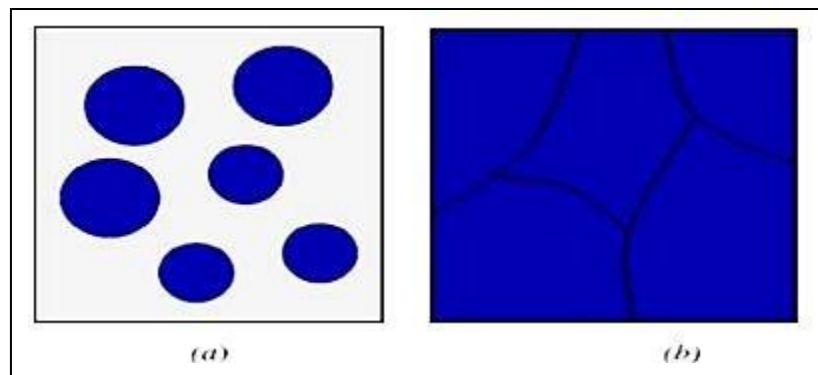


Figure I.8 growth of thin films[26]

I.9 Steps of thin film deposition process

We can see in figure1.9 all steps of thin film deposition process

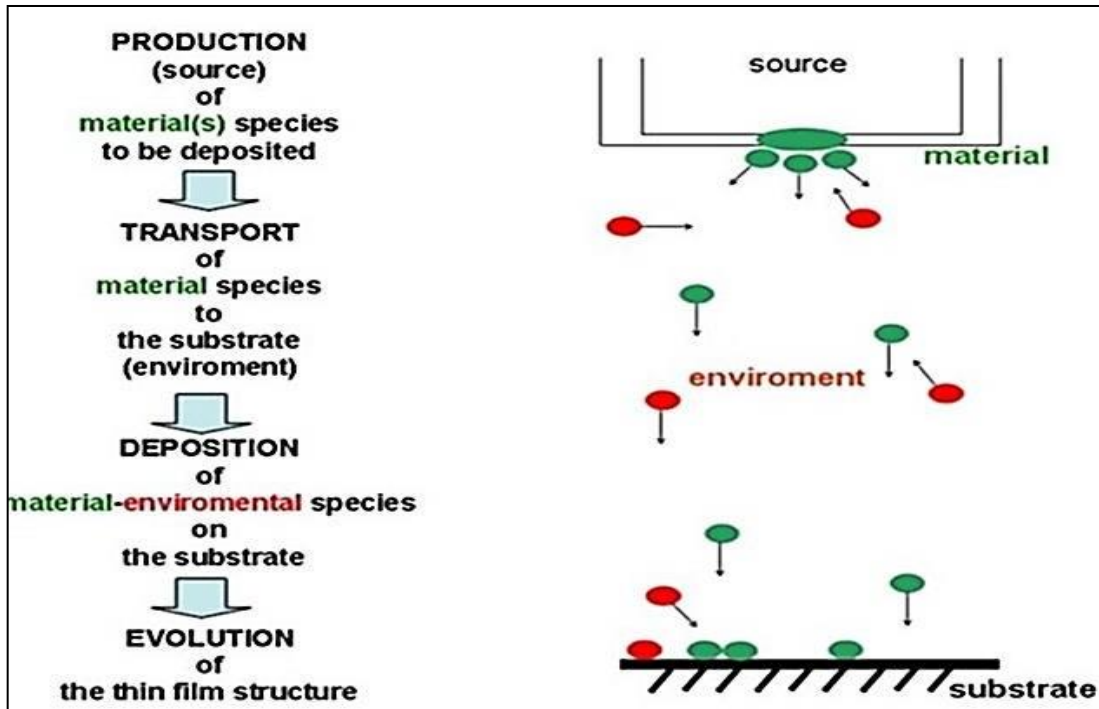


Figure I.9 steps of thin films process

I.9.1 Source

The material that constitutes the base of the thin film to be elaborated can be a solid, a liquid, a vapor, or a gas. When the material is solid, its transport to the substrate is carried out by vaporization. This can be achieved by thermal evaporation, electron beam, laser ablation, or by positive ions "sputtering."

All 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. The processes that use gases, evaporated liquids, or solid materials evaporated by chemical means as the base material are known as chemical vapor deposition, CVD.[23].

I.9.2 Transport

In the transport step, the uniformity of the species flux arriving on the substrate surface is an essential element, and several factors can affect this uniformity depending on the environment in which the transport occurs, whether under a high vacuum or in a fluid (primarily gases).

In the case of a high vacuum, the molecules from the source to the substrate travel in straight lines, while in a fluid medium, they undergo several collisions during transport. As a result, in a vacuum, the reaction's geometry determines the uniformity of the flux arriving on the substrate. In contrast, a fluid determines by the gas flow and the diffusion of the source molecules into the other gases present. Often, processes that use high vacuum are equivalent to PVD processes, while those that use fluid flow are CVD processes. However, this definition is only sometimes confirmed.

Several physical vapor deposition processes operate under high vacuum, while others, such as laser ablation and sputtering, often operate at high-pressure characteristics of fluids. Likewise, most CVD deposition processes operate at moderate pressures, while chemical beam epitaxy (CBE) operates in a high vacuum.

In this phase, several thin film deposition processes use a plasma medium. Indeed, the high energy content in this medium allows the activation of layer formation at low temperatures. The working pressure of a plasma can be that of a fluid.[23].

I.9.3 Deposition

The third step in the thin film fabrication process is the deposition of the film onto the substrate surface. This phase goes through nucleation and coalescence steps. The deposition behavior is determined by source and transport factors, as well as the primary conditions of the substrate surface: surface state (roughness, contamination level, etc.), the reactivity of the material arriving on this surface (adhesion coefficient), and substrate temperature.[25].

I.9.4 The analysis

The final step in the manufacturing process is the need for analysis of the obtained film. The initial level of material control involves conducting direct measurements of its essential properties. If the analysis results are insufficient, it becomes necessary to employ specific experiments to resolve any ambiguities in a particular process [24].

I.10 Interest and Characterization techniques

In studies conducted on thin films, characterization techniques play a fundamental role in understanding the behavior of the films produced. Each characterization technique is intended to analyze a particular property of the material. Many materials characterization techniques are based on different basic physical principles: radiation-matter interactions, thermodynamics, and mechanics. [25]

The interest in thin films comes mainly from the economical use of materials in relation to their physical properties and the simplicity of the technologies used to create them (easy and inexpensive elaboration...). Various materials are used to produce these thin films, including metals, alloys, oxides, polymers, etc.

The second essential characteristic of a thin film is that, regardless of the process used for its fabrication, a thin film is permanently bonded to a substrate on which it is built. Thus, a thin film of the same material and thickness can have significantly different physical properties depending on whether it is deposited on an insulating amorphous substrate such as glass or a monocrystalline silicon substrate, for example. [26].

I.11 Types of electrical materials

Electronic materials are of great interest due to their potential to be applied in a broad range of critical electronic devices, including transistors, sensors, solar cells, etc. To improve the electronic performance and development of new electronic materials for future technologies, understanding the electronic processes in these materials and devices is of fundamental importance.

For this reason, advanced characterization techniques and theoretical models are necessary to gain detailed knowledge regarding the properties of electronic materials. [27].

I.11.1 Conductors

An electrical conductor is a substance or material that allows electricity flow. In a conductor, electrical charge carriers, usually electrons or ions, move quickly from atom to atom when voltage is applied. Most metals, like copper, are considered good conductors, while nonmetals are considered bad conductors and insulators.

In general, conductivity refers to the capacity of a substance to transmit electricity or heat. A conductor conducts electricity since it offers little or no resistance to the flow of electrons, thus leading to a flow of electrical current. Metals, metal alloys, electrolytes, and even nonmetals, like graphite and liquids, including water, are good electrical conductors. Pure elemental silver is one of the best electrical conductors. Other good electrical conductors include the following: copper, steel, gold, silver, platinum, aluminum, and brass.

Humans body are also good conductors of electricity, so touching someone experiencing an electric shock causes the toucher to experience the same shock. Conductors in electrical and electronic systems comprise solid metals molded into wires or etched onto printed circuit boards.

Essential features of an electrical conductor include the following:

- ✓ It ensures the free movement of electrons or ions through it.
- ✓ It has a zero electric field inside, which permits the movement of electrons or ions.
- ✓ Outside the conductor, the electric field is perpendicular to the conductor's surface.
- ✓ It has a zero charge density, ensuring that the positive and negative charges cancel each other and free charges exist only on the surface.

In addition, conductors have low resistance and high thermal conductivity. Further, a conductor placed in a magnetic field does not store energy. Finally, both ends of the conductor are at the same potential. Electricity flows through the conductor when the potential is changed at one end, which allows electrons to start flowing from one end to another.[29].

I.11.2 Semiconductors

Semiconductors are materials that have electrical conductivity values between those of conductors and insulators. They are an important class of materials because they form the basis of modern electronic devices such as transistors, solar cells, light-emitting diodes (LEDs), and integrated circuits (ICs).

The electrical conductivity of semiconductors can be controlled by introducing impurities into their crystal structure, a process known as doping. This creates an excess of either negative (n-type) or positive (p-type) charge carriers, increasing the material's electrical conductivity.

One of the most common semiconductors is silicon, widely used in the semiconductor industry due to its abundance and high purity. Other important semiconductors include germanium, gallium arsenide, and indium phosphide.

Semiconductors are characterized by their band gap, which is the energy difference between the valence band (the highest energy level of electrons bound to the atoms) and the conduction band (the lowest energy level of electrons free to move through the material). Materials with a small band gap, such as silicon and germanium, are known as narrow-band gap semiconductors. In contrast, those with a more significant band gap, such as gallium arsenide, are known as wide-band gap semiconductors.[12].

I.11.3 Insulators

Insulators, also known as non-conductors, resist the flow of electric charge. They have high electrical resistance, so they do not allow electrons to move freely through them. Insulators protect electrical equipment and wiring from damage or short circuits caused by electric current flowing in unintended directions.

Examples of insulators include rubber, glass, air, and certain types of plastics. In contrast to conductors, often used in electrical wiring and other applications where electricity needs to flow freely, insulators prevent electricity from flowing where it is not intended to go. The properties of insulators are essential in many fields, including electronics, materials science, and electrical engineering.

Materials whose resistivity is typically greater than $10^8 \Omega/\text{cm}$ are considered insulators

I.12 Thin film Challenges and future strange

Thin films have emerged as an important area of research due to their widespread applications in various fields, such as electronics, optics, energy, and catalysis. However, several challenges are associated with thin film production, characterization, and utilization. Some of the significant challenges and prospects are discussed below:

- Thin film growth is a complex process, and obtaining high-quality films with desired properties is often difficult. Several factors, such as substrate temperature, pressure, and gas flow rate, influence thin film growth. Developing new growth techniques such as atomic layer deposition, pulsed laser deposition, and molecular beam epitaxy has enabled the fabrication of high-quality thin films with precise thickness and composition.
- The characterization of thin films is another challenge, as the thickness of the film is typically in the range of nanometers to micrometers. Characterization techniques such as X-ray diffraction, scanning electron microscopy, and atomic force microscopy are commonly used to investigate thin films' structural, morphological, and electrical properties.
- Thin films are often susceptible to environmental degradation, such as oxidation or corrosion, affecting their performance and lifetime. To overcome this challenge, the researchers are exploring the use of protective coatings or encapsulation techniques to improve the stability of thin films.
- Integration of thin films with other materials and devices is another challenge, as the thin films must be compatible with the substrate and other materials. Integration challenges can be overcome by selecting appropriate deposition techniques, optimizing the interface properties, and developing new bonding and interconnect technologies.

Despite the challenges, the future of thin films is promising, as they offer many advantages, such as high performance, low cost, and flexibility. In electronics, thin films are expected to play a critical role in developing next-generation electronic devices such as flexible displays, sensors, and high-performance transistors. In the energy field, thin films are expected to contribute

to developing more efficient solar cells and energy storage devices. Additionally, thin films are expected to have optics, catalysis, and biomedicine applications.[31].

I.13 Importance of thin films

Modern technologies and their components, such as cellphones, laptops, and smartwatches, rely on cutting-edge technology to be manufactured. Therefore, they typically require small parts obtained from miniaturized wafers using thin-film technology.

Thin films have become increasingly important in modern technology due to their unique properties and versatility. One of the main advantages of thin films is their ability to provide a large surface area with a small volume of material, making them ideal for use in miniaturized electronic devices. Additionally, thin films can be engineered to have specific electrical, optical, magnetic, or mechanical properties, allowing them to be used in various applications, including sensors, solar cells, displays, and coatings.

Thin films also offer numerous benefits over their bulk counterparts. For example, they can exhibit improved mechanical, electrical, and optical properties due to their crystalline structure and can be fabricated with exact thickness and composition control. Thin films can also create unique material combinations that are difficult or impossible to achieve using traditional bulk processing techniques.

Thin films have the potential to revolutionize various industries, including medicine, by enabling the development of implantable sensors and drug-delivery devices. They can also improve the efficiency of energy storage and conversion systems, such as batteries and fuel cells, and enhance the performance of electronic devices, such as transistors and integrated circuits.

The importance of thin films lies in their unique and tunable properties, making them indispensable in various modern applications and technologies. The continued development of thin film materials and processing techniques promises to yield even more advanced and innovative applications.[30].

I.14 Conclusion

Thin films are critical in numerous technological applications due to their unique properties, flexibility, transparency, and high surface area-to-volume ratio. Thin film technology has been widely used in various fields, including microelectronics, optoelectronics, energy storage, and biomedical engineering.

The generality of thin films involves a broad range of topics, including the fundamentals of thin film deposition techniques, the characterization and analysis of thin films, and the applications of thin films in various fields. Understanding the principles and properties of thin films is critical for developing new materials, devices, and technologies.

In this chapter, we have discussed the fundamental concepts of thin films, including the types of thin films, the techniques for thin film deposition, and the characterization methods for thin films. By further exploring the possibilities of thin film technology, we can continue to innovate and advance in various fields and improve our daily lives.

Chapter 02:

Sputtering process

II.1 Introduction

The production of thin films is based on a certain number of varieties of vacuum techniques, classified into two large families according to the process used: Physical methods (PVD deposition processes) and chemical methods (CVD Deposition processes). [32].

In the first chapter, we discussed thin film application and the differences in deposition, so in this chapter, we will discuss PVD deposition by electrical discharge, which is sputtering. Sputtering is a process in which atoms or molecules are ejected from a solid or liquid target material due to the bombardment of high-energy particles. This process is widely used in producing thin films and coatings for various applications such as microelectronics, optics, and energy storage.

Understanding the principles and mechanisms of sputtering is essential for developing efficient and high-quality thin-film deposition techniques. This chapter will discuss the fundamental concepts of sputtering, including the physical principles, types of sputtering, and factors that affect the process. Additionally, we will examine the various applications of sputtering in industry and research.

II.2 Brief history of PVD

Physical vapor deposition (PVD) methods are mainly based on the principle of accumulation, by evaporation and/or sputtering, of solid-state coating material on a base material.

The coating made by Faraday by evaporating a metal wire under a vacuum in 1857 is accepted as the first PVD coating application. Optical property examinations were performed with thin films produced by Kuntz with this method in 1888. The method was limited to physics studies for many years, but it became widespread when it was used on cutting tool surfaces to delay tool wear after the 1960s [33].

At this time, an advance in the vacuum coating process was required. This has been brought about by the development of well-known technologies such as sputtering, vacuum, plasma technology, magnetic fields, gas chemistry, thermal evaporation, arc, and power control, as described in detail in Powell's book [34].

Over the past three decades, plasma-enhanced PVD (PAPVD) has been classified into various power technologies, such as direct current (DC) diodes, triodes, radio frequency (RF), pulsed plasma, and ion beam-assisted coatings. Initially, there were some difficulties in understanding the process at a fundamental level. However, the necessary improvements provided advantages such as excellent adhesion of coatings to substrates, structural control, and deposition of materials at low temperatures. Changes have been introduced. [35].

II.3 PVD Definition

PVD technology is a thin film deposition process that grows a coating on a substrate, atom by atom. As shown in the figure below, PVD is the atomization or vaporization of material from a reliable source, generally called a target.

Thin films typically have layers with thicknesses ranging from a few atomic layers to several micrometers' thick films. This process changes the surface properties and the transition zone between the substrate and the deposited material. On the other hand, film properties can also be influenced by substrate properties. Atomic deposition processes can be performed in vacuum, gas, plasma, or electrolytic environments. Additionally, the vacuum environment within the deposition chamber reduces gas contamination to deficient levels during the deposition process [36].

These techniques are constantly evolving and continue to serve as a source of inspiration for many studies. Many books and articles widely disseminate information about these variants, making it difficult to quantify all existing techniques. Sputtering (or cathodic spray) and evaporation are the most commonly used PVD methods for thin film deposition [37].

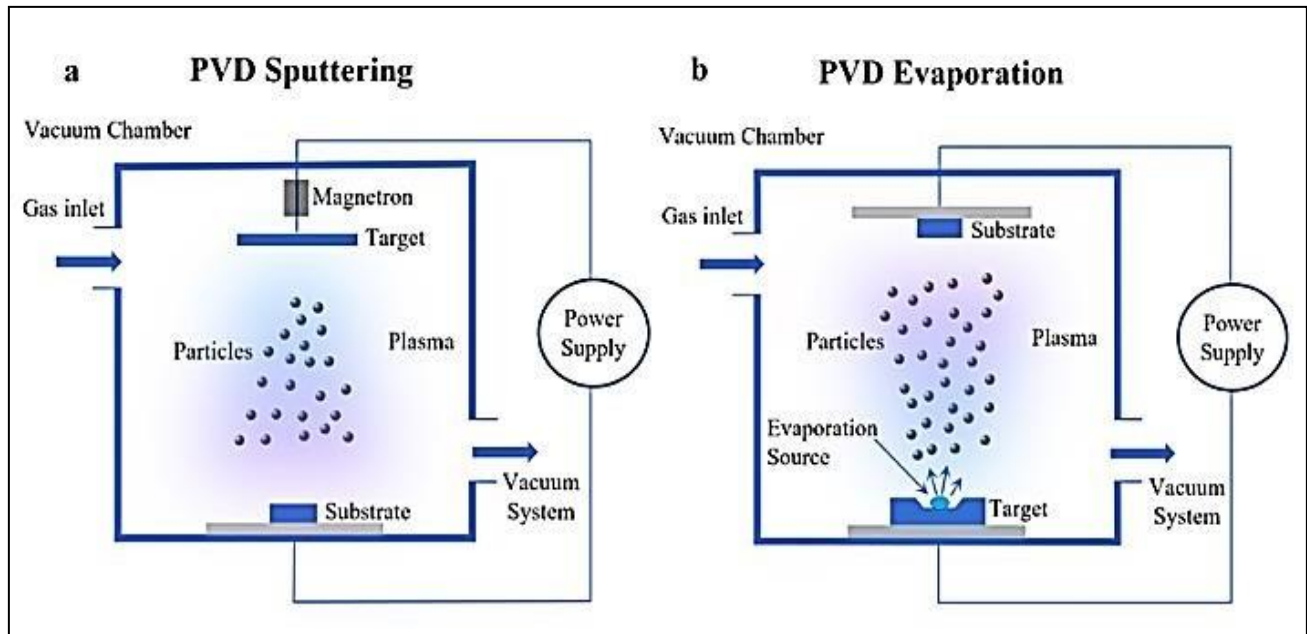


Figure II.1 Schematic of two conventional PVD processes: (a) Sputtering (b) Evaporation [37]

II.3.1 Advantages and disadvantages of PVD

Physical vapor deposition (PVD) creates layers of different thicknesses using unrelated precursors. This technique makes it possible to deposit any solid, except for specific polymers, onto any other solid (substrate). [38] PVD has several advantages. On the other hand, inclusion also has disadvantages.

a) Advantages

- Improves hardness, wear resistance, and oxidation resistance.
- The environmental impact is shallow as no chemical reagents or post-treatment cleaning is required.
- PVD can be applied to all kinds of inorganic materials.
- Coatings obtained by PVD exhibit excellent adhesion, resistance, and durability.
- PVD technology allows reasonable control over coating composition and thickness [39].

b) Disadvantages

- The PVD process uses complex equipment with a very high cost
- The production speed of PVD coatings is slow compared to other coating deposition processes.
- The PVD technique is more suited to substrates with complex geometries [39]

II.4 Steps of PVD

Physical Vapor Deposition (PVD) is a process used to deposit thin films of materials onto a substrate through a physical process. The general steps involved in a PVD process are as follows:

- **Cleaning the substrate:** The substrate surface is cleaned thoroughly to remove any impurities or contaminants that could interfere with the deposition process.
- **Loading the substrate:** The cleaned substrate is loaded into the vacuum chamber.
- **Creating a vacuum:** The vacuum chamber is sealed, and the air inside is removed to create a vacuum.
- **Heating the source material:** The source material (e.g., metal, ceramic) is heated to its vaporization temperature, causing it to evaporate and form a vapor.
- **Ionization of the vapor:** The vapor is ionized by bombarding it with high-energy ions or electrons, making it highly reactive.
- **Deposition on substrate:** The ionized vapor condenses on the substrate, forming a thin film of the desired material. The substrate may be heated to increase adhesion or modify the deposited film's properties.
- **Monitoring the process:** The deposition process is monitored to achieve the desired film thickness and properties.
- **Cooling the substrate:** After the deposition, the substrate is cooled to room temperature before being removed from the vacuum chamber.
- **Unloading the substrate:** The coated substrate is removed from the vacuum chamber and may undergo further processing or use in its intended application.

Overall, the PVD process is a sophisticated and precise technique for depositing thin films with high quality, uniformity, and reproducibility.

II.5 The components of PVD

Physical vapor deposition (PVD) is a well-known technique widely used for the deposition of thin films under many requirements, where the coating is grown atom by atom on the substrate. We represent the PVD components as follows:

II.5.1. Vacuum

The word "vacuum" comes from the Latin word "vacua" which means "empty". However, no space exists in nature, and no "ideal vacuum" exists. A vacuum is a partial space in which some of the air and other gases have been removed from a volume containing gas ("gas" comes from the Greek word "chaos," meaning infinite space). So vacuum means "everyone." A volume that contains fewer gas particles, atoms, or molecules than the surrounding air (lower particle density and gas pressure). A vacuum is therefore a gaseous environment with pressure below atmospheric pressure. [40].

II.5.2. Plasma

Plasma is primarily ionized gas. A liquid is usually formed when a solid is heated to the point where the thermal motion of atoms destroys the crystal lattice structure. A gas is formed when a liquid is overheated and evaporates from the surface faster than the atoms can recondense. Plasma is formed when the gas is heated enough that the atoms collide and the electrons are separated [41].

Plasma is, therefore, one of the four primary states of matter, the others being solid, liquid and gas (see Figure 2.2 below). Under normal conditions, Plasma does not exist freely on the Earth's surface. Plasmas can only be artificially generated by heating neutral gases or exposing them to solid electromagnetic fields until ionized gaseous substances become highly conductive [42].

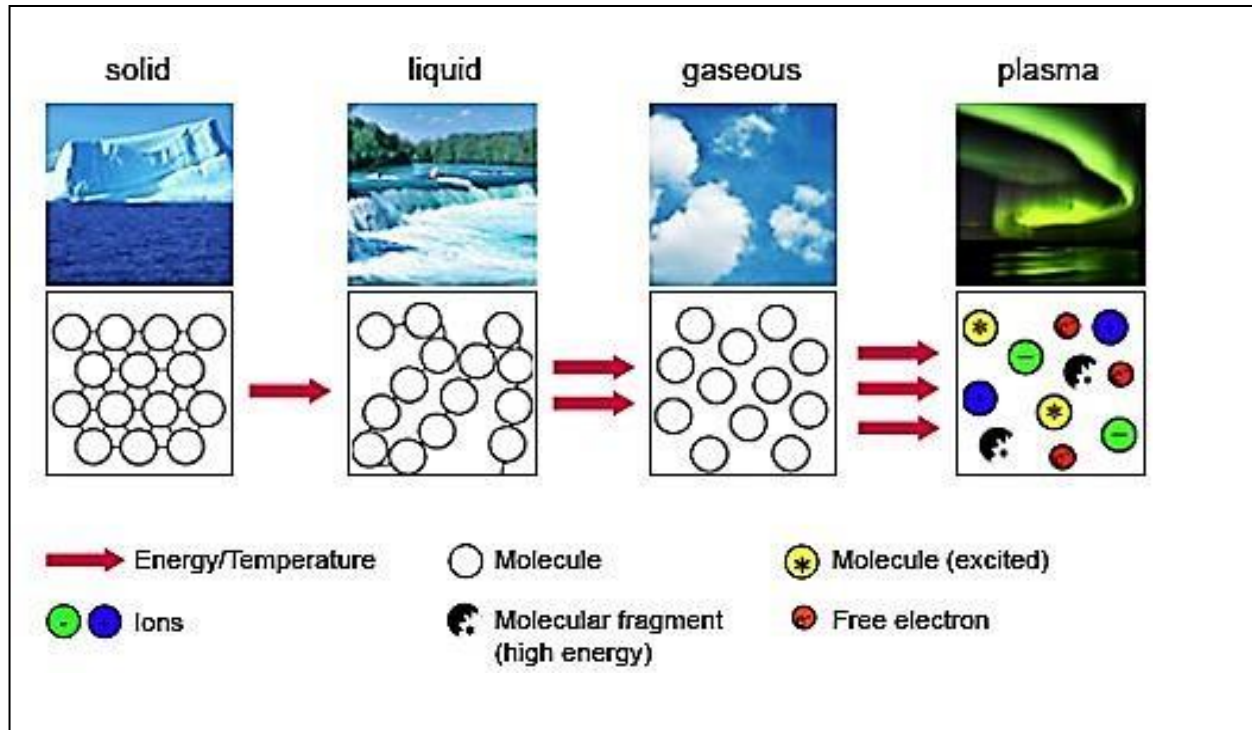


Figure II.2 the four fundamental states of matter. [42]

II.5.3 Vacuum chamber

A vacuum chamber is a rigid enclosure from which a vacuum pump removes air and other gases. This creates a low-pressure environment inside the chamber, commonly called a vacuum. In a vacuum environment, researchers can conduct physical experiments and test mechanical devices that must be used in space and processes such as vacuum drying and vacuum coating.

Chambers are typically made of metal that may or may not shield an applied external magnetic field, depending on the wall thickness, frequency, resistivity, and permeability of the materials used. Only some materials are suitable for vacuum use. Chambers often have multiple ports covered by vacuum flanges, allowing for the integration of instruments and windows into the chamber walls.

For low to medium vacuum applications, these are sealed with elastomeric O-rings. For high vacuum applications, a hardened steel knife is welded to the flange and cuts into the copper gasket when the flange is bolted. One type of vacuum chamber commonly used on spacecraft is

the thermal vacuum chamber, which provides a thermal environment that reflects what the spacecraft experiences in space. [1] Figure 2.3 below shows a vacuum chamber for thin film deposition.



Figure II.3 Vacuum chambers for the deposition of thin film.

II.5.4 Substrate

A thin film substrate (see FigureII.4 below) is a layer of material deposited using thin film techniques. Many industrial and technical devices require coating with specific chemicals or thin layers of substances. [43].

Thin-film technology uses semiconductor and microsystem technology processes to fabricate circuits on ceramic or organic materials. The vacuum process used in the metal deposition process and its flexibility, especially with respect to metallization thickness and type, set thin film technology apart from printed circuit board technology. Thin-film technology connection carriers (substrates) enable extreme connection density, precise geometries of conductor and insulator materials, and high thermal conductivity with maximum reliability [44].

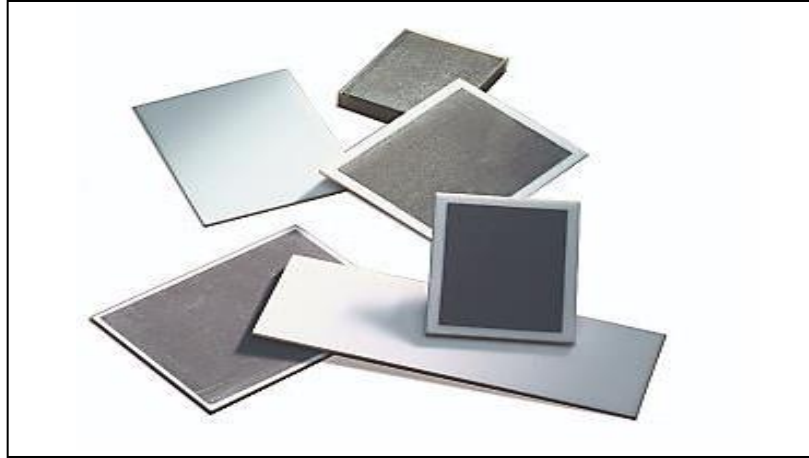


Figure II.4 Thin-Film Substrates for Microelectronics.

II.5.5 Target

It is a material (it can be a conductor or semiconductor) used in the sputtering deposition, which uses the energy of the plasma (ionized gas) on the surface of this target (cathode) to tear off one by one the atoms of the material and deposit them on the substrate. Target materials, such as disks, cylinders, or rectangles, are typically made of high-purity materials to ensure a high-quality deposition process. The target's shape and size can affect the thin film's deposition rate and uniformity. In sputtering, it is bombarded with high-energy ions, typically generated by plasma, which causes atoms or molecules to be ejected from the surface of the target. These ejected particles travel through the vacuum chamber and condense onto the substrate to form a thin film. The properties of the thin film can be controlled by adjusting the energy of the ions and the properties of this material.

In evaporation, the target material is heated to a high temperature, causing it to vaporize and condense onto the substrate. The properties of the thin film can be controlled by adjusting the temperature of the target material and the deposition rate.

The choice of target material can also affect the properties of the resulting thin film. For example, a target material with a different crystal structure or composition can produce a thin film with different properties, such as electrical conductivity and optical or magnetic properties. The target is an essential component in thin film deposition, and selecting the appropriate target material

and deposition process can significantly affect the properties and performance of the resulting thin film.

II.6 Sputtering history and application

Grove and Plucker showed that when an electrical discharge occurs between two conductive electrodes placed in an enclosure with reduced static gas pressure, a thin layer of the compound forming the opposed electrode appears. This phenomenon was long thought to be a tube lifetime-limiting effect on gas but was finally revived after 100 years, studied, and further developed for thin film growth. This technique, known as sputtering, makes it possible to obtain highly uniform thin films [45].

Around the same time, P.J. Clarke and J.S. Chapin developed the first sputtering source in the late 1960s and early 1970s. Clark arranged the cathode in a ring around the anode, but Chapin chose a planar structure and invented the planar magnetron. However, these ion sources were unsuitable for industrial applications due to their low ionization and coating rates. A.M. Drodnov took a different approach and introduced a closed-ring magnet arrangement in a plasma accelerator for surface metallization [46]. This deposition technique is often used in industry to manufacture electronic components based on thin layers.

II.7 Sputtering definition

In sputtering, atoms are ejected by bombarding a solid or liquid target with energetic particles (usually ions). This is caused by collisions between energetic incident particles and/or the resulting collisions between recoiled and surface atoms. A measure of the surface atom removal rate is the sputter yield Y , defined as the ratio of the number of atoms ejected by sputtering to the number of incident projectiles [47].

The principle of sputtering is to use the energy of the plasma (partially ionized gas) on the surface of the target (cathode) to extract the material's atoms one by one and deposit them on the substrate. For this purpose, plasma is generated by ionizing a pure gas (usually argon) using a potential difference (pulsed direct current) or electromagnetic excitation (MF, RF). This plasma

consists of Ar^+ ions, accelerated and confined around the target by a magnetic field (see Figure 2.5 below). Each ionized atom transfers energy as it hits the target, destroying those atoms with enough energy to be projected onto the substrate [48].

Sputtering is a thin film manufacturing process used in many industries, such as semiconductor processing, precision optics, and surface finishing. Sputtered thin films feature excellent uniformity, density, and adhesion, making them ideal for a wide range of applications.

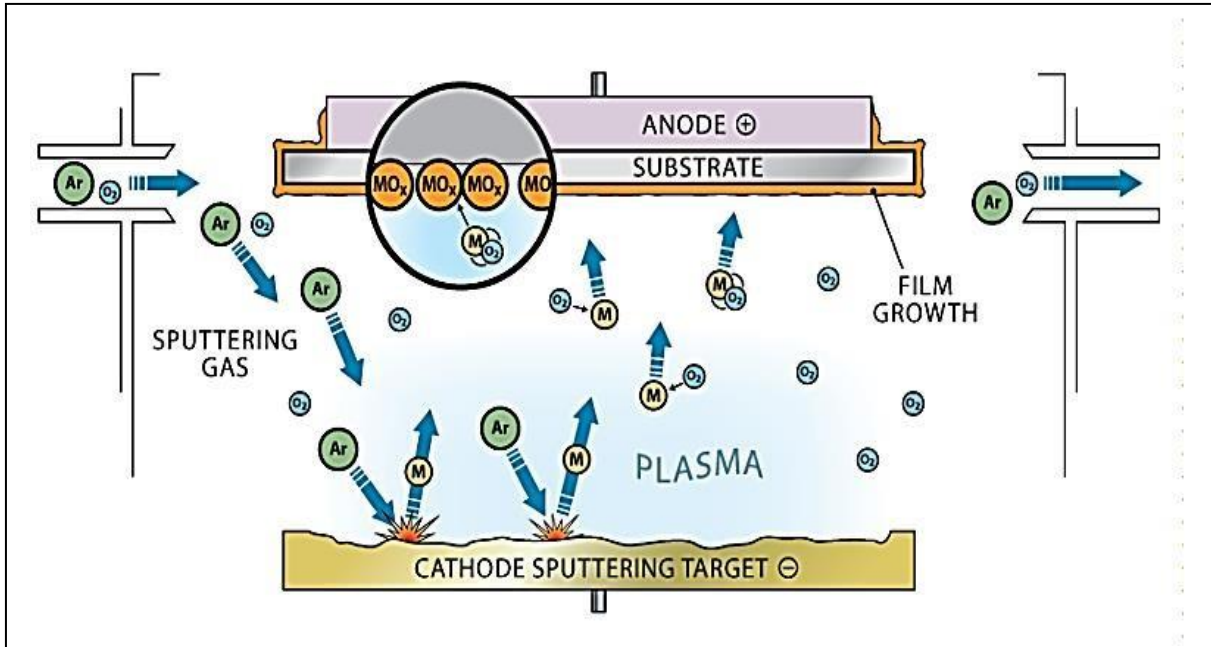


Figure II.5 Sputtering deposition.[48]

II.8 Mechanism of sputtering

Several hypotheses have been put forward regarding the sputtering mechanism, which is only partially acceptable. The sputtering rate depends on the ion mass and its energy and is highly sensitive to the incident angle of the bombarding ions. There is an energy threshold below which sputtering phenomena do not occur. Atoms emitted by the sputtering mechanism have higher energies than atoms emitted by vacuum thermal evaporation. Atoms sputtered from a single crystal target come from directions with high atomic density. The ions penetrate deeply into the crystal structures at very high energies, slowing down the sputtering rate—low secondary emission rate due to the influence of ions. Electron impact sputtering only occurs at very high energies.

Therefore, the sputtering process can be quantified based on spray performance. The sputtering process occurs when the surface of a material is bombarded with ions. When an ion enters a solid with an energy of 1 KeV, it releases its energy through collisions with atoms and electrons of the solid (Fig. 2.6). Those atoms that have started to move can move other atoms, and so on. This results in a new local distribution of species [49].

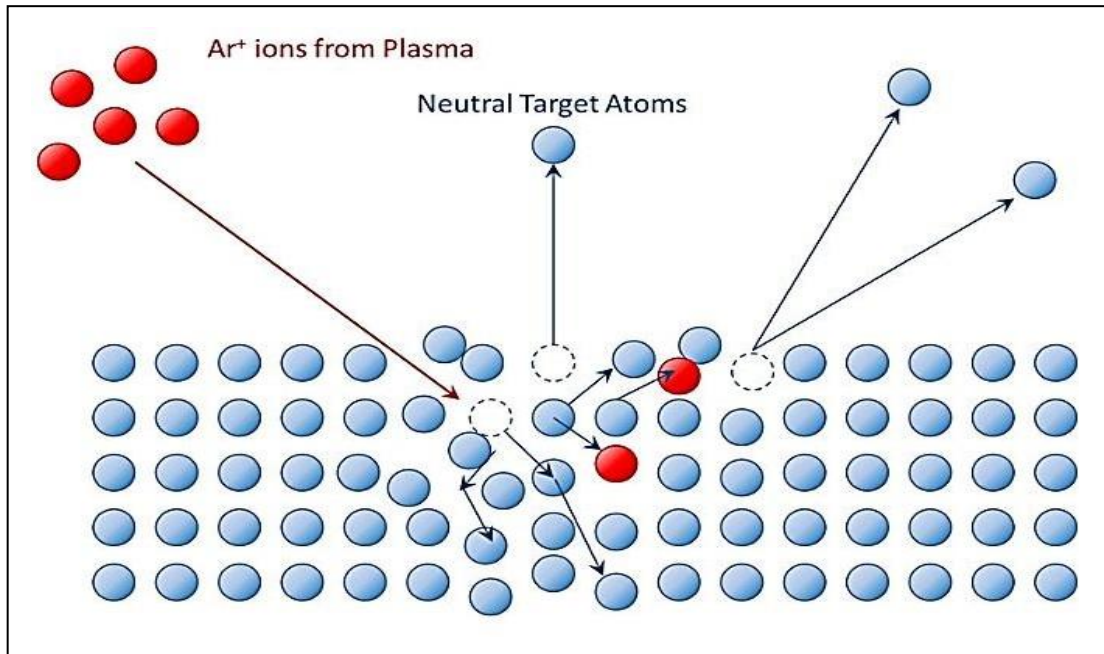


Figure II.6 A schematic of the basic mechanism of sputtering. [49]

II.9 Types of sputtering

Cathode sputtering systems come in many different types:

II.9.1. DC diode

DC sputtering is a technique that a direct current creates between two electrodes (Figure 2.7). The applied voltage is as high as 3-5 kV, so only conductive or semi-conductive materials can be deposited. The sputtering of insulating materials causes rapid polarization of the target, resulting in the accumulation of positive charges on the surface of the target. The electrons do not neutralize

these, so the voltage across the electrodes drops, the plasma quickly extinguishes, and the spray stops [50].

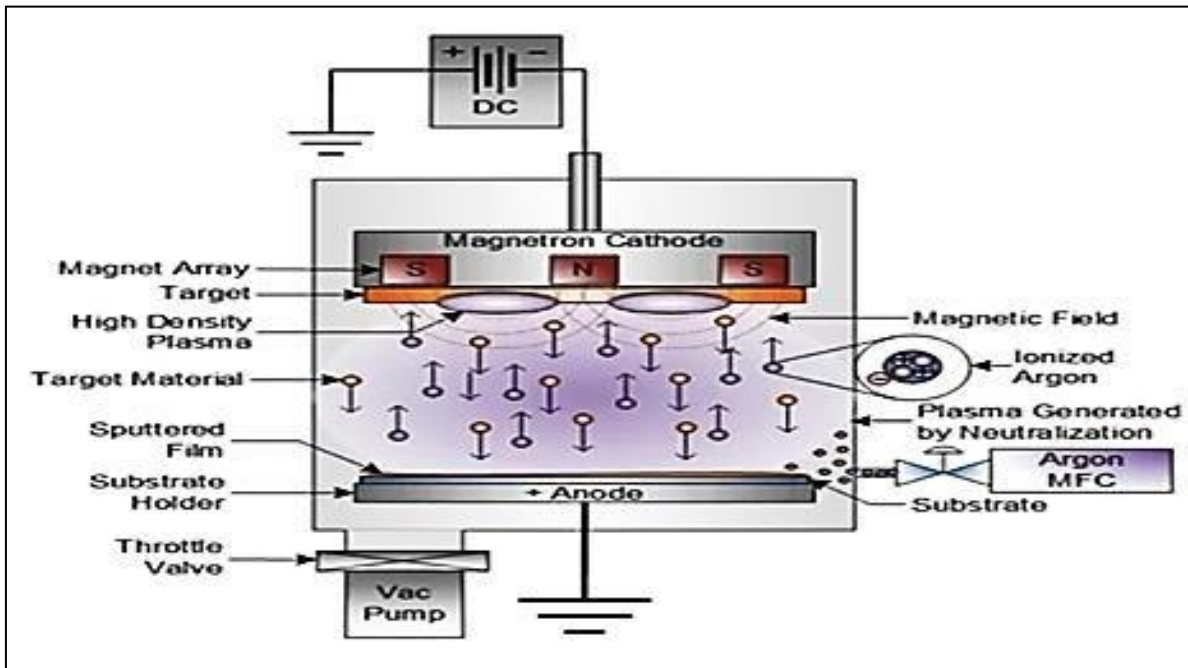


Figure II.7 Diagram of the DC Magnetron Sputtering Process. [51]

II.9.2 Radio frequency

The build-up of charge generated by ions bombarding an insulating target prevents a DC diode system from sputtering dielectric material. For this purpose, these charges must be neutralized. Using AC voltage is best for this task. This system behaves like a DC diode system during negative transitions.

During the positive transition, the charge accumulated on the target (cathode) is neutralized by electrons attracted to its positive potential. Problems arise at this level: Since the two electrodes (target holder and substrate holder) act as anode and cathode simultaneously during the two alternations, both target and substrate are pulverized. However, this is only observed at low line voltage frequencies. Therefore, the ions alternately reach one of the electrodes and have enough time to cause sputtering.

It has been reported that at radio frequencies around 13.56 MHz, ions are much more massive than electrons and thus remain immobile. In contrast, electrons oscillate with enough energy to initiate gas ionization. This results in a large number of electrons reaching the surface of the target during the positive alternation, followed by a decrease in the flux of positive ions during the negative alternation. Since the target (insulator) is capacitively coupled to the voltage generator, self-polarization produces a negative charge on its surface. Ultimately, this results in behavior similar to the DC process but with significantly higher deposition rates. [51]

In other words, the technology replaces the continuous electric field with a variable, high-frequency, very high-intensity alternating electric field. Figure 2.8 below illustrates this technique in more detail.

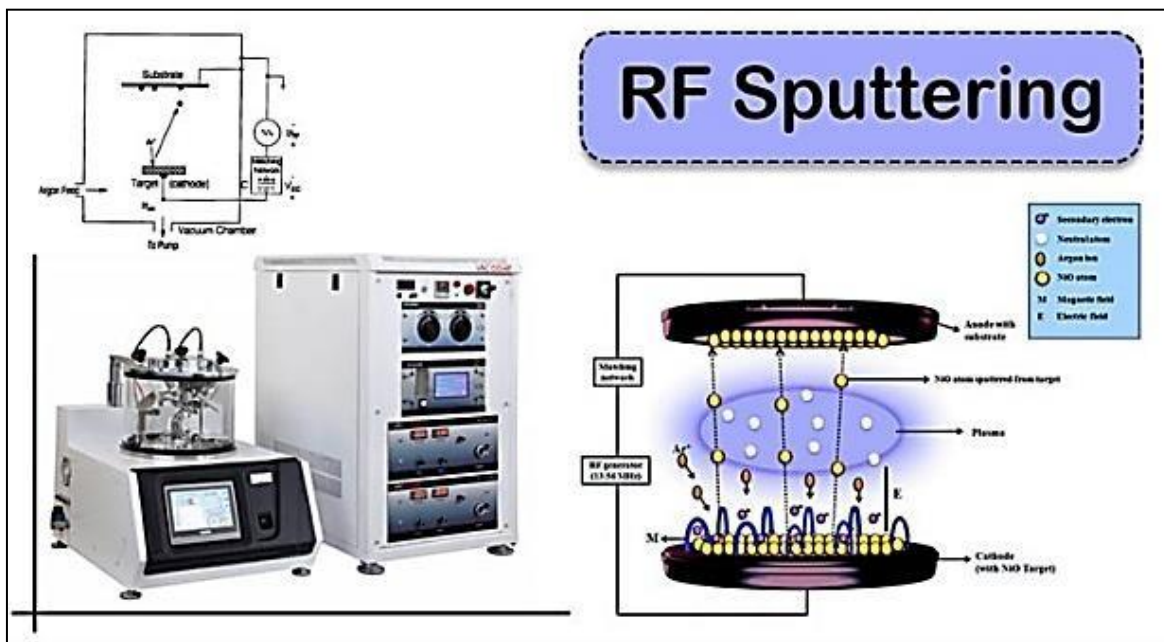


Figure II.8 RF Sputtering Processes.

a) Benefits

1. All kinds of materials can be deposited by high-frequency sputtering. Conductors, semiconductors, or insulators can all be sputtered, whether simple or composite (such as boron nitride).
2. Substrate heat generation is low

3. electron oscillation means the sputtering rate is about ten times higher than DC sputtering at the same chamber pressure.

b) Limitations

1. Relatively low coating rate.
2. The RF generation is more expensive than a DC voltage source
3. For large rectangular cathodes ($> 1\text{m}$), irregularities in plasma density (layer thickness distribution) can occur. [52]

II.9.3 Reactive Sputtering

Using a conductive and usually metallic target makes powering the magnetron much easier, as several alternatives are now possible. However, the range of materials that can be applied using this technique is limited; To resolve this problem, reactive gases can be added to the discharge. Reactive gases such as nitrogen, oxygen, hydrogen sulfide, etc., can react with the sputtered material to form compounds on the substrate. However, adding reactive gases to the discharge adds complexity to the overall process and affects the deposition process in several ways. [53]. This technique is illustrated in Figure 2.9 below.

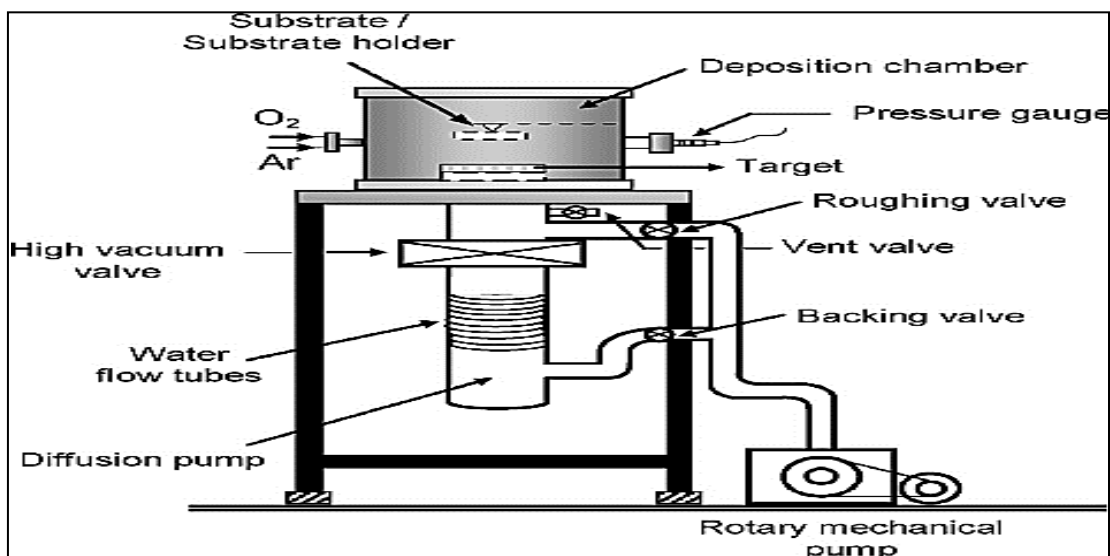


Figure II.9 Schematics of reactive sputtering system for coating deposition. [53]

II.9.4 Triode DC

The triode sputter deposition process uses a different heating filament to increase the electron density in the plasma through thermionic emission, as shown in Figure 2.12.

Using the triode increases the ionization efficiency of the plasma. It produces a powerful sputtering discharge, allowing higher discharge rates at lower target voltages and pressures than conventional PVD sputtering using DC. In some cases, the filament reacts with the working gas to form deposits, which tend to erode rapidly during deposition, thus reducing the sputtering rate. This method is used for thick coatings, but it is difficult to maintain uniform coatings because there is no electronic path-guiding mechanism to confine the plasma [54].

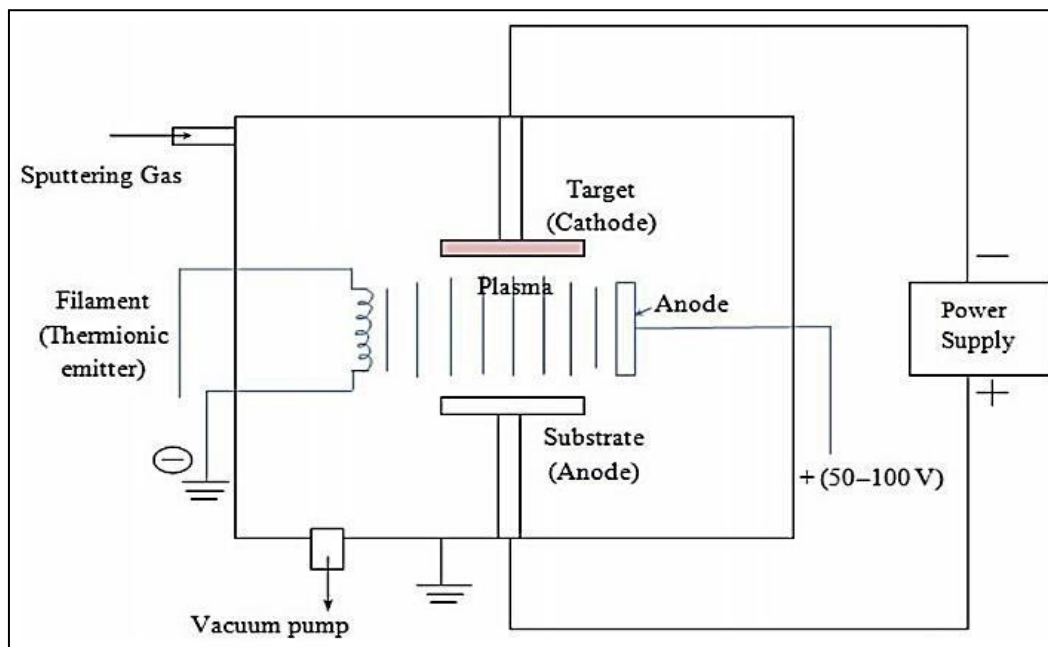


Figure II.10 working principle of triode-sputtering deposition process. [54]

II.9.5 Magnetron Sputtering

In simple sputtering systems, the plasma is maintained by secondary electrons ejected from the target by ion bombardment. Some electrons are removed from the cathode and attracted to the anode so they do not collide with gas molecules. Therefore, the ionization rate is relatively low. To solve this problem, it is possible to mount a magnetron device under the target [55].

By applying a closed magnetic field parallel to the target surface in bipolar sputtering, secondary electrons are confined to specific regions of the target surface using the orthogonal electromagnetic field formed on the target surface, increasing the ionization efficiency, density, and energy—realization high-speed sputtering. The above is the concept of magnetron sputtering.

Magnetron sputtering is the dominant technique for growing thin films because it can produce large amounts of thin films with relatively high purity and low cost. Material is deposited onto a "substrate" such as a silicon wafer from a "target" that acts as a source. [56].

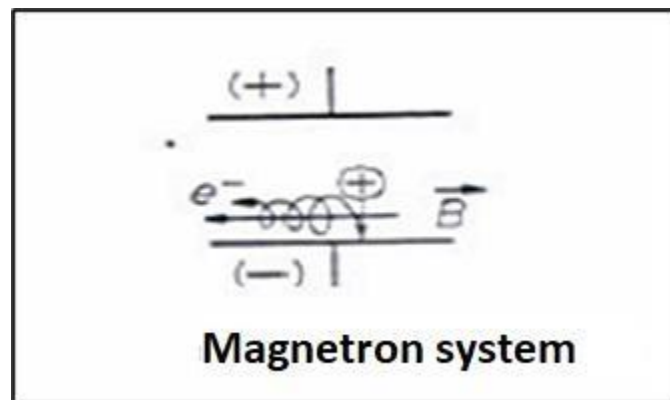


Figure II.11 Schematic representation of the diode and magnetron system. [56]

This leads to stronger ionization of the gas. Included in the enclosure, and leads to an increased deposition rate and decreased plasma holding pressure. This device adds nothing to the energy of consequent ions on the target, and it just increases the number of ions for a given target polarization voltage [57]. This technique is made more evident in the following illustration.

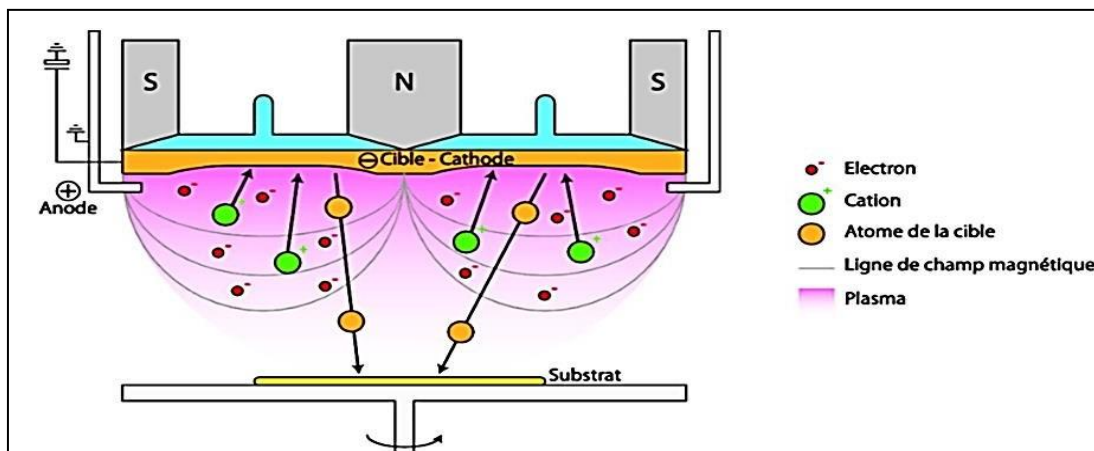


Figure II.12 Principle of magnetron sputtering [57]

II.9.5.1 Advantages

- The deposition speed is fast, the temperature rise of the substrate is limited, and the damage to the film is minor.
- Most materials can be sputtered as long as the scraped material can be made.
- Films obtained by sputtering adhere well to the substrate.
- A film obtained by sputtering has high purity, high density, and excellent film formation uniformity.
- The sputtering process has good reproducibility, and a uniform film thickness can be obtained even on a large-area substrate.
- At the same time, you can control the particle size of the film by changing the parameters.
- Various metals, alloys, and oxides can simultaneously be mixed and sputtered onto the substrate.
- Easy to industrialize.[58].

II.9.5.2 Disadvantages

- The ring magnetic field used in magnetron sputtering causes secondary electrons to move around the ring magnetic field. Therefore, the region controlled by the annular magnetic field will be where the plasma density is highest.
- Plasma instability.
- Low-temperature, high-speed sputtering of ferromagnetic materials is impossible because most magnetic flux cannot flow through the magnetic target, and an external enhancing magnetic field cannot be applied near the target surface [55].

II.10 Advantages of sputtering

- Deposition can be performed at low substrate temperatures, minimizing substrate microstructural issues and property changes due to the coating process.
- Uniform film thickness over a large area
- Good film adhesion
- Well accepted, industrially scalable and environmentally friendly process [59]

- Deposition can be performed with low background.

II.11 Disadvantages of sputtering

- Slow deposition rate (typically less than 300 nm/min)
- The line-of-sight method may not be suitable for small-diameter tubes or significant components.
- Substrate surface preparation is critical to adhesion and performance.
- High set-up cost and low energy efficiency due to the vacuum (over 70% of his input energy is used to heat the target) [59].

II.12. Conclusion

In this chapter, we have discussed the deposition of thin films, PVD, by the sputtering process. We discussed these different types in detail.

In conclusion, sputtering processes play a role in many vital areas, such as manufacturing, high-energy physics, and space science applications. This is the leading technique for depositing growth thin films, ensuring better film quality and uniformity.

Chapter 03:

Results and Discussions

III.1 Introduction

Sputtering yields have been significant in many fields where materials are in contact with plasmas. Early work concerned interactions in vacuum devices before the semiconductor age and, more recently, the design of fusion reactors and space research. Over a significant part of this timescale, sputtering has also been used as an applied method in conjunction with surface analysis methods in order to obtain composition–depth profiles in the outermost layers [65]

This chapter will delve into the simulation of sputtering yield using various computational methods. Utilizing esteemed software tools such as SRIM and SIMTRA, which are based on the Monte-Carlo method calculations, will enable us to comprehensively investigate the underlying principles governing the sputtering phenomenon. Our exploration will encompass an in-depth analysis of crucial aspects, including the intricate interplay between ions and the target surface, the intricate energy transfer mechanisms dictating the sputtering yield, the influences of incident angles, and the distinctive characteristics of different plasma gases. Additionally, we will examine the computation of sputter yield utilizing the Yamamura and Tawara models, subsequently juxtaposing their outcomes with those obtained from the SRIM simulations. This comparative analysis will provide valuable insights and facilitate a comprehensive understanding of the subject.

III.2 Monte Carlo Simulation

The Monte Carlo simulation is a computerized mathematical technique using random numbers to simulate a mathematical or physical problem to find the desired solution. ("Monte Carlo simulation" means using the chance to study deterministic problems. This also means that when solving a particular problem, for example, using purely mathematical, this is almost unavoidable if the solution is too complex (especially if there are too many variables involved) or if the problem is too significant (mainly because there are too many variables). Numerical approximation techniques can be used in a reasonable amount of time.

This technique is one of the most widely used in all areas of applied mathematics: Physics, Chemistry, Biology, Economics, Sociology, etc. Take the prediction, for example. Monte Carlo simulations are used to address a wide variety of problems in many areas, such as

investment, economics, physics, and engineering. Also called multiple probability simulation. [60].

III.3 History of Monte Carlo

The Monte Carlo method owes its name to Nicholas Metropolis and Stanislaw Ulla in the 1940s. These authors were the first to describe the use of this method for calculations related to the Manhattan First Design Project atomic bombs. Its name dates from the 1944's and refers to the principality of Monaco and its casino, a hotspot for gambling. In the immediate post-war period, Von Neumann, Fermi, and Ulam introduced the possibility of applying the Monte Carlo method in the scientific field; for example, for approximating the eigenvalues of the Schrödinger equation.

The systematic study was carried out by Harris and Khan in 1948. After an eclipse due to too intensive use during the 1950s, the Monte Carlo method has returned to favour many problems: in the physical sciences, in economics, for electoral forecasts, etc., wherever simulation processes are successful.

The Monte Carlo technique is particularly suitable for calculating integrals of all sizes. Indeed, the strength of this method is that the calculation error does not depend on the number of variables in the problem.[61].

The Monte Carlo codes are becoming an essential tool in the physics of radiation-matter interaction, both in the field of radiation protection and medical physics, especially radiation therapy. The possibility of including a large part of the physics of elementary interaction in the form of increasingly elaborate numerical models makes them more predictive, precise, and reliable. They also allow the determination of quantities inaccessible by experience. [62].

III.4 The principle of the Monte Carlo method

The basic principle of the Monte-Carlo method consists in estimating the average result of an amount of interest generated by a series of stochastic events. In the physics of particle transport (photons, electrons, etc.), Monte Carlo methods describe the history of each particle traversing a single trajectory resulting from a series of interactions. The selection of each interaction results from a random process that can be described by a probability density

function for obtaining the average energy absorbed by the medium and thus determining the dose delivered to the medium. Figure (2.10) gives an overview of the basic principles of the Monte Carlo method. [63].

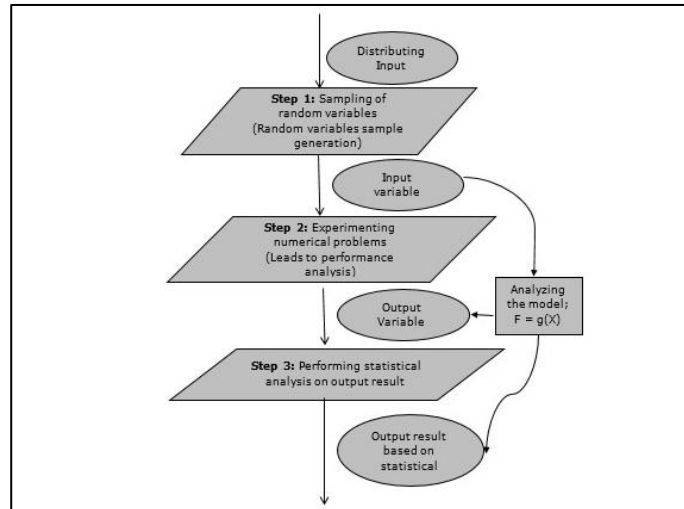


Figure III.1 Monte Carlo principal diagram

III.5 Advantages and disadvantages of the Monte Carlo method

A Monte Carlo simulation estimates the probability of a given income. As such, it is widely used by investors and financial analysts to assess the possibility of success of an investment they are considering. It has several advantages and disadvantages [60]:

a) Advantages

- The main advantage of these methods is that they offer the possibility of simulating second-order duets of larger systems, more extensive than those accessible by quantum or dynamic methods.
- The Monte Carlo method reflects the exact evolution of the system. If the simulation is performed precisely and accurately, the final result can be directly compared and, in some cases, indistinguishable from the experience.
- Relevance to experimental procedures.
- Thermodynamic equilibrium is not required for this category.
- No saving of objects.
- Time follows the change of mechanism.

- Monte Carlo simulation was developed to overcome the perceived disadvantage of other methods of estimating probable outcomes.
- The difference is that the Monte Carlo method tests and averages several random variables rather than starting with an average. [60].

b) Disadvantages

- The activation mechanisms and related ranges need to be known in advance.
- Hard work for efficient coding of dome mechanisms and structures.
- Arrhenius's law may need to be revised, for instance, when kinetic energy is accumulated during the healing of an obstacle and can be used for other obstacles. [64]
- Like all financial simulations, the Monte Carlo method uses historical price data to project future price data. It then disrupts the pattern by introducing random variables represented by numbers. Finally, he averages these figures to estimate the risk that the model will be disturbed in real life. [30].

III.6 SRIM software

SRIM is a group of programs that calculate the stopping and range of ions (up to 2 GeV/amu) into matter using a quantum mechanical treatment of ion-atom collisions (assuming a moving atom is an "ion" and all target atoms as "atoms"). Statistical algorithms make This calculation very efficient, allowing the ion to make jumps between calculated collisions and then average the collision results over the intervening gap.

During the collisions, the ion and atom have a screened Coulomb collision, including exchange and correlation interactions between the overlapping electron shells. The ion has prolonged range interactions creating electron excitations and plasmons within the target. These are described by describing the target's collective electronic structure and interatomic bond structure when the calculation is set up (tables of nominal values are supplied). The charge state of the ion within the target is described using the concept of effective charge, which includes a velocity dependent charge state and extended range screening due to the collective electron sea of the target.

A full description of the calculation is found in our tutorial book "SRIM - The Stopping and Range of Ions in Solids" by J. F. Ziegler and J. P. Biersack in 1985. This book presents the

physics of ion penetration into solids in a simple tutorial manner, then presents the source code for SRIM programs with a full explanation. Further chapters document the accuracy of SRIM and show various applications.

TRIM (the Transport of Ions in Matter) is the most comprehensive program, and will accept complex targets made of compound materials with up to eight layers, each of different materials. It will calculate the final 3D distribution of the ions and all kinetic phenomena associated with the ion's energy loss: target damage, sputtering, and ionization. All target atom cascades in the target are followed in detail. [66]

III.6.1 Inputs and Outputs of SRIM

Figure 3.1 shows the interface of SRIM software with the various available options and different parameters to input for the calculation.

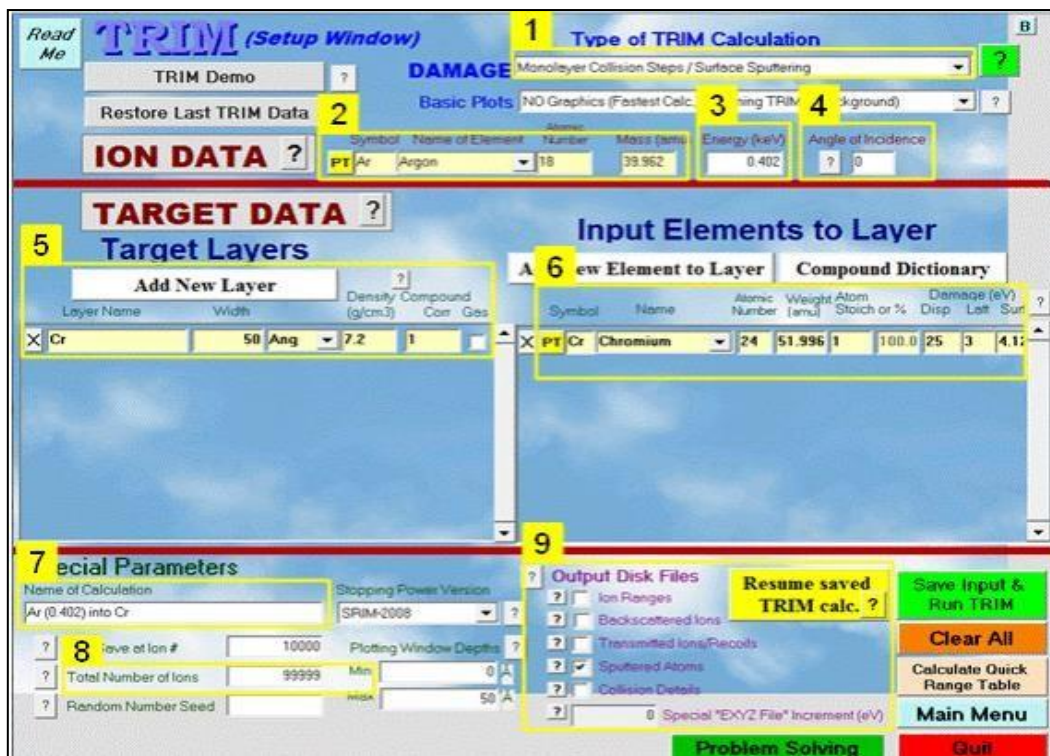


Figure III.2. SRIM software interface

The TRIM software interface has several options. Options 1 to 9 allow you to choose the input and output parameters grouped in table III-1.

Table III.1 Input and output parameters of TRIM.

Option	Paramètres
1	It allows you to choose the phenomena to study among: <ul style="list-style-type: none"> • Target damage and ion distribution, • Ion implantation, • Sputtering, • Specific energy/angle/depth of ions, • ...
2	Incident ion data: name, symbol, atomic number, atomic mass.
3	Ion Energy in keV.
4	The angle of incidence of ions between 0 and 90 degrees.
5	The nature of the material subjected to ion bombardment.
6	The name, atomic number, stoichiometry of the bombarded material, and the binding energy of atoms.
7	Simulation name: gas (energy in keV) - target.
8	The number of injected ions (the maximum number can reach 10^7 , and the default value is set to 716,381 ions).
9	Range.txt: Table of the final distribution of ions and recoil target atoms. Backscat.txt: Kinetics of all backscattered ions (energy, location, and trajectory). Transmit.txt: Kinetics of all transmitted ions (energy, location, and trajectory). Sputter.txt: Kinetics of all target atoms sputtered by cathodic sputtering. Collision.txt: Table of all atomic collisions between ions and targets leading to target damage.

III.7 SIMTRA Software

SiMTra, Simulation of the Metal Transport, was developed by Koen Van Aeken for the simulation of trajectories of gas-phase particles in a definable 3D configuration where the interatomic collision modeling, the potentials, and thermal motion of the background atoms are included in the code. It has known as a binary collision Monte Carlo program that allows the simulation of the transport of sputtered particles through the gas phase flux during sputtering [66]

In this chapter, we delve into applying SIMTRA (Simulation of Material Transport) software for studying the transport and deposition of particles in various systems. SIMTRA is a powerful computational tool that utilizes advanced numerical techniques to simulate the intricate processes of particle transport, diffusion, and deposition. Using SIMTRA, we can unravel the underlying mechanisms driving particle deposition, optimize coating processes, and improve the efficiency of particle-based systems.

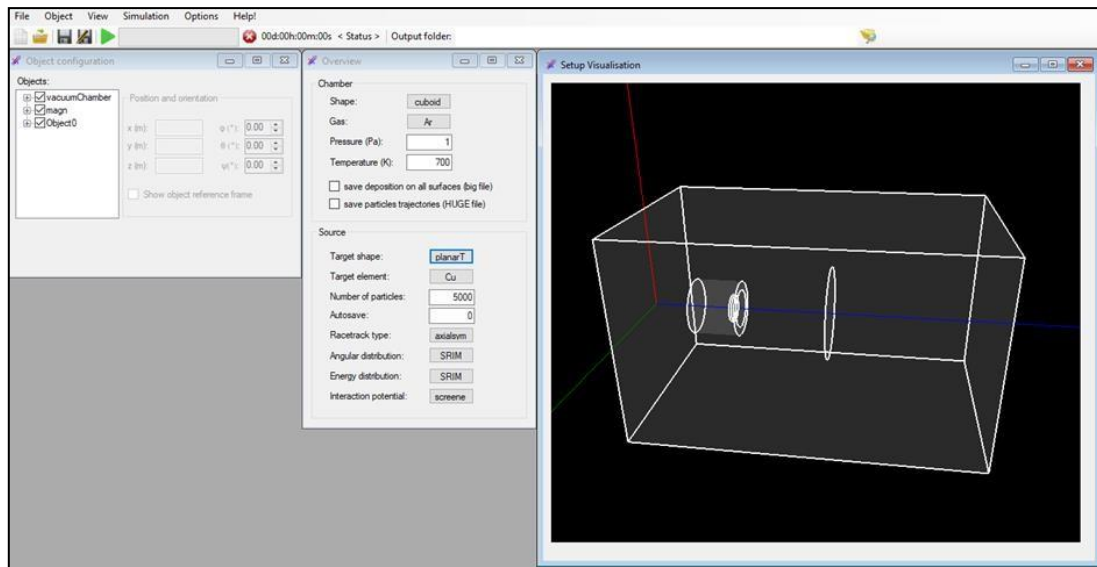


Figure III.3 SIMTRA software interface

III.8 Modeling of sputtering yield

III.8.1 Yamamura and Tawara model

The Yamamura and Tawara model, also known as the Yamamura-Tawara model, is a widely used mathematical model in the field of materials science and engineering. It is specifically applied to the simulation and analysis of cathodic sputtering processes, an empirical fitting formula for multi-component materials $Y(E)$ is proposed:

$$Y(E) = 0,042 \times \frac{(Z_2)\alpha(\frac{M_1}{M_2})}{U_S} \times \frac{S(E)}{1+\Gamma K e e^{0,3}} \times (1 - \sqrt{\frac{E_{th}}{E}})^s \tag{1}$$

: The reduced energy

:is an energy independent function of the ration of ions and target masses

: The nuclear stopping power of the target

U_s : the surface binding energy

Γ : parameter that factor in the contribution of reflected ions to the recoil cascade and takes the form:

$$\Gamma = \frac{(Z_2)}{1 + (\frac{M_1}{7})^3} \quad (2)$$

And we have

$$W = 0,35 \times U_s \quad (3)$$

where Z_1 and M_1 are the atomic number and mass of the probe ion (here argon) and Z_2 and M_2 are those for the target atoms. E_{th} is the threshold energy

$$E_{th} = \left\{ \begin{array}{ll} (1 + 5,7 \times \frac{M_1}{\gamma}) \times \frac{U_s}{\gamma} & \text{when } M_1 < M_2 \\ 6,7 \times (\frac{M_2}{\gamma}) & \text{when } M_1 > M_2 \end{array} \right. \quad (4)$$

With the elastic collisions is

$$\gamma = \frac{4 \times M_1 \times M_2}{(M_1 + M_2)^2} \quad (5)$$

Here we use the nuclear stopping power of the target given by

$$S_n(E) = 84,78 \frac{Z_1 \times Z_2}{(Z_1^{2/3} + Z_2^{2/3})^{1/2}} \times \frac{M_1}{M_1 + M_2} \times S_n(\varepsilon) \quad (6)$$

where Z_1 and Z_2 are the atomic number and mass of the probe ion and M_1 and M_2 are similarly for the target atoms where the inelastic electronic stopping power is

$$S_n(\varepsilon) = \frac{3,441 \times \sqrt{s} \times \ln(s + 2,718)}{1 + 6,355 \times \sqrt{s} + (6,882 \times \sqrt{s} - 1,708)} \quad (7)$$

And if E is in eV we have

$$\varepsilon = \frac{0,03255}{Z_1 \times Z_2 (Z_1^{2/3} + Z_2^{2/3})^{1/2}} \times \frac{M_2}{M_1 + M_2} \times E \quad (8)$$

The expression of α When $M_1 \geq M_2$

When $M_1 \leq M_2$

$$\alpha = 0,249 \times \left(\frac{M_2}{M_1}\right)^{0,56} + 0,0035(M_1)^{1,5} \quad (10)$$

Where:

$$K_e = 0,079 \times \frac{(M_1+M_2)^2}{M_1^2 \times M_2^2} \times \frac{Z_1^3 \times Z_2^2}{(Z_1^3+Z_2^3)^4} \quad (11)$$

The nuclear stopping power of the target is defined as:

$$S_n(E) = 84,78 \times \frac{Z_1 \times Z_2}{(Z_1^3+Z_2^3)^2} \times \frac{M_1}{M_1+M_2} \times S_n(\varepsilon) \quad (12)$$

And we have

$$S_n(\varepsilon) = \frac{3,441 \times \sqrt{s} \times \ln(s-1,708)}{1+6,355 \times \sqrt{s} + s(6,882 \times \sqrt{s}-1,708)} \quad (13)$$

Where:

$$\varepsilon = \frac{0,03255}{2} \times \frac{M_2}{M_1+M_2} \times (ev) \quad (14)$$

$$Z_1 \times Z_2 \times (Z_1^3+Z_2^3)^2$$

III.9 comparison between modulization and SRIM calculation

In our previous investigation, we focused on the sputtering behavior of copper (Cu) materials, specifically examining the impact of varying ion energy on the sputtering yield. Our findings revealed the following values for different energy levels:

Table III.2 simulation and theoretical results of sputtering yield

E(Kev)	Theoretical results of Y(atoms/ion)	Experimental results of Y(atoms/ion)
0,1	0,645	0,652
1	3,77	3,71
10	8,84	8,13
100	5,76	5,94

Chapter 03	2,04	Results and Discussions
10000	0,104	0,369

Through the comparison between the results obtained from SRIM and the results of the Yamamura and Tawara models, the consistency and accuracy of SRIM in simulating ion energy loss can be evaluated. This comparative analysis validates the fundamental physical principles and assumptions utilized by SRIM and assesses the suitability of the Yamamura and Tawara models in capturing ion-matter interactions. The agreement between the results from SRIM and the Results of the Yamamura and Tawara models in Table III.2 strengthens the confidence in the dependability and precision of SRIM simulations for comprehending and forecasting ion energy loss and sputtering yield phenomena.

III.10 Materials used in the simulation

III.10.1 Copper (Cu)

Copper possesses numerous advantages due to its ease of processing and excellent electrical and thermal conductivity. Historically abundant, copper has played a vital role in various industries. However, recent closures of copper mines have created uncertainty regarding future supplies. This comes when the demand for copper materials continuously increases, particularly in renewable energy generation, lithium batteries, and next-generation power transmission infrastructure development. Additionally, copper foil is widely used in lithium batteries, further exacerbating the demand. As a result, copper prices have surged, transforming copper into a "precious" metal. In response, innovative approaches have been developed to maximize the utilization of thin copper film.[67].

III.6.2 Silicon (Si)

Silicon is widely regarded as a fundamental material in semiconductor technology, owing to its exceptional electronic properties, high charge carrier mobility, and well-established fabrication processes. Its significance in modern technology, such as thin film solar cells, emerged during the 1970s. These photovoltaic cells, which employ silicon, offer several advantages over traditional silicon wafer solar cells.

One notable advantage is the reduced silicon material required in thin-film solar cells. This efficiency in material usage is achieved due to the shorter conduction distance between electrons and holes, thereby mitigating the severe dependence on the purity of the silicon material. Consequently, this aspect contributes to a decline in material costs.

Furthermore, unlike other semiconductor materials being explored for photovoltaic cell development, silicon does not necessitate an exceptionally high absorption efficiency. This characteristic enables researchers to focus on optimizing other aspects of the cell design and manufacturing processes, potentially leading to further advancements in developing semiconductor photovoltaic cells [68].

III.10.3 Indium oxide (In₂O₃)

The significance of indium tin oxide (ITO) thin films in the field of optoelectronics has spurred a multitude of research studies. ITO films are widely recognized as n-type semiconductors, exhibiting a resistivity ranging from 10^{-3} to 10^{-4} ohm-cm [69].

The applications of ITO thin films are vast and encompass various fields. They find utility as photovoltaic cell components in transistors, transparent conductive electrodes in solar cells, photochemical and photoconductive devices in liquid crystal displays, gas sensor devices, and organic light-emitting diodes (OLEDs). Over time, several methods have been employed for synthesizing ITO films, including R.F. magnetron sputtering, thermal evaporation, chemical vapor deposition, laser pulse deposition, sol-gel processes, spray pyrolysis, and the spin coating technique.

It is important to note that the characteristics and applications of ITO thin films continue to be the subject of ongoing research and development in the pursuit of improved performance and expanded functionality. ITO thin films have immense applications such as photovoltaic cell in transistors, transparent conductive electrode for solar cell photochemical and photoconductive devices in liquid crystal display gas sensor devices organic light emitting diodes (OLED) Till today so many methods were adopted to synthesize doped or un-doped ITO films such as R.F. Magnetron Co-sputtering, Thermal Evaporation, Chemical Vapor Deposition, Laser Pulse deposition, sol-gel, Spray Pyrolysis and spin coating technique. [69].

III.11 Results and simulation of SRIM software

The main purpose is to calculate the sputtering yield $Y(E)$ using the Monte Carlo simulation program SRIM, which uses the binomial collision approximation (BCA) for ion-solid interactions. It is an open-source program suitable for practical use. Different angles of incidence were used ($\theta = [0^\circ, 15^\circ, 30^\circ, 45^\circ, 60^\circ, 75^\circ, 85^\circ]$). The sputtering yield varied with

the applied energy ($E = [100 \text{ eV}, 1 \text{ KeV}, 10 \text{ KeV}, 100 \text{ KeV}, 1000 \text{ KeV}]$), and the target was bombarded by gas ions (argon and xenon) in the vacuum chamber. Materials (Si, Cu, In_2O_3). Incident angle and impact energy must be considered for optimum results with any material. Therefore, we focus on the collision energy and angle of incidence that give the highest sputter yield. They are named E_{max} and θ_{max} , respectively. These two parameters represent the maximum number of emitted atoms extracted from the target.

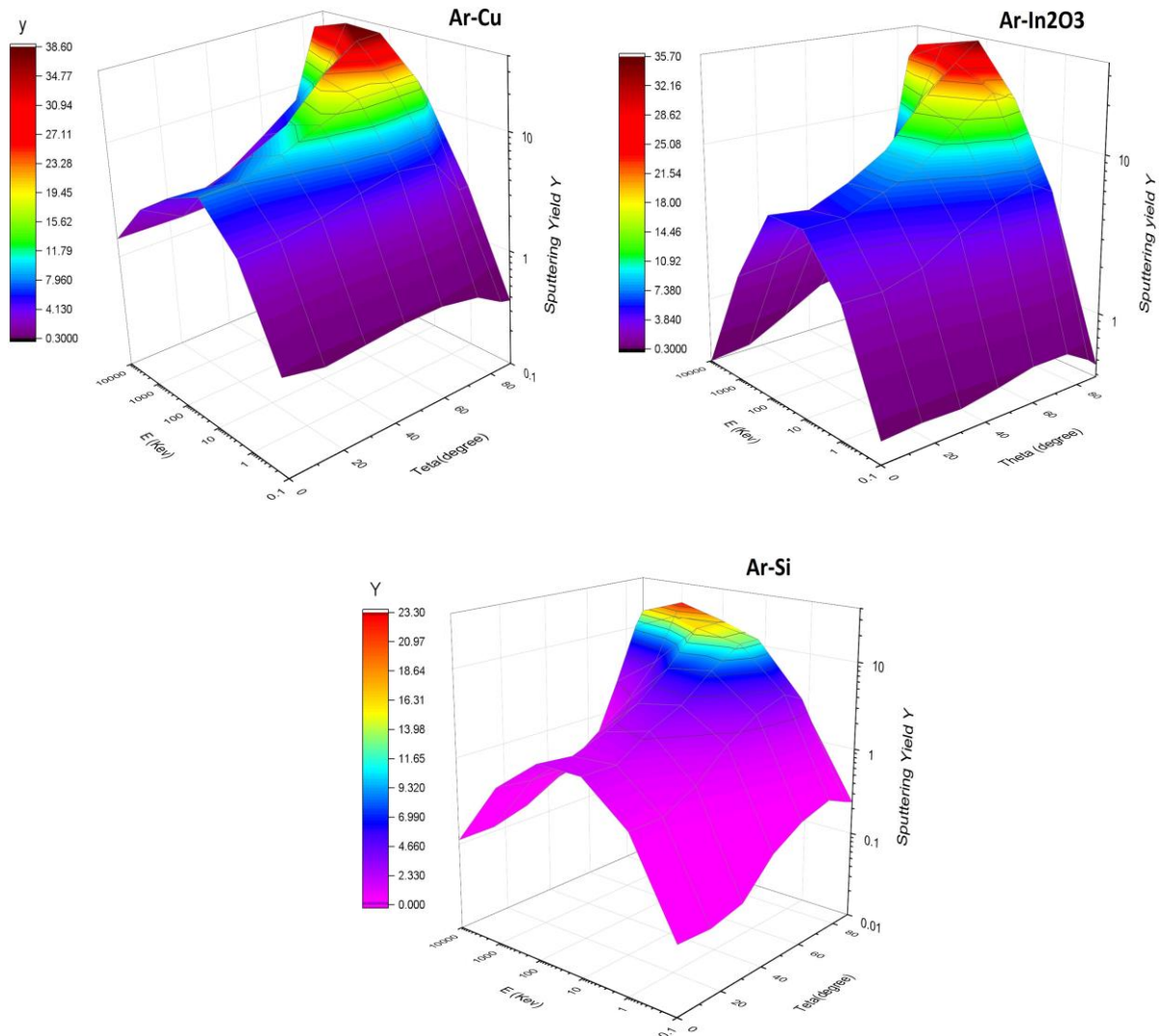


Figure III.4 sputtering yield as a function of energy for materials (Cu-Si-In2O3) bombarded by Argon.

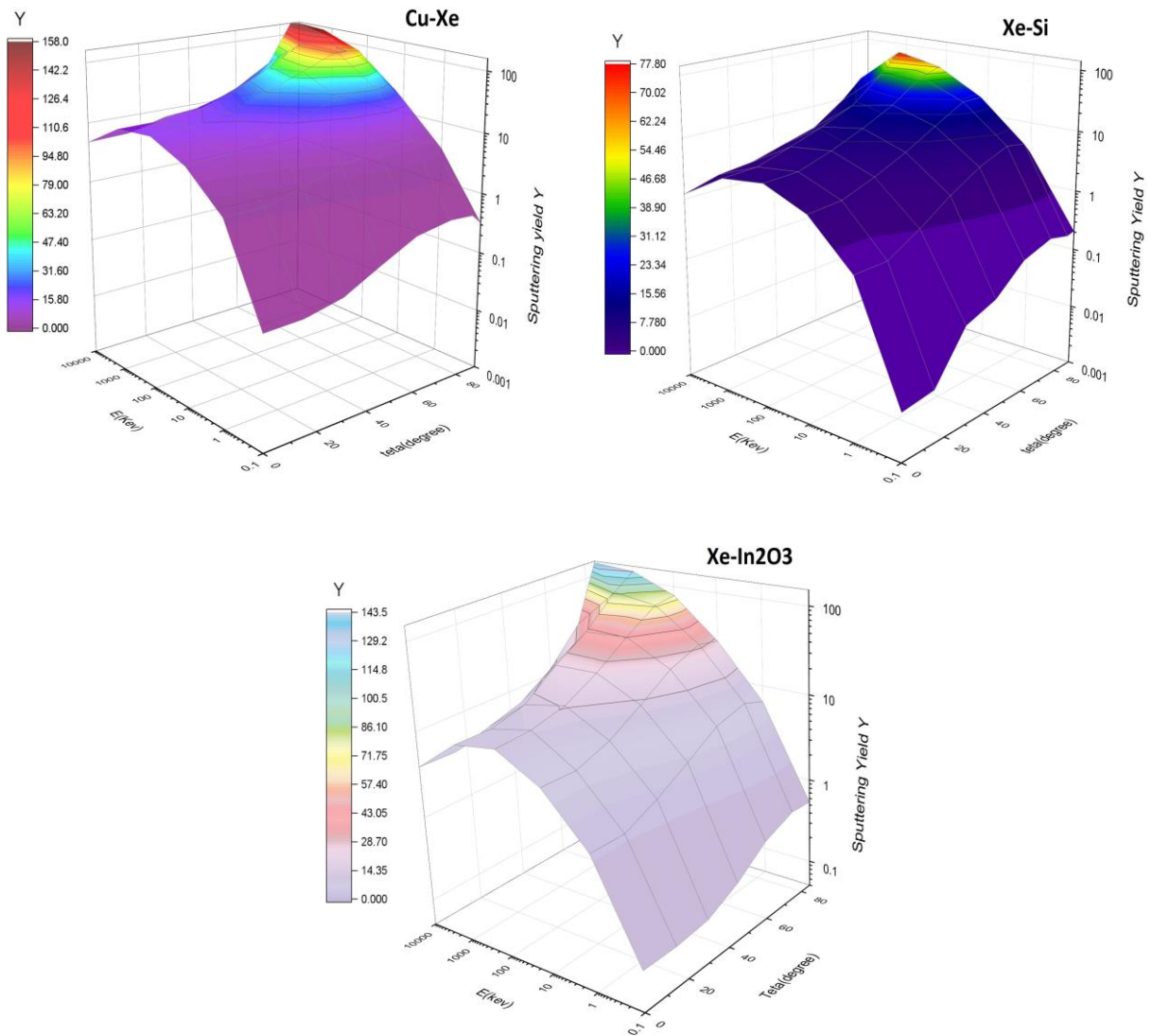


Figure III.5 sputtering yield as a function of energy for materials (Cu-Si-In₂O₃) bombarded by Xenon.

The sputtering yield rates for Si, In₂O₃, and Cu materials attacked by Ar and Xe vacuum chamber plasma gas, using various energy and incidence angle values, are shown in Figures 3.3 and 3.4 below so we can observe that the sputtering yield increases up to an energy max, and then decreases beyond that value beam interacts with the target surface can be used to explain this observation. At energies max, the ion's energy is sufficient to dislodge molecules or atoms off the target surface, increasing the sputtering yield. After that value, the sputtering decreases because the ion energy will be powerful to damage the materials.

The results demonstrate the behavior of Ar and Xe gases, so we can also observe that bombarding with Xe ions produced a higher sputtering yield than bombarding with Ar ions because xenon has a larger atomic mass.

We can observe from the previous figures that the sputtering yield can vary depending on the materials used, and we see that a low sputtering yield is present in silicon. This indicates that it is less likely to be ejected from the target surface when interacting with an ion beam. As we know, silicon is a semiconductor with an ordered crystalline structure, making it more difficult for them to be ejected from the target surface when interacting with the ion beam. When we compare copper to silicon, we notice that Cu has a higher sputtering yield than Si. Copper is more easily ejected from the target surface because it has a less ordered crystalline structure, and its atoms are less tightly bound and more mobile, making it a popular choice for sputtering in producing electrical conductors. In the case of indium oxide, it demonstrates a relatively high sputtering yield. As a result, during the sputtering process, thin films are effectively and uniformly deposited, and that is because of their chemical and crystalline structure. In₂O₃ has a low resistivity which promotes better electrical conduction during the sputtering process.

A) Simulation results obtained from the SRIM simulation

Between 100 eV and 1.5 keV are the typical operating voltages utilized in commercial and industrial sputtering applications. $E_{opt}=1.5$ KeV was chosen as the ideal energy source as a result. The ideal incidence angle for the sputtering yield for both gases was $\theta_{opt} = 75$.

Table III.3 Sputtering yield for 1,5 KeV of the energy of the bombardment ions (Ar and Xe) as a function of various incidence angles of Si, In₂O₃ and Cu materials.

Gas \ Angles		0°	15°	30°	45°	60°	75°	85°	89°
Ar	Cu	4.70	4.92	5.57	6.59	7.84	7.35	5.21	3.51
	Si	0.703	0.704	1.21	2.11	3.87	5.39	4.42	2.79
	In ₂ O ₃	3.25	3.35	3.62	4.87	6.81	7.86	6.43	4.07
Xe	Cu	2,72	2,73	3,90	6,26	8,86	9,24	6,85	4,65
	Si	0,521	0,582	1,16	2,36	4,74	7,54	6,44	3,99
	In ₂ O ₃	2.32	2.313	3.02	5.20	8.34	10,60	8,76	5,78

III.12 Conclusion

As a thin film production process, sputtering deposition is affected by a number of variables, including the target material, sputtering gas, incidence angle, and ion beam energy. The composition, structure, adhesion, and surface characteristics of the resultant thin films are greatly influenced by these variables. The manufacturing of high-quality films with distinctive qualities appropriate for varied applications is made possible by optimizing these parameters. Enhancing the performance and dependability of thin films in a variety of applications, such as electronics, optics, and functional coatings, requires a complete knowledge of the relationships among these variables.

III.13 Simulation of Metal transfer (SIMTRA)

We choose $\theta_{opt} = 75$ and $E_{opt} = 1.5$ KeV as the default incidence angle and energy entrance settings for the SIMTRA program, respectively, and run the simulation to see how these ejected particles move under various temperature and pressure and distance conditions.

a) The impact of changing pressure

The results of the SIMTRA (Simulation of Metal Transfer) simulation are presented in the curves below. In this part, we examine the impact of high pressure by introducing three different pressures (0.5, 1, and 2 Pa) while keeping the vacuum chamber's temperature constant at 300 K. Fig. 6 shows the consequences of bombarding the target with the same gases (argon, xenon) and materials (Cu, In₂O₃, and Si).

- Argon

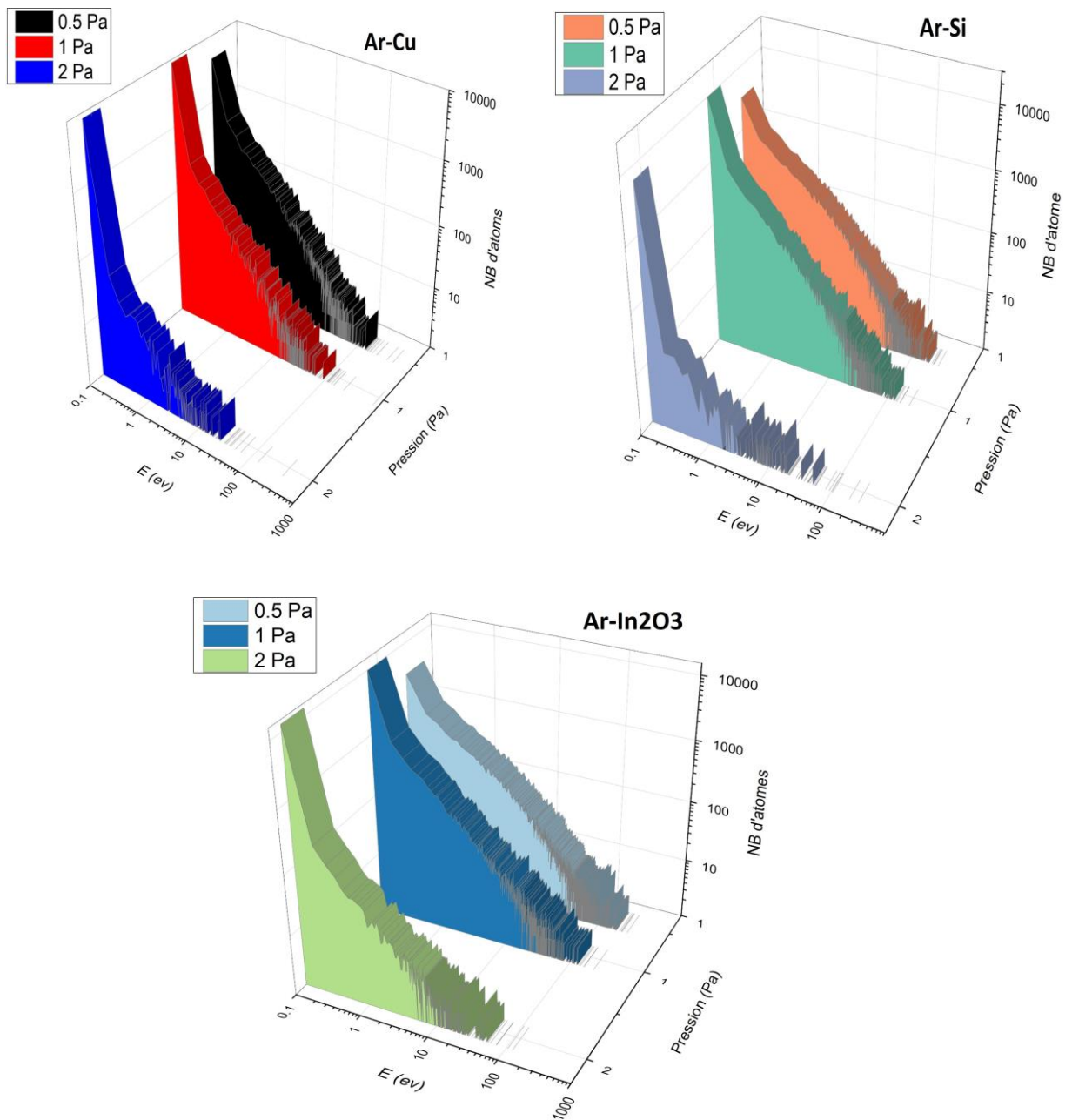


Figure III.6 Depending on the pressure in the chamber, the energy distribution of: a) Cu, Si, In₂O₃, arrives at the substrate levels and is bombarded by Ar ion beam.

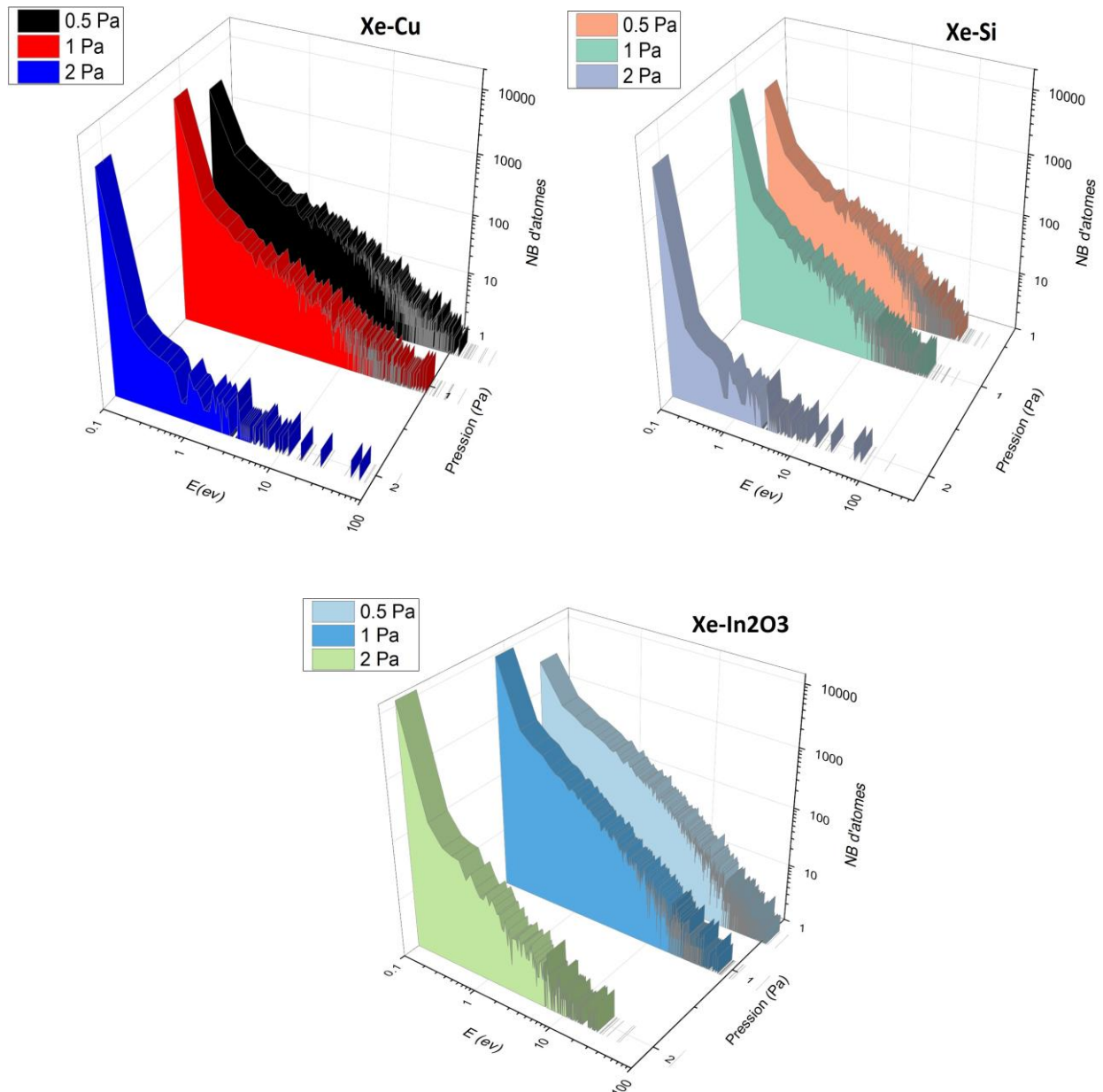


Figure III.7 Depending on the pressure in the chamber, the energy distribution of: (Cu, Si, In2O3) arrives at the substrate levels and is bombarded by Xe ion beam.

The results are important because they clearly demonstrate the impact of energetic bombardment on the stress, microstructure, and surface roughness of the deposited films. The majority of atoms arrived with energies in the range of 0.1 to 1 eV, while only a small number of atoms were observed in the higher energy tail extending up to 100 eV. At higher pressures, collisions between atoms and the surrounding gas occur more frequently, resulting in a different energy distribution. Pressure can also influence atom diffusion in the sputtering environment. Higher pressures can lead to more constrained diffusion, reducing the number of

atoms observed at various energies. Additionally, elevated pressures typically result in increased collisions between ejected atoms and nearby gas molecules.

- **The number of atoms arriving on the substrate depends on the applied pressure**

Table III.4 shows the total number of atoms sprayed on the substrate depending to the pressure.

Table III.4 The total number of atoms reaching the substrate

	Pressure	Copper	Indium oxide	Silicon
Argon	0,5	13821	20854	12698
	1	12983	19711	10658
	2	9122	15073	6821
Xenon	0,5	9683	13539	10187
	1	8479	11552	8243
	2	5487	7456	5589

In atom count with an increase in pressure. Increasing the pressure causes the number of atoms to decrease. The likelihood of collisions between the ejected atoms and the gas molecules in the surroundings has increased, which might cause this drop. The possibility of the expelled atoms reaching the substrate decreases because of these collisions, which change their trajectories. Increased pressure promotes atom diffusion, leading to dispersion inside the sputtering chamber and a reduction in direct atom-to-substrate collisions. In addition, increased pressure increases gas density, which hinders atom diffusion and lowers the number of atoms that may diffuse toward the substrate. Moreover, we can also observe a difference between xenon and argon concerning the number of atoms arriving at the substrate. We can see that xenon's number of atoms is higher than argon, and we can explain it by their effect on atom diffusion.

B) The impact of temperature

The following curves show the number of atoms that arrive on the substrate for each considered temperature when the selected pressure is 0.5 Pa and with the temperature fluctuation (100, 500, and 700 K), as determined using SIMTRA code simulation.

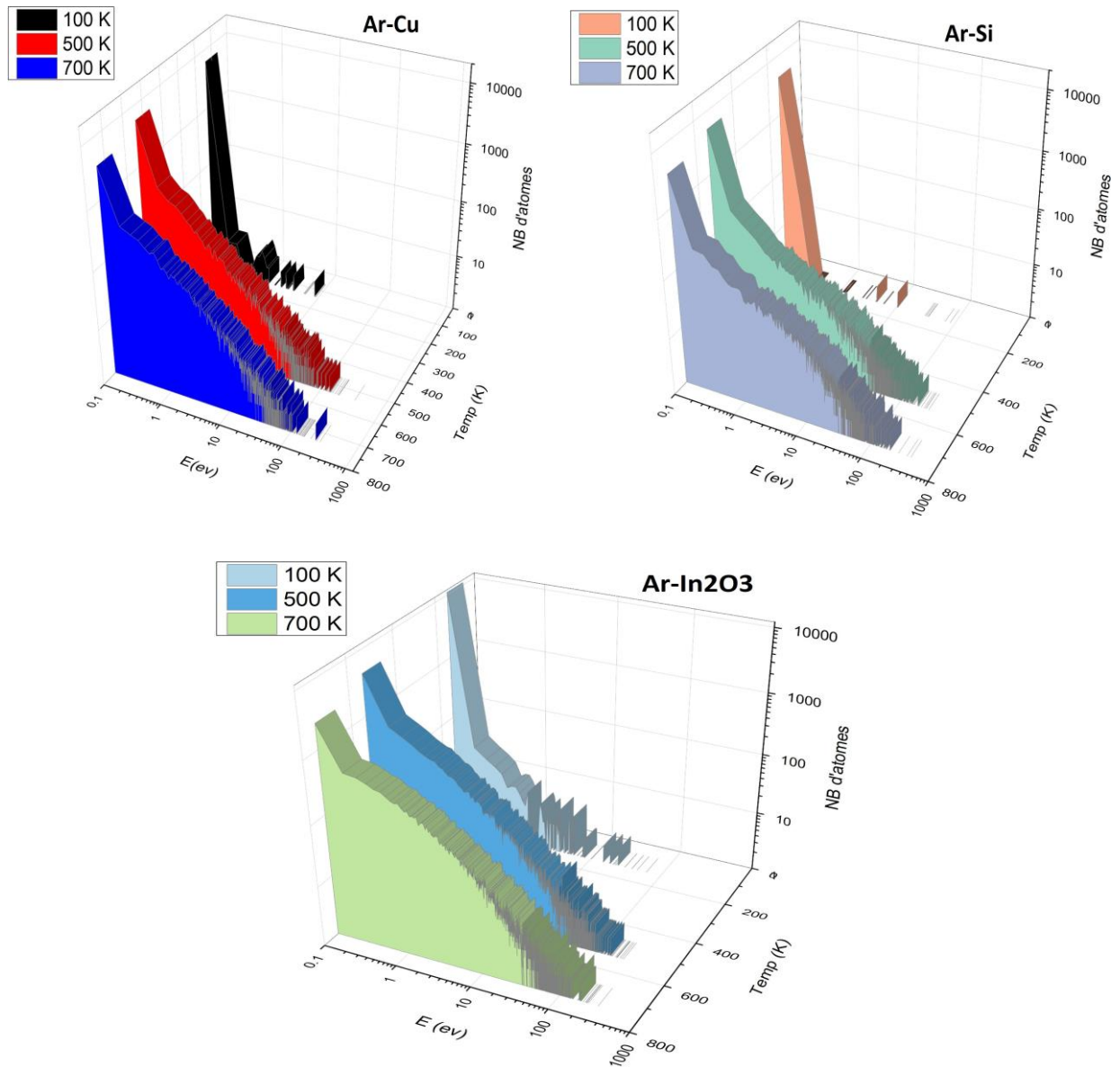


Figure III.8 Depending on the temperature in the chamber, the energy distribution of: (Cu, Si, In₂O₃) arrives at the substrate levels and is bombarded by Ar ion beam

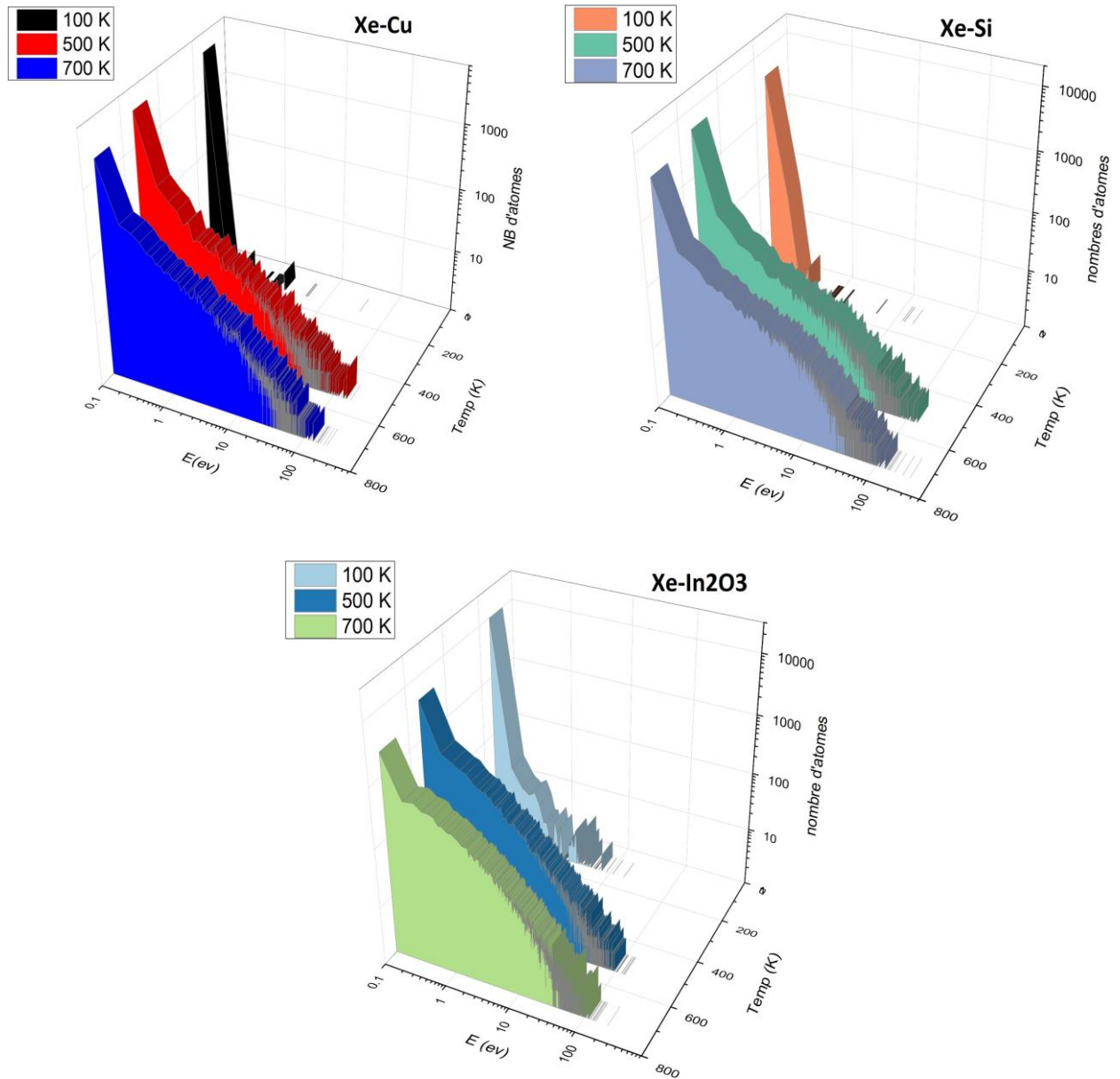


Figure III.9 Depending on the temperature in the chamber, the energy distribution of: (Cu, Si ,In2O3) arrives at the substrate levels and is bombarded by Xe ion beam.

We noticed that an increase in temperature leads to an increase in the number of expelled atoms and their distribution in the system. This results from the increased kinetic energy of the atoms and its effect on collisions with gas molecules and other surfaces in the system, increasing the possibility of reaching the substrate. Temperature can also significantly impact how atoms are distributed and interact in the evaporation process. This observation from the results can be of great importance in optimizing evaporation processes and determining

optimal operating conditions to obtain excellent performance and desirable properties in the deposited thin films.

- **The number of atoms arriving on the substrate depends on the applied Temperature**

Table III.05: Total number of atoms arrived on the substrate depending to the temperature.

	Temperature	copper	Indium oxide	Silicon
Argon	100	6457	11376	4532
	500	13874	20306	11552
	700	14799	20584	12981
Xenon	100	3720	4939	3767
	500	9369	12943	9714
	700	9914	14039	10591

c) The impact of distance

According to simulation results from the SIMTRA program, the following graphs represent the number of atoms that reach the substrate for each distance under consideration when the chosen pressure is 1 Pa, the temperature is 300K, and the distance is varied (3 cm, 6 cm, and 9 cm).

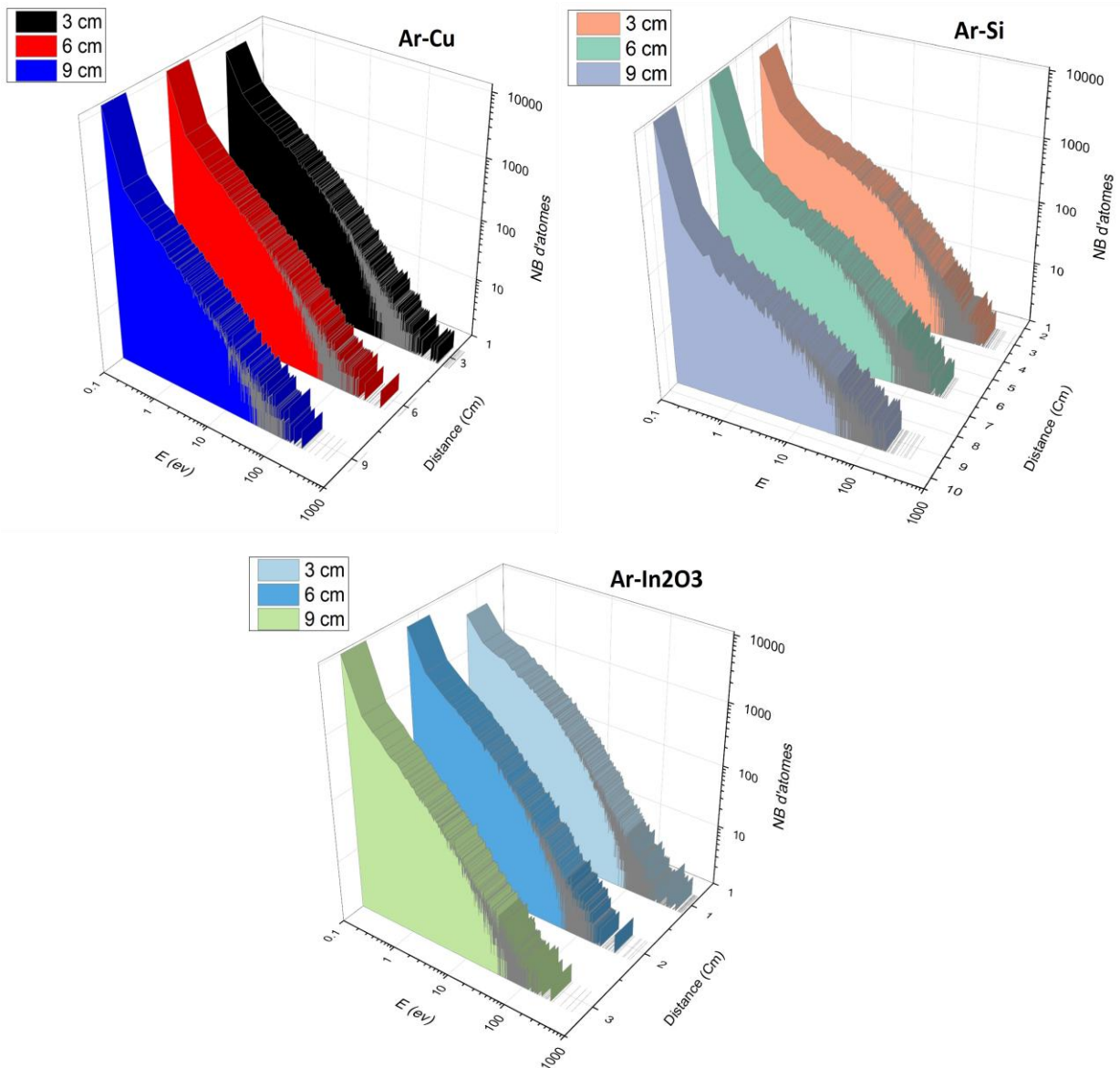


Figure III.10 The energy distribution of the (Cu, Si, In₂O₃) atoms arriving at the substrate bombarded by Ar ion with distance variations

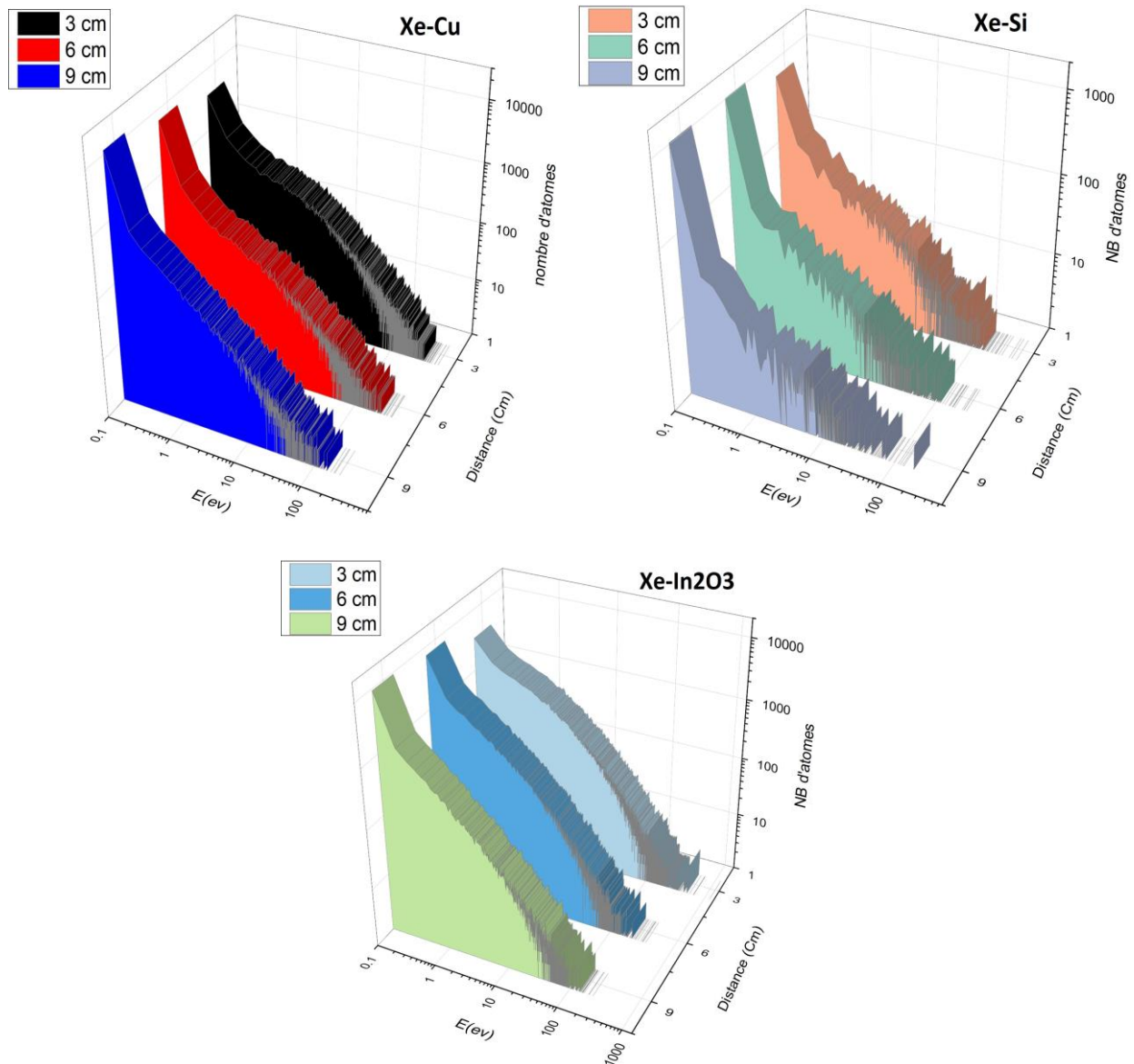


Figure III.11 The energy distribution of: (Cu,Si ,In2O3) atoms arriving to the substrate bombarded by Xe ion with distance variation.

We observed that the number of atoms arriving at the substrate decreases at a distance of 9cm between the substrate and the source. In comparison, at distances of 3cm and 6cm, the number is higher, and also from the observations we obtained about the effect of distance on the number of atoms and energy that increasing the distance between the source and the surface leads to a decrease in the number of atoms that reach the substrate. When the target is farther from the substrate, the expelled atoms are subject to more significant scattering and further spacing between them, which leads to a lower efficiency in reaching the substrate. As the distance

increases, the total number of atoms interacting with and reaching the substrate decreases. In addition, the energy distribution of the expelled atoms can be affected as the distance increases, as the atoms can lose part of their energy through diffusion in the space between the target and the substrate.

- **The number of atoms arriving on the substrate depends on the applied distance**

Table III.6 shows the total number of atoms sprayed on the substrate depending to the distance

	Distance	copper	Indium oxide	Silicon
Argon	3cm	54879	64090	48286
	6cm	36024	45296	30633
	9cm	23958	32495	19785
Xenon	3cm	40901	48969	41872
	6cm	24926	31721	25462
	9cm	15863	20972	16106

III.10 Conclusion

The SimTra simulation's findings have shown how vital factors such as pressure, temperature, distance, type of gas, and material affect cathodic sputtering. These results underline the importance of considering these factors when designing and refining cathodic sputtering procedures to achieve deposition quality and performance goals.

General

Conclusion

Thin film material technology is widely used for nanomaterial processing. Thin films are created by depositing atoms of a material (target) onto a substrate. Thin films are defined as low-dimensional materials formed by the continuous densification of atomic/molecular/ionic species of matter.

The performance of thin film optical coatings is typically enhanced when the thin film coating consists of multiple layers having varying thicknesses and refractive indices.

A thin film is a layer of material ranging in thickness from a fraction of a nanometer (monolayer) to several microns.

Our work focuses on the research and fabrication of thin materials using sputtering deposition techniques, considering various parameters that influence the morphology of these films. So:

- **First step:** We calculated the sputtering yield theoretically using various formulas of Yamamura and Tawara and compared it with the simulation results with SRIM software by manipulating the ion incident angle and energy. We find almost the same value. As a result, the Yamamura and Towara theorem confirmed the SRIM simulation.
- **Next step:** Adopt the optimal incident angle and energy value results that give excellent sputtering yield (85° and 100 KeV are found). A simulation using SIMTRA software gives the number of atoms arriving at the substrate and their energies. We varied the pressure, fixed the temperature (300 Kelvin), fixed the pressure (1 Pa), varied the temperature, and finally varied the distance between the target and substrate.

In summary, to get a thin, thick, perfect layer, one has to choose the material to use for the target (in terms of this evaluation of available materials and from an economic point of view, copper seems to give a perfect yield. Economic Side is not expensive), For bombardment gas, tests were done with two Xenon and Argon, under regulatory conditions of temperatures above 300 Kelvin and pressures of 0.5 Pa. The wrong choice of this parameter will affect the target and the thin film morphology and also will affect the substrate.

Argon is the best because of its high molecular weight and its availability.

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ملخص

الأفلام الرقيقة تمثل قفزة نوعية في تطوير وتصغير المجال الإلكتروني وإنتاج المكونات الإلكترونية؛ وأحد الأساليب المستخدمة لإنتاج هذه الأفلام الرقيقة هو التبخير الإلكتروني. تعتبر الطاقة الذرية وتوزيع الزوايا أكثر المؤشرات فعالية لتحسين عملية الرش وبالتالي الترسيب. الهدف الرئيسي لعمليتنا هو دراسة تأثير عوامل أخرى مثل الضغط العالية والمسافة والحرارة العالية، التي تؤثر بشكل هام في تكوين الأفلام الرقيقة. لقد استخدمنا غازين في عمليتنا لمعرفة أيها يعطينا نتائج أفضل، بالإضافة إلى ثلاثة مواد كما استخدمنا برامج محاكاة في عمليتنا مثل SRIM و SIMTRA. من خلال هذه الدراسات، سعينا لاكتشاف تأثيرات الظروف المثلى لإنتاج أفلام رقيقة عالية الجودة

Abstract

Thin films have revolutionized the field of electronics by enabling miniaturization and advanced electronic component production. Sputtering is a widely employed technique for fabricating these films. Enhancing sputtering and deposition processes necessitates understanding atomic energy and angular distribution. In our study, we aimed to investigate the impact of high pressure and high temperature, key factors influencing thin film formation. Additionally, we examined two gases and three materials to determine their effectiveness. To facilitate our research, we employed simulation programs such as SRIM and SIMTRA. Through these investigations, we aimed to uncover optimal conditions for producing high-quality thin films

Resumé

Les couches minces représentent une avancée qualitative dans le développement et la miniaturisation du domaine électronique ainsi que dans la production de composants électroniques. L'une des méthodes utilisées pour produire ces couches minces est la pulvérisation cathodique (sputtering). L'énergie atomique et la distribution angulaire sont des indicateurs essentiels pour améliorer la pulvérisation et, par conséquent, le dépôt. L'objectif principal de notre travail est d'étudier les effets d'autres facteurs tels que la haute pression et la haute température et la distance, qui jouent un rôle important dans la formation des films minces. Nous avons utilisé deux gaz dans notre étude pour déterminer lequel nous donne de meilleurs résultats, ainsi que trois matériaux. Nous avons également utilisé des programmes de simulation, tels que SRIM et SIMTRA, dans notre travail. À travers ces recherches, nous avons cherché à déterminer les conditions optimales pour produire des films minces de haute qualité