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Monte Carlo simulation of the influence of temperature and pressureon the transport of particlesin the plasma discharge for thin filmsdeposition

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Dedication

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Our brothers and sisters,

To all our family,

Our friends who encourage and support us,

Summary

SUMMARY

INTRODUCTION 2

Chapter I : Thin film preparation

1.PLASMA 5
1.1. History 5
1.2. Definition 5
1.3. Common forms of plasma 6
1.3.1. Terrestrial plasmas 6
1.3.2. Space and astrophysical plasmas 6
1.4.Plasma parameters: Three fundamental parameters characterize a plasma: 8
1.4.1. the particle density n: 8
1.4.2. the temperature T: 8
1.4.3. the steady state magnetic field B: 9
1.5. Plasma classification 9
1.5.1. Pseudo-plasmas vs real plasma 9
1.5.2. Cold warm and hot plasmas: 9
1.5.2.1. Hot plasma (thermal plasma) 9
1.5.2.2. Cold plasma (non-thermal plasma) 10
1.5.2.3. Ultra cold plasma 10
1.5.3. Plasma ionization 10
1.5.4. Plasma densities 10
1.5.5. Active and passive plasma 10
1.5.5.1. Passive plasma 10
1.5.5.2. Active plasma 11
1.5.6. Ideal and non-ideal plasma 11
1.6. Types of plasma 11
1.7. HOW ARE PLASMAS MADE? 11
1.8. Plasma applications 12
2. Interaction 12
2.1. History 12
2.1.1. Classical theory 12

2.2. Interaction between particles 13
2.3. Collision between particles 13
2.3.1. Elastic collision 13
2.3.2. Inelastic collision 14
2.3.3. Comparison between Elastic and inelastic 14
3. Thin films 15
3.1. Definition 15
3.2. Thin films deposition 15
3.2.1. Physical vapor deposition (PVD) 16
3.2.1.1. Physical evaporation 16
3.2.1.2. Vacuum thermal evaporition 16
3.2.1.3. SPUTTER DEPOSITION 17
3.2.2. Chemical vapor deposition 18
3.2.2.1. Plasma-enhanced chemical vapor deposition (PECVD) 18
3.3. Importance of deposition technology in modern fabrication processes 19
3.4. Deposition Technologies and Applications 19

Chapter II : Sputtering

1. Sputtering 22
1.1.Introduction 22
1.2.Generality 22
1.1 Sputtering Process 24
2. Sputtering yield formulas 25
2.1 Sigmund formula 26
2.2 Improvements made by other authors 26
2.3 Sputter yield formula obtained by Yamamura 27
3.Various Sputtering Regimes 28
3.1 Single Knock-On 28
3.2 Linear Collision Cascade 29
4.General sputtering methodology 29
4.1Reactive sputtering 29
4.2RF (radio frequency) sputter deposition 29
4.3. Magnetron sputtering 30
4.4. Direct sputtering (DC sputtering) 31
4.5. Confocal sputtering 32

4.6. Pulsed DC Sputtering....33
4.7. Ion Beam Sputtering....34
5. Vacuum chamber 35
6. Sputter deposition advantages.... 36
6.1 Advantages....36
6.2. Disadvantages 37
7. Sputtering system applications.... 37

Chapter III : Results and discussion

1. Monte Carlo method 40
1.1.Introduction 40
1.2.History 40
1.3. Generality....41
2. Monte Carlo Simulation.... 41
3. SRIM 2013 (TRIM) 42
3.1. Generality....42
4.Part one 42
4.1.Results found by SRIM simulation 42
4.1.1. Variation of the ions sputtering yield for different metals 42
4.1.2. Variation of the ions sputtering yield for different gas 45
5. Effects of Incidence Angle.... 46
6. Part tow 48
6.1.SIMTRA (SImulation of Metal TRAnsport) 48
6.2 Influence of divers parameters on the number of sputtered atoms arriving at the substrate and their energy....48
6.2.1 Variation of chamber temperature. 48
General conclusion....54

List of Figures

Chapter I :Thin film preparation

Figure 1.1 Schematic representation of plasma -the fourth state of matter-……………………….…5

Figure 1.2 Schematic representation an examples for plasma…………………………..……..…7

Figure1.3 Schematic representation the 2nd parameter of plasma – the temperature-…….……..…8

Figure 1.4 Schematic representation of an elastic head-on collision between two particles……....14

Figure 1.5 Schematic representation of a perfectly inelastic head-on collision between two particles..14

Figure 1.5 Schematic representation of thin film deposition…………………..………………...15

Figure 1.6 Schematic representation of vacuum evaporation………………………………………17

Figure 1.7 Schematic representation of sputter deposition…………………………………………17

Figure 1.8 Schematic representation of chemical vapor deposition (CVD)………………………..18

Figure 1.9 PECVD (Plasma-enhanced chemical vapor deposition) machine……………………….19

Chapter II: Sputtering

Figure 2.1 sputtering system……………………………..………………………………………23

Figure 2.2 Diagram of the Sputtering Process…………………..………………………….……24

Figure 2.3 Schematic representation of Single Knock-On……………………...……………….28

Figure 2.4 Schematic representation of linear collision cascade……………..…..………...……29

Figure 2.5 Diagram of the RF Sputtering Process…………………………….……..………….30

Figure 2.6 Schematic representation of Magnetron sputtering system…………….……………31

Figure 2.7 Direct sputtering (DC sputtering)…………………………………….……………….…..32

Figure 2.8 Schematic diagram of dc magnetron co-sputtering system……………………….……….33

Figure 2.9 Schematic diagram of Pulsed DC sputtering system…………………………………...34

Figure 2.10 Schematic representation of ion beam sputtering system………………….……….35

Figure 2.11 A large vacuum chamber…………………………………………………..…….36

Chapter III: Result and discussion

Figure 3.1 Variation of sputtering yield of Aluminum for different ions found by SRIM simulation……………………………………………………………………………..…………..……**42**
.

Figure 3.2 Variation of sputtering yield of Germanium for different ions found by SRIM simulation………………………………………………………………………..……………..…..**43**

Figure 3.3 Variation of sputtering yield of silver for different ions found by SRIM simulation……………………………………………………………………..…………….…..……..**43**

Figure 3.4 Variation of sputtering yield of copper for different ions found by SRIM simulation…………………………………………………………………..…………………………..**43**

Figure 3.5 Variation of sputtering yield of Antimony for different ions found by SRIM simulation…………………………………………………………………………………...…..…..**44**

Figure 3.6 Variation of sputtering yield of Boron for different ions found by SRIM simulation……………………………………………………………………..……………..……**44**

Figure 3.7 Variation of sputtering yield of Niobium for different ions found by SRIM simulation………………………………………………………………………………………...…**44**

Figure 3.8 Sputtering yield of silver, aluminum, Germanium, Boron, Niobium, Antimony and copper for an xenon ion beam at normal incidence calculating………………..…….…………..**45**

Figure 3.9 Sputtering yield of silver, aluminum, Germanium, Boron, Niobium, Antimony and copper for an Argon ion beam at normal incidence calculating............……………………….**45**

Figure 3.10 Sputtering yield of silver, aluminum, Germanium, Boron, Niobium, Antimony and copper for an Silicon ion beam at normal incidence calculating ……………..……………..……**45**

Figure 3.11 Sputtering yield of silver, aluminum, Germanium, Boron, Niobium, Antimony and copper for an Helium ion beam at normal incidence calculating ……………………………..…**45**

Figure 3.12 Sputtering yield of silver, aluminum, Germanium, Boron, Niobium, Antimony and copper for an Neon ion beam at normal incidence calculating ………………..…………..…**46**

Figure 3.13 Variation of sputtering yield of Xenon for different angle found by SRIM simulation………………………………………………………………………...………..**47**

Figure 3.14 Variation of sputtering yield of Neon for different angle found by SRIM simulation……………………………………………………………………………………..**47**

Figure 3.15 Variation of sputtering yield of Argon for different angle found by SRIM simulation…………………………………………………………………………………..…**47**

Figure 3.16 Variation of sputtering yield of Silicon for different angle found by SRIM simulation……………………………………………………………………………..………**47**

Figure 3.17 (Color online) The energy distribution for arriving Ag atoms as a function of temperature………...**49**

Figure 3.18 (Color online) The energy distribution for arriving Al atoms as a function of temperature……………………………………………………………………………..………...**49**

Figure 3.19 (Color online) The energy distribution for arriving B atoms as a function of temperature…………………………………………………………………………………..…**50**

Figure 3.20 (Color online) The energy distribution for arriving Cu atoms as a function of temperature……………………………………………………………………………………....**50**

Figure 3.21 (Color online) The energy distribution for arriving Ge atoms as a function of temperature………………………………………………………………………………………**51**

Figure 3.22 (Color online) The energy distribution for arriving Si atoms as a function of temperature……………………………………………………………………..……..……..…**51**

General Introduction

This work is devoted to the study of sputtering and the deposition of thin film by plasma. Film preparation using sputtering phenomena is classified in the physical vapor deposition (PVD) process, and has been widely used in these days. The thin film deposition is a technic that deposits a thin film of material onto a substrate or onto previously deposited layers. Most deposition techniques allow reaching a layer thickness of several nanometers. More industrial applications are based on this technology that is very useful to create compounds that cannot be manufactured by chemical mass (traditional methods). The optimization of the deposition parameters to films owning the desired properties (thickness homogeneity and identical composition to the evaporated material) is conducted through the implementation of numerous experiments. To reduce the duration of the optimization process, it became necessary to develop a simulation of physical processes involved in the transport of species when making a deposit in order to predict thickness distributions and composition of a layer. Sputtering deposition has been widely used technique for fabricating a variety of thin films of metals. It has also been used for Cu2O semiconductor films deposition, and dielectric materials, including magnetic films and high critical temperature superconducting films on all different kinds of substrates, and is particularly useful for the preparation of multilayered films because of its good controllability of each thickness in multilayered structures. In film deposition applications, sputtering can be the mode by which thin film coatings of target material are applied to surfaces to enhance their mechanical, thermal or optical properties. The plasma sputtering technology has been used for the deposition of solar selective coating with less environmental pollution than electrochemical methods. Thin film are widely used in many fields, such as optics, microelectronics, biomedical, magnetic materials and so on. In earlier researches of other groups, they discussed that the energy of the particles arriving at the substrate is in close relation with the transport process from the target to the substrate. Several research groups have published Monte Carlo models, but generally speaking, they do not allow the target nature when we use metals, semiconductors and dielectrics and it is very important to know the difference to use each one of them. We are using Monte Carlo models that allow one to calculate the sputtered atoms and their energies, and on the other hand to implement the vacuum chamber geometry, and to use a wide variety of interaction potentials to calculate the number of atoms and their energy arriving at the substrate.

The objective of the work presented here is to simulate with two programs which are

SRIM2013 ("**S**topping and **R**ange of **I**ons in **M**atter") calculates sputtering yield and SIMTRA (**SI**mulation of **M**etal **TRA**nsport).

This thesis is divided into three parts:

In Chapter 1, we speak about thin film preparation, plasma and interaction between particles.

The 2nd chapter is devoted to sputtering. We will make a few brief reminders on the theory, the different sputtering regimes and general sputtering methodology.

In the last chapter, we will present the principle of Monte-Carlo techniques, simulation with SRIM2013 and SIMTRA software. and the influence of temperature on the sputtering process for metal and semiconductor layers

CHAPTER I

Thin Film Preparation

1.PLASMA

1.1. History

Plasma was first identified in a Crookes tube, and so described by Sir William Crookes in 1879 (he called it "radiant matter").**[1][2]** The nature of the Crookes tube "cathode ray" matter was subsequently identified by British physicist Sir J.J. Thomson in 1897.**[3]** The term "plasma" was coined by Irving Langmuir in 1928,**[4][5]** perhaps because the glowing discharge molds itself to the shape of the Crookes tube .[4] Langmuir described his observations as:

"Except near the electrodes, where there are sheaths containing very few electrons, the ionized gas contains ions and electrons in about equal numbers so that the resultant space charge is very small. We shall use the name plasma to describe this region containing balanced charges of ions and electrons."**[4]**.

1.2. Definition

Plasma is one of the four fundamental states of matter, the others being solid, liquid, and gas. Yet unlike these three states of matter, plasma does not naturally exist on the Earth under normal surface conditions, and can only be artificially generated from neutral gases.**[6]** The term was first introduced by chemist Irving Langmuir**[7]** in the 1920s.**[8]**.

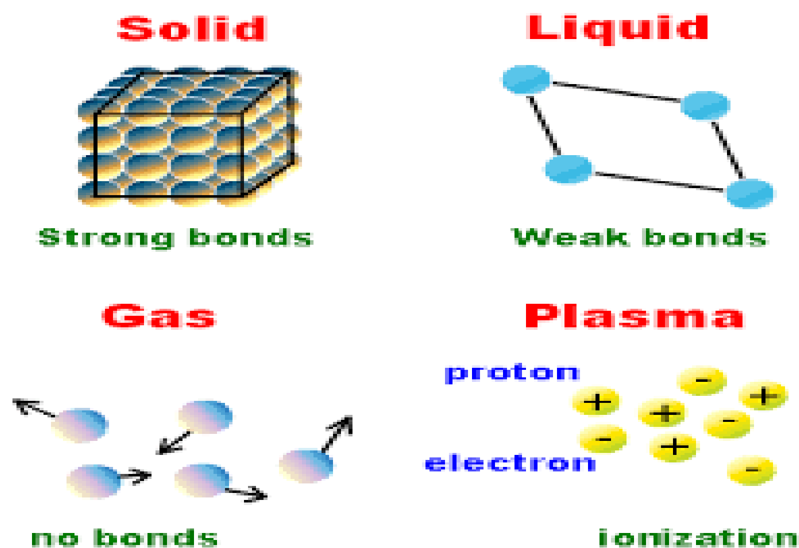

Figure 1.1 Schematic representation of plasma -the fourth state of matter-

- Plasma exists in many forms in nature and has a widespread use in science and technology. It is a special Kind of ionized gas and in general consists of:

- Positively charged ions (“positive ions”).

- electrons, and

- neutrals (atoms, molecules, radicals).

(Under special conditions, plasma may also contain negative ions. But here we will not discuss this case further. Thus in what follows the term ‘ion’ always means ‘positive ion’.)

We call an ionized gas ‘plasma’ if it is quasi-neutral and its properties are dominated by electric and/or magnetic forces. **[9]**

1.3. Common forms of plasma

Plasmas can appear in Nature in various forms and locations.

1.3.1. Terrestrial plasmas

- Lightning.
- St. Elmo's fire.
- Upper-atmospheric lightning (e.g. Blue jets, Blue starters, Gigantic jets, ELVES).
- Sprites.
- The ionosphere.
- The plasmasphere.
- The polar aurorae.
- The polar wind, a plasma fountain.

1.3.2. Space and astrophysical plasmas

- The Sun and other stars (plasmas heated by nuclear fusion).
- The solar wind.
- The interplanetary medium (space between planets).
- The interstellar medium (space between star systems).
- The Intergalactic medium (space between galaxies).
- The Io-Jupiter flux tube.
- Accretion discs.
- Interstellar nebulae.

1.3.3. Artificially produced :

- Those found in plasma displays, including TV screens.
- Inside fluorescent lamps (low energy lighting), neon signs.
- Rocket exhaust and ion thrusters.
- The area in front of a spacecraft's heat shield during re-entry into the atmosphere.
- Inside a corona discharge ozone generator.
- Fusion energy research.
- The electric arc in an arc lamp, an arc welder or plasma torch.
- Plasma ball (sometimes called a plasma sphere or plasma globe).
- Arcs produced by Tesla coils (resonant air core transformer or disruptor coil that produces arcs similar to lightning, but with alternating current rather than static electricity).
- Plasmas used in semiconductor device fabrication including reactive-ion etching, sputtering, surface cleaning and plasma-enhanced chemical vapor deposition.
- Laser-produced plasmas (LPP), found when high power lasers interact with materials.
- Inductively coupled plasmas (ICP), formed typically in argon gas for optical emission spectroscopy or mass spectrometry.
- Magnetically induced plasmas (MIP), typically produced using microwaves as a resonant coupling method.
- Static electric sparks.

Figure 1.2 Schematic representation an examples for plasma.

1.4.Plasma parameters:

Three fundamental parameters characterize a plasma:

1.4.1. the particle density n:

(measured in particles per cubic meter),

Owing to the presence of free charge carriers, plasma reacts to electromagnetic fields, conducts
electrical current, and possesses a well-defined space potential.

Positive ions may be singly charged or multiply charged. For a plasma containing only singly charged ions, the ion population is adequately described by the ion density *n*i;

$$n_i = \frac{number\ of\ particles}{volume}, \quad [n_i] = cm^{-3}\ or\ [n_i] = m^{-3} \qquad (1)$$

Besides the ion density, we characterize a plasma by its electron density **ne** and the neutral density **na.**

1.4.2. the temperature T:

(usually measured in eV, where 1 eV=11,605 K),

Plasma temperature is commonly measured in kelvins or electronvolts and is, informally, a measure of the thermal kinetic energy per particle. High temperatures are usually needed to sustain ionization, which is a defining feature of a plasma. The degree of plasma ionization is determined by the electron temperature relative to the ionization energy (and more weakly by the density), in a relationship called the Saha equation. At low temperatures, ions and electrons tend to recombine into boundstates atoms[22]and the plasma will eventually become a gas.

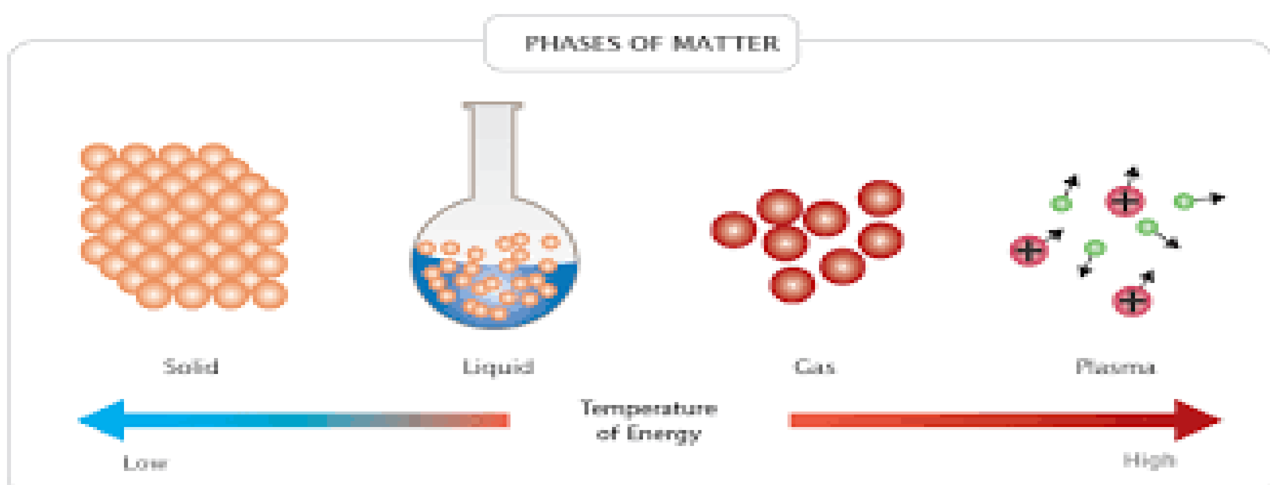

Figure1.3 Schematic representation the 2nd parameter of plasma – the temperature-

1.4.3. the steady state magnetic field B:

(measured in Tesla).

Plasma with a magnetic field strong enough to influence the motion of the charged particles is said to be magnetized. A common quantitative criterion is that a particle on average completes at least one gyration around the magnetic field before making a collision, i.e., where is the "electron gyrofrequency" and is the "electron collision rate". It is often the case that the electrons are magnetized while the ions are not. Magnetized plasmas are ***anisotropic***, meaning that their properties in the direction parallel to the magnetic field are different from those perpendicular to it. While electric fields in plasmas are usually small due to the high conductivity, the electric field associated with a plasma moving in a magnetic field is given by (where is the electric field, is the velocity, and is the magnetic field), and is not affected by Debye shielding.**[10]**

1.5. Plasma classification

Plasmas are described by many characteristics, such as temperature, degree of ionization, and density, gives rise to plasmas that may be classified in different ways.

1.5.1. Pseudo-plasmas vs real plasma

A real plasma may have complex characteristics that exhibited complex phenomena. pseudo-plasma may or may not be an adequate representation of a real plasma ;Pseudo-plasmas tend to neglect double layers, instabilities, electric currents, and other potentially important properties.

1.5.2. Cold warm and hot plasmas:

In the laboratory in the positive column of a glow discharge tube:

"A plasma is sometimes referred to as being "hot" if it is nearly fully ionized, or "cold" if only a small fraction, (for instance 1%) of the gas molecules are ionized, but other definitions of the terms "hot plasma" and "cold plasma" are common. Even in cold plasma the electron temperature is still typically several thousand centigrade."**[11]**

1.5.2.1. Hot plasma (thermal plasma)

A hot plasma in one which approaches a state of local thermodynamic equilibrium (LTE). A hot plasma is also called a thermal plasma, but in Russian literature, a "low temperature" plasma in order to distinguish it from a thermonuclear fusion plasma.**[12]** Such plasmas can be produced by atmospheric arcs, sparks and flames.**[13]**

1.5.2.2. Cold plasma (non-thermal plasma)

A cold plasma is one in which the thermal motion of the ions can be ignored. Consequently there is no pressure force, the magnetic force can be ignored, and only the electric force is considered to act on the particles.**[14]** Examples of cold plasmas include the Earth's ionosphere (about 1000K compared to the Earth's ring current temperature of about 10^8K).**[15]**, the flow discharge in a fluorescent tube, **[16]**

1.5.2.3. Ultra cold plasma

An ultracold plasma is one which occurs at temperatures as low as 1K.**[17]** and may be formed by photoionizing laser-cooled atoms. Ultracold plasmas tend to be rather delicate, experiments being carried out in vacuum.**[18]**

1.5.3. Plasma ionization

The degree of ionization of a plasma is the proportion of charged particles to the total number of particles including neutrals and ions, and is defined as: $\alpha = n^+/(n + n^+)$where n is the number of neutrals, and n^+ is the number of charged particles. (**α** is the Greek letter alpha).

1.5.4. Plasma densities

In this category there is three types High density plasma, Medium density plasma and Low density plasma.

1.5.5. Active and passive plasma

Hannes Alfvén writes: "**Passive plasma regions**, which can be described by classical hydrodynamic theory. They transmit waves and high energy charged particles but if the field-aligned currentsexceed a certain value they are transferred into.

Active plasma regions: These carry field-aligned currents which give them filamentary or sheet structure with thickness down to a few cyclotron radii (ionic or even electronic). They transmit energy from one region to another and produce electric double layers which accelerate particles to high energies. Active regions cannot be described by hydromagnetic theories. Boundary conditions are essential and may be introduced by circuit theory"**[19]**

1.5.5.1. Passive plasma

Alfvén continues:

"These regions may transmit different kinds of plasma waves and flow of high energy particles. There may be transient currents perpendicular to the magnetic field changing the state of motion of the

plasma but not necessarily associated with strong electric fields and currents parallel to the magnetic field. A plasma of this kind fills most of space."

1.5.5.2. Active plasma

"Besides the passive plasma regions there are also small but very important regions where filamentary and sheet currents flow (Alfvén, 1977a)**[20]**. By transferring energy and producing sharp borders between different regions of passive plasmas, they are of decisive importance to the overall behavior of plasmas in space. There are two different - but somewhat related - types of such regions which we shall call plasma cables and boundary current sheets."

1.5.6. Ideal and non-ideal plasma

An ideal plasma is one in which Coulomb collisions are negligible, otherwise the plasma is non-ideal.

"At low densities, a low-temperature, partly ionized plasma can be regarded as a mixture of ideal gases of electrons, atoms and ions. The particles travel at thermal velocities, mainly along straight paths, and collide with each other only occasionally. In other words, the free path times prove greater than those of interparticle interaction. With an increase in density, mean distances between the particles decrease and the particles start spending even more time interacting with each other, that is, in the fields of surrounding particles. Under these conditions, the mean energy of interparticle interaction increases. When this energy becomes comparable with the mean kinetic energy of thermal motion, the plasma becomes non-ideal."**[21]**

1.6. Types of plasma

Among plasmas types we have:

1.Ionized gas (More understanding).

2.Ionized solid state (example: ionized semiconductors).

3.Ionized liquid (example: breakdown of water or oil).

4.Dust plasma.

5.Cluster plasma (example: evaporated plasma in electron source).

1.7. HOW ARE PLASMAS MADE?

A plasma is not usually made simply by heating up a container of gas. The problem is that for the most part a container cannot be as hot as a plasma needs to be in order to be ionized-or the container itself would vaporize and become plasma as well. Typically, in the laboratory, a small

amount of gas is heated and ionized by driving an electric current through it, or by shining radio waves into it. Either the thermal capacity of the container is used to keep it from getting hot enough to melt-let alone ionize during a short heating pulse, or the container is actively cooled (for example with water) for longer-pulse operation. Generally, these means of plasma formation give energy to free electrons in the plasma directly, and then electron-atom collisions liberate more electrons, and the process cascades until the desired degree of ionization is achieved. Sometimes the electrons end up quite a bit hotter than the ions, since the electrons carry the electrical current or absorb the radio waves. **[22]**

1.8. Plasma applications

There are all sorts of uses for plasmas. To give one example, if we want to make a short-wavelength laser we need to generate a population inversion in highly excited atomic states. Generally, gas lasers are 'pumped' into their lasing states by driving an electric current through the gas, and using electron-atom collisions to excite the atoms. X-ray lasers depend on collisional excitation of more energetic states of partially ionized atoms in a plasma. Sometimes a magnetic field is used to hold the plasma together long enough to create the highly ionized states.

A whole field of 'plasma chemistry' exists where the chemical processes that can be accessed through highly excited atomic states are exploited. Plasma etching and deposition in semiconductor technology is a very important related enterprise. Plasmas used for these purposes are sometimes called 'process plasmas'.

Perhaps the most exciting application of plasmas such as the ones we will be studying is the production of power from thermonuclear fusion. **[22]**

2. Interaction

2.1. History

2.1.1. Classical theory

In his 1687 theory, "Isaac Newton" postulated space as an infinite and unalterable physical structure existing before, within, and around all objects while their states and relations unfold at a constant pace everywhere, thus absolute space and time. Inferring that all objects bearing mass approach at a constant rate, but collide by impact proportional to their masses, Newton inferred that matter exhibits an attractive force. His law of universal gravitation mathematically stated it to span the entire universe instantly (despite absolute time), or, if not actually a force, to be instant interaction among all objects (despite absolute space.) As conventionally interpreted, Newton's theory of motion modelled a central force without a communicating medium.**[23]** Thus Newton's theory violated the

first principle of mechanical philosophy, as stated by Descartes, No action at a distance. Conversely, during the 1820s, when explaining magnetism, Michael Faraday inferred a field filling space and transmitting that force. Faraday conjectured that ultimately, all forces unified into one.

2.2. Interaction between particles

When electrons interact with atoms or molecules, energy of the incident electron is lost through inelastic collisions with the target. The target atom can undergo ionization or excitation. Secondary electrons released during the ionization process will trigger further collisions. These electrons lose energy via further collisions in the gas. This kind of electron energy degradation process is of great importance in understanding phenomena, like electron beam propagation in the atmosphere, population inversion process in a large group of gas lasers, optical emissions occurring in the upper atmosphere, such as aurora and airglow, which happen due to the precipitation of high-energy electrons, etc. **[24]**

2.3. Collision between particles

The concept of collision is described by the use of conservation of momentum and momentum. The conservation of momentum is based on the conservation of energy and kinetic energy concept. The collision takes place between two or more objects. When objects collide with each other than each object feels small amount of force for a small period of time. This force alters the momentum of the colliding objects. But in case of isolated system of particles, the momentum is in conservative state. So the momentum of individual particle is changed but total momentum of system remains constant. The detection procedure of collision is only depending on the type of collision. There are two types of collision that can be is **elastic** or **inelastic**. **[25]**

2.3.1. Elastic collision

An elastic collision between two objects is one in which total kinetic energy (as well as total momentum) is the same before and after the collision. Billiard-ball collisions and the collisions of air molecules with the walls of a container at ordinary temperatures are approximately elastic. Truly elastic collisions do occur, however, between atomic and subatomic particles. Collisions between certain objects in the macroscopic world, such as billiard-ball collisions, are only approximately elastic because some deformation and loss of kinetic energy take place. **[25]**

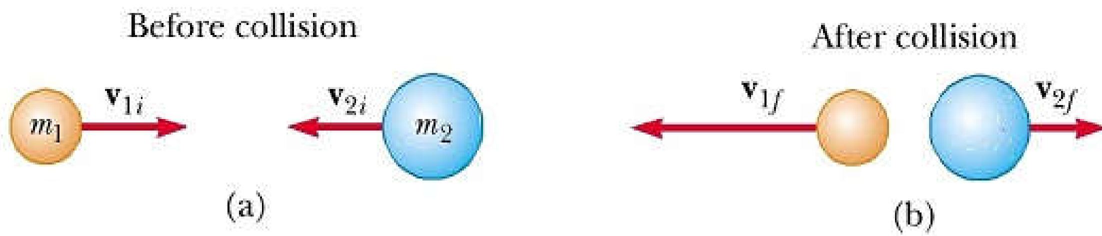

Figure 1.4 Schematic representation of an elastic head-on collision between two particles: (a) before collision and (b) after collision.

2.3.2. Inelastic collision

An inelastic collision is one in which total kinetic energy is not the same before and after the collision (even though momentum is constant). Inelastic collisions are of two types. When the colliding objects stick together after the collision, as happens when a meteorite collides with the Earth, the collision is called perfectly inelastic. When the colliding objects do not stick together, but some kinetic energy is lost, as in the case of a rubber ball colliding with a hard surface, the collision is called inelastic collision. **[25]**

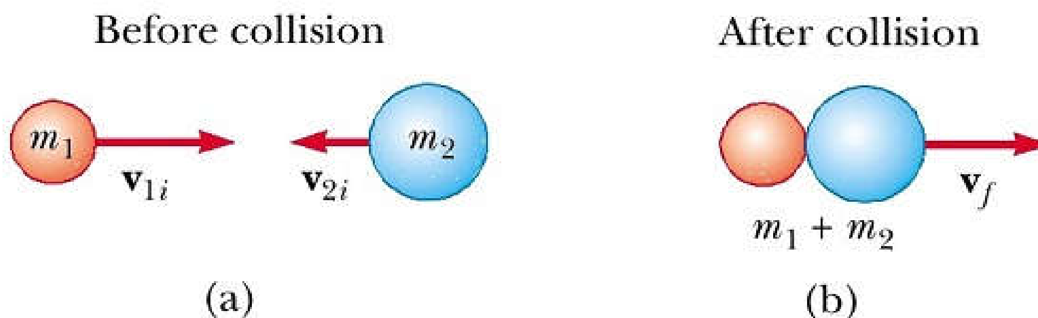

Figure 1.5 Schematic representation of a perfectly inelastic head-on collision between two particles: (a) before collision and (b) after collision.

2.3.3. Comparison between Elastic and inelastic

The comparison between Elastic and inelastic collision is given below:

ELASTIC COLLISION	INELASTIC COLLISION
Momentum Conserved	Momentum Conserved
Kinetic energy Conserved	Kinetic energy not conserved
Example: Bouncing ball	example: Bullet shot in wood
Cannot be Perfect	Can be Perfect.

3. Thin films

The technology of thin film deposition has advanced dramatically during the past 30 years. This advancement was driven primarily by the need for new products and devices in the electronics and optical industries. The rapid progress in solid-state electronic devices would not have been possible without the development of new thin film deposition processes, improved film characteristics and superior film qualities. Thin film deposition technology is still undergoing rapid changes which will lead to even more complex and advanced electronic devices in the future. The economic impact of this technology can best be characterized by the worldwide sales of semiconductor devices. **[26]**

3.1. Definition

Thin film is a microscopically thin layer of material that is deposited onto a metal, ceramic, semiconductor or plastic base. Typically, less than one micron thick, thin films can be conductive or dielectric (non-conductive) and are used in myriad applications. For example, the top metallic layer on a chip and the coating on magnetic disks are thin films. Thin films of photovoltaic material using silicon, cadmium telluride and other elements are used to make solar panels and solar roof shingles.**[27]**

3.2. Thin films deposition

Physical vapor deposition (PVD) and chemical vapor deposition (CVD) are the most common methods for transferring material atom by atom from one or more sources to the growth surface of a film being deposited onto a substrate. Vapor deposition describes any process in which a solid immersed in a vapor becomes larger in mass due to transference of material from the vapor onto the solid surface. The deposition is normally carried out in a vacuum chamber to enable control of the vapor composition. If the vapor is created by physical means without a chemical reaction, the process is classified as PVD; if the material deposited is the product of a chemical reaction, the process is classified as CVD. Many variations of these basic vapor deposition methods have been developed in efforts to balance advantages and disadvantages of various strategies based on the requirements of film purity, structural quality, the rate of growth, temperature constraints and other factors. **[27]**

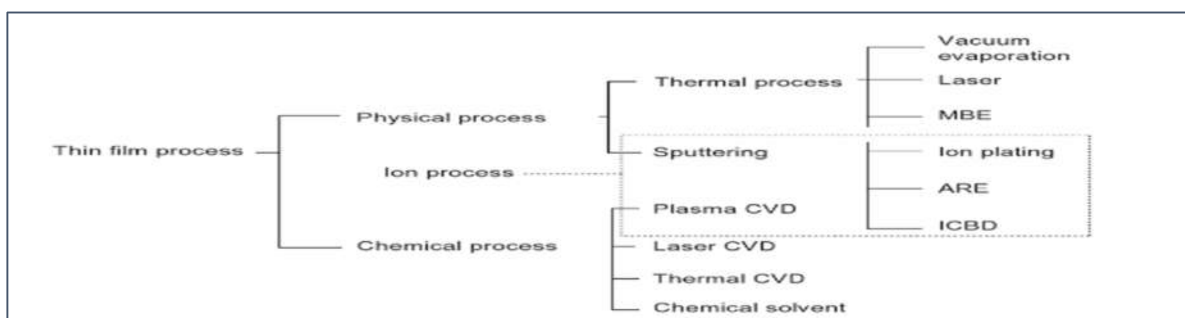

Figure 1.5 Schematic representation of thin film deposition.

3.2.1. Physical vapor deposition (PVD)

Physical vapor deposition is a technique whereby physical processes, such as evaporation, sublimation or ionic impingement on a target, facilitate the transfer of atoms from a solid or molten source onto a substrate. Evaporation and sputtering are the two most widely used PVD methods for depositing films. It used for decorative coating, tool coating, and other equipment coating applications. It is fundamentally a vaporization coating process in which the basic mechanism is an atom by atom transfer of material from the solid phase to the vapor phase and back to the solid phase, gradually building a film on the surface to be coated. In the case of reactive deposition, the depositing material reacts with a gaseous environment of co-deposited material to form a film of compound material, such as a nitride, oxide, carbide or carbonated. **[28]**

3.2.1.1. Physical evaporation

Physical evaporation is one of the oldest methods of depositing metal films. Aluminum, gold and other metals are heated to the point of vaporization, and then evaporate to form to a thin film covering the surface of the substrate. All film deposition takes place under vacuum or very carefully controlled atmosphere.**[29]**

3.2.1.2. Vacuum thermal evaporition

Vacuum evaporation is also known as vacuum deposition and this is the process where the material used for coating is thermally vaporized and then proceeds by potential differences to the substrate with little or no collisions with gas molecules. Normal vacuum levels are in the medium to high vacuum range of 10-5 to 10-9 mbar.In thermal evaporation techniques, different methods can be applied to heat the material. The equipments available in the laboratory use either resistance heating or bombardment with a high energy electron beam, usually several KeV, from an electron beam gun (electron beam heating).

In the **Resistance heating technique**, the material is heated until fusion by means of an electrical current passing through a filament or metal plate (Evaporator) where the target material is deposited. The evaporated material is then condensed on the substrate.

The **Electron beam heating technique** is based in the heat produced by high energy electron beam bombardment on the material to be deposited. The electron beam is generated by an electron gun, which uses the thermionic emission of electrons produced by an incandescent filament.**[28]**

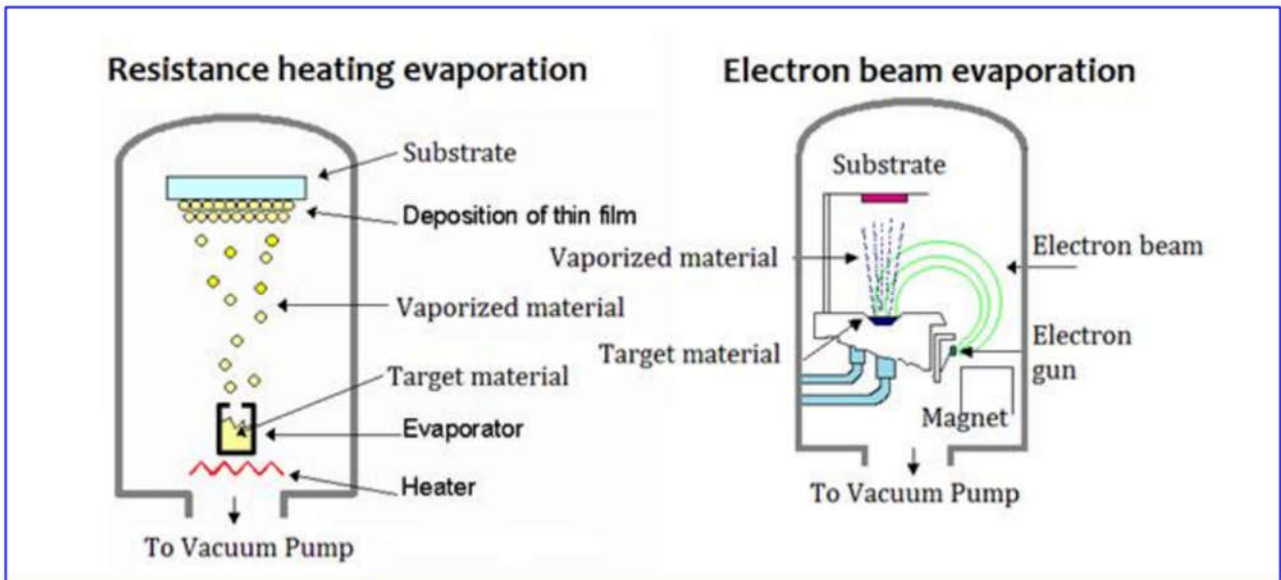

Figure 1.6 Schematic representation of vacuum evaporation

3.2.1.3. SPUTTER DEPOSITION

Sputter deposition are methods of depositing thin films by sputtering. They involve ejecting material a “target” that is a source onto a “substrate” such as a silicon wafer. Sputtered atoms ejected from the target have a wide energy distribution, typically up to tens of eV. The sputtered ions (typically only a small fraction — order 1% — of the ejected particles are ionized) can ballistically fly from the target in straight lines and impact energetically on the substrates. The sputtering gas is often an inert gas such as argon. For efficient momentum transfer, the atomic weight of the sputtering gas should be close to the atomic weight of the target, so for sputtering light elements neon is preferable, while for heavy elements krypton or xenon are used. He compound can be formed on the target surface, inflight or on the substrate depending on the process parameters. **[28]**

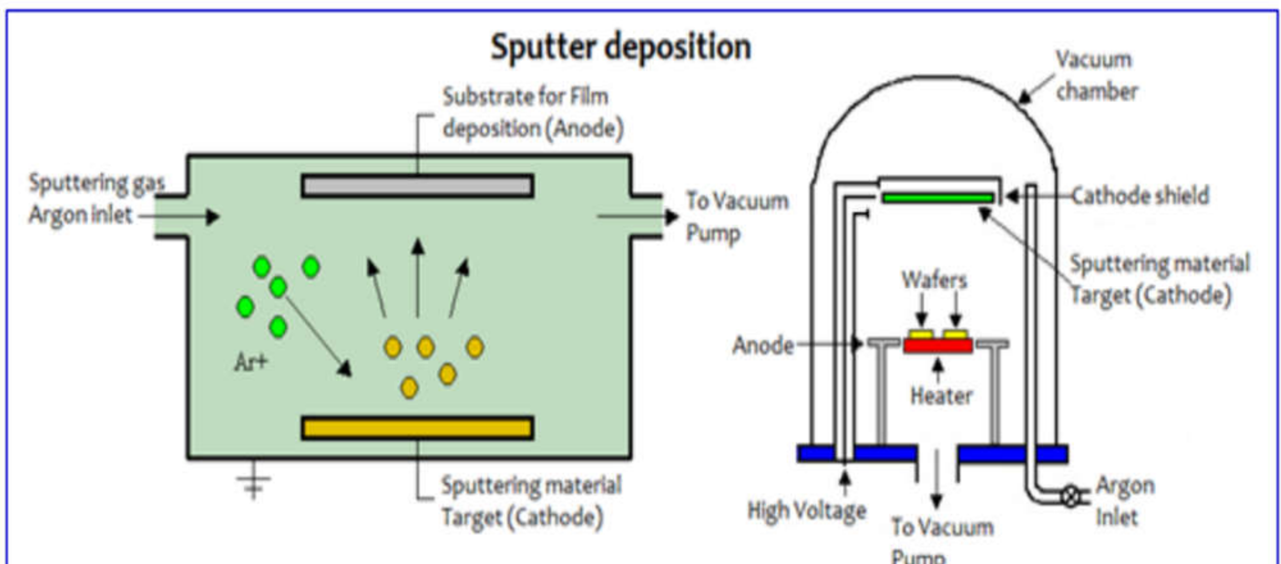

Figure 1.7 Schematic representation of sputter deposition

3.2.2. Chemical vapor deposition

Chemical vapor deposition is a versatile deposition technique that provides a means of growing thin films of elemental and compound semiconductors, metal alloys and amorphous or crystalline compounds of different stoichiometry. The basic principle underlying this method is a chemical reaction between a volatile compound of the material from which the film is to be made with other suitable gases so as to facilitate the atomic deposition of a nonvolatile solid film on a substrate. **[29]**

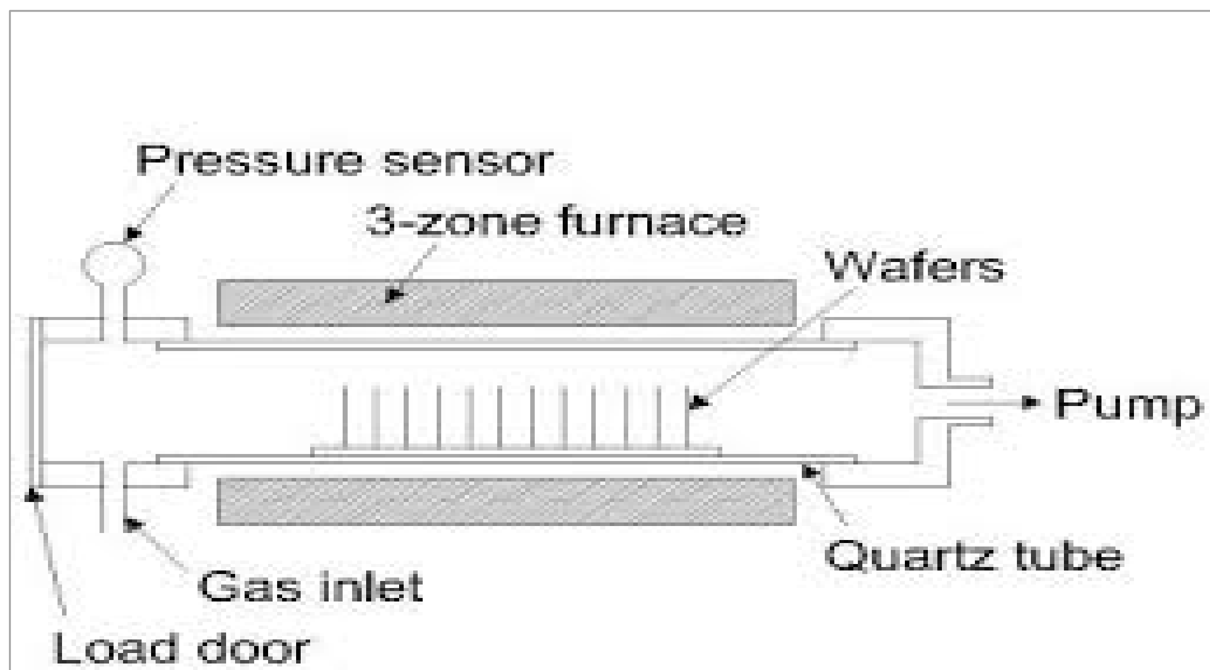

Figure 1.8 Schematic representation of chemical vapor deposition (CVD).

CVD relies on chemical reactivity between ionized vaporized gas within the deposition chamber. Ionized gas is injected through control valves into the deposition chamber where a chemical reaction occurs between the precursor and substrate.**[29]**

3.2.2.1. Plasma-enhanced chemical vapor deposition (PECVD)

is a chemical vapor deposition process used to deposit thin films from a gas state (vapor) to a solid state on a substrate. Chemical reactions are involved in the process, which occur after creation of a plasma of the reacting gases. The plasma is generally created by radio frequency (RF) (alternating current (AC)) frequency or direct current (DC) discharge between two electrodes, the space between which is filled with the reacting gases. **[29]**

Figure 1.9 PECVD (Plasma-enhanced chemical vapor deposition) machine.

3.3. Importance of deposition technology in modern fabrication processes

Deposition technology can well be regarded as the major key to the creation of devices such as computers, since microelectronic solid-state devices are all based on material structures created by thin-film deposition. Electronic engineers have continuously demanded films of improved quality and sophistication for solid-state devices, requiring a rapid evolution of deposition technology. Equipment manufacturers have made successful efforts to meet the requirements for improved and more economical deposition systems and for in situ process monitors and controls for measuring film parameters. Another important reason for the rapid growth of deposition technology is the improved understanding of the physics and chemistry of films, surfaces, interfaces, and microstructures made possible by the remarkable advances in analytical instrumentation during the past twenty years. A better fundamental understanding of materials leads to expanded applications and new designs of devices. **[29]**

3.4. Deposition Technologies and Applications

A good example of the crucial importance of deposition technology is the fabrication of semiconductor devices, an industry that is totally dependent on the formation of thin solid films of a variety of materials by deposition from the gas, vapor, liquid, or solid phase. The starting materials, epitaxial films of semiconductors, are usually grown from the gas phase. Chemical vapor deposition of a single-crystal silicon film on a single-crystal silicon substrate of the same crystallographic

orientation, a process known as homoepitaxy, is accomplished by hydrogen reduction of dichlorosilane vapor. If a single-crystal film of silicon is deposited on a non-silicon crystal substrate, the process is termed heteroepitaxy. Layers of single-crystal compound semiconductors are created to a thickness of a few atom layers by molecular beam epitaxy. Subsequent steps in the fabrication process create electrical structures that require the deposition of an insulating or dielectric layer, such as an oxide, glass, or nitride, by one of several types of chemical vapor deposition (CVD) processes, by plasma-enhanced chemical vapor deposition (PECVD), or by any one of a number of sputtering deposition methods. The deposition of conductor films for contact formation and interconnections can be accomplished by vacuum evaporation or sputtering. CVD processes are especially suitable if polysilicon, polycides, or refractory metals are to be deposited. **[28]**

CHAPTER II

Sputtering

1. Sputtering

1.1. Introduction

Sputtering is a technique used to deposit thin films of a material onto a surface ("substrate"). By first creating a gaseous plasma and then accelerating the ions from this plasma into some source material ("target"), the source material is eroded by the arriving ions via energy transfer and is ejected in the form of neutral particles - either individual atoms, clusters of atoms or molecules. As these neutral particles are ejected they will travel in a straight line unless they come into contact with something - other particles or a nearby surface. If a "substrate" such as a Si wafer is placed in the path of these ejected particles it will be coated by a thin film of the source material**. [30]**

- So in sputtering, the target material and the substrate is placed in a vacuum chamber.
- A voltage is applied between them so that the target is the cathode and the substrate is attached to the anode.
- A plasma is created by ionizing a sputtering gas (generally a chemically inert, heavy gas like Argon).
- The sputtering gas bombards the target and sputters off the material we would like to deposit.

1.2.Generality

Sputtering is the thin film deposition manufacturing process at the core of today's semiconductors, disk drives, CDs, and optical devices industries. On an atomic level, sputtering is the process whereby atoms are ejected from a target or source material that is to be deposited on a substrate - such as a silicon wafer, solar panel or optical device - as a result of the bombardment of the target by high energy particles.

The verb "To Sputter" comes from the Latin word Sputare meaning to "To emit saliva with noise." While the word sputtering sounds funny to those who associate it with stammering and speech impediments, in 1970 Peter J. Clarke changed the course of history when he developed the first "Sputter gun" that catapulted the semiconductor industry by enabling the accurate and reliable deposition of materials on an atomic level using a charged plasma stream of electrons and ions in a vacuum environment.

The sputtering process begins when a substrate to be coated is placed in a vacuum chamber containing an inert gas - usually Argon - and a negative charge is applied to a target source material that will be deposited onto the substrate causing the plasma to glow.

Free electrons flow from the negatively charged target source material in the plasma environment, colliding with the outer electronic shell of the Argon gas atoms driving these electrons off due to their like charge. The inert gas atoms become positively charged ions attracted to the negatively charged target material at a very high velocity that "Sputters off" atomic size particles from the target source material due to the momentum of the collisions. These particles cross the vacuum deposition chamber of the sputter coater and are deposited as a thin film of material on the surface of the substrate to be coated.

Sputtering only takes place when the kinetic energy of the bombarding particles is extremely high, much higher than normal thermal energies in the "Fourth state of nature" plasma environment. This can allow a much more pure and precise thin film deposition on the atomic level than can be achieved by melting a source material with conventional thermal energies.

The number of atoms ejected or "Sputtered off" from the target or source material is called the sputter yield. The sputter yield varies and can be controlled by the energy and incident of angle of the bombarding ions, the relative masses of the ions and target atoms, and the surface binding energy of the target atoms. Several different methods of physical vapor deposition are widely used in sputter coaters, including ion beam and ion-assisted sputtering, reactive sputtering in an Oxygen gas environment, gas flow and magnetron sputtering.**[31]**

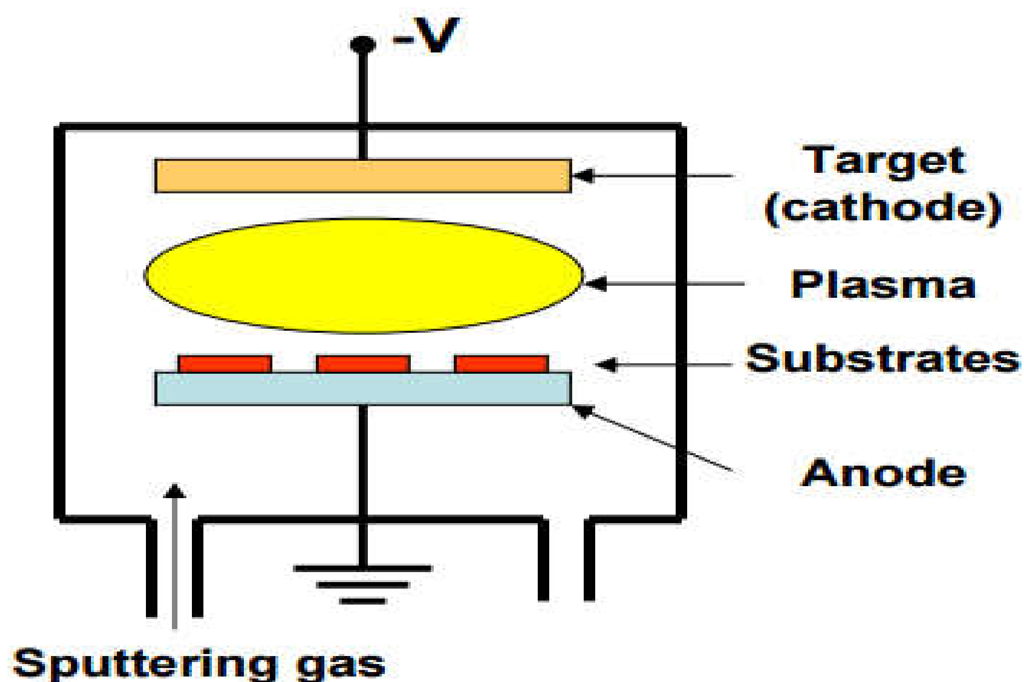

Figure 2.1 sputtering system

1.1 Sputtering Process

Over the years, a vast amount of sputter phenomena have been published. Based on analytical models, semi-empirical formulas and computer simulation programs have been developed and published. In the field of theoretical study of sputtering, Thompson's work for energy distribution and Sigmund's for the sputtering yield. After their work, Monte Carlo codes (SIMTRA, SRIM, etc.) have been developed, and have been applied to obtain various properties of sputtering.

As sputter deposition has become popular, problems of it have also been recognized, e.g. the inhomogeneity of the deposition rate on substrate positions. In addition, it has also been understood that the sputtered particles have much larger energies compared to the particles in vacuum evaporation, and affect the properties of deposited films in various ways. Therefore, it is interesting to know how sputtered particles are transported to the substrate, and what energy, flux and incidence angle they reach therewith[38] The Monte Carlo simulation is one of these studies. **[1]**

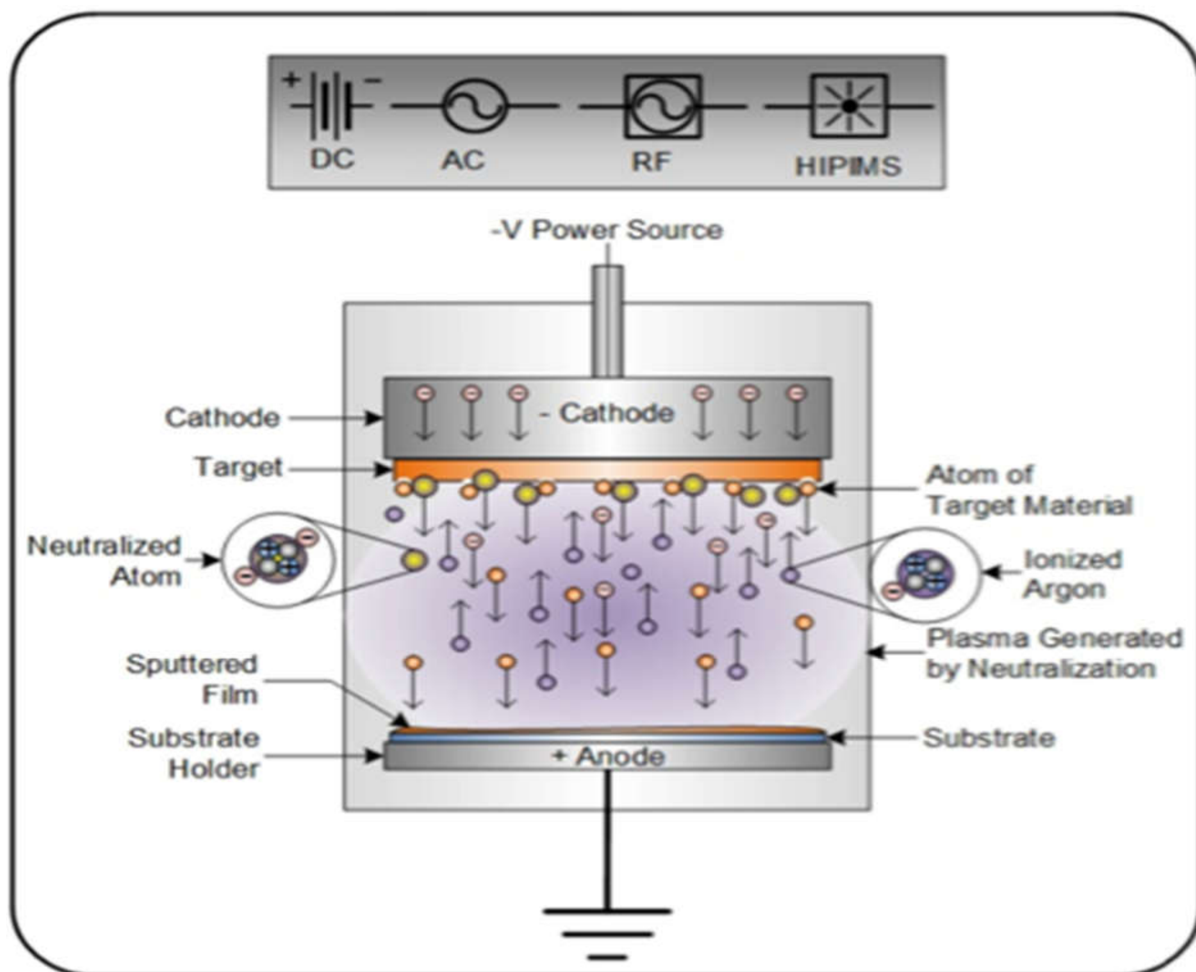

Figure 2.2 Diagram of the Sputtering Process

In sputter deposition processes (figure 2.2), ions are commonly employed as energetic species because their energy can be easily controlled by using electric fields. Ions can be provided by an ion source but the most common way is by ionizing inert gas (typically Ar) atoms (i.e. generating a glow discharge/plasma) in an evacuated vessel (referred to as chamber). The inert gas ionization occurs by applying a potential difference between the target (serving as a cathode) and an anode. Then positively charged Ar ions are accelerated towards the cathode (negatively biased) providing the energy and momentum necessary for sputtering. Magnetic fields can be used along with an electric field to confine the plasma close to the target and improve efficiency of the process. Reactive gases can be added to trigger chemical reactions (primarily on the substrate surface) and thus facilitate synthesis of multicomponent (compound) films. Sputter deposition is a widely used technique, since it combines versatility, control over the composition and microstructure, relatively high deposition rates and conceptual simplicity. Moreover it has the advantage of scalability, to develop deposition processes and films on a laboratory and transfer them to an industrial environment**. [1]**

2. Sputtering yield formulas

The average number of atoms ejected from the target per incident ion is called the sputter yield and depends on several variable parameters such as the energy of the ion, the ion incident angle, the masses of the ion and target atoms, the surface binding energy of atom sin the target, and target's material. **[4]**

$$S = \frac{Number\ of\ sputtered\ atoms}{Number\ of\ incident\ ions} \quad (2)$$

- S depends on
  - – type of target atom
  - – binding energy of target atoms
  - – relative mass of ions and atoms
  - – incident ion energy
  - – angle of incidence of ions
- S can range from 0.1 to 10.

2.1 Sigmund formula

It would take too long to develop the calculations that helped get the sputtering yield. In 1969 , Sigmund published a theoretical analysis of sputtering . He presented a systematic theory of sputtering on the basis of minimum assumptions and without adjustable parameters. He developed the sputtering yield equation (Y) for yield from the Boltzmann transport equation that is a function of collision cross sections, and atomic binding energies.

He arrived in solving analytically the Boltzmann equation by making a number of approximations (approximation of binary collisions, infinite medium, etc.), this which overcomes a digital resolution. A general analytical formula for the sputter yield reads

$$Y(E) = A\alpha n_t \, S_n(E) \qquad (3)$$

where A is a material constant that includes the range of a displaced target atom and the probability of ejection of an atom at the surface, **α** is a dimensionless correction factor that depends on the mass ratio $\frac{\mathbf{M1}}{\mathbf{M2}}$ in the elastic collision regime where **M1** and **M2** are the atomic masses of the impinging particles (ions) and of the target atoms, respectively, **nt** is the atomic density of the target and **Sn(E)** is the stopping power of the ion.

$$y(E) = A\alpha n_t \, (E) \qquad (4)$$

This yield expression applies for low and high energy bombardment particles. For normal incidence of bombarding ions/particles with energies smaller than **1keV**, equation (4) can be simplified to

$$Y(E) = \left(\frac{3}{4\pi^2}\right)\frac{yE^{1-2n}}{U_{sb}}\alpha \qquad (5)$$

In which **γ** is the energy transfer mass factor, **E** the energy of the impinging particle, Usb is the surface binding energy of the target material, and the parameter m depends on the energy of the impinging ions and ranges from **m=1** at high energies (keV range) down to **m=0** at low energies (eV range).**[1][4]**

2.2 Improvements made by other authors

Many discrepancies have been observed in relation to the theory developed by Sigmund. The formula given by him to calculating the sputtering yield does not reflect well the experiments performed with light ions or incident particles having energies near their threshold sputtering. In1984, Matsunamietal. offered a first semi empirical formula that takes into consideration the threshold

sputtering for normal incidence. In 1981, Meyer, Schuller and Falco gave a first compilation of sputtering yield for different pairs (incident ion-atom) of the target.

The formula includes the cross section of electronic stopping power, which allows making calculations even for light ions. Bohdansky took the same approach to calculate the sputtering yield coefficient near threshold and for light incident particles. He obtains a new expression for the sputtering yield according to the energy of the incident particle**. [1]**

2.3 Sputter yield formula obtained by Yamamura

Another rapproach to calculate the sputter yield is by using semi-empirical equations developed by Yamamura metal. in. Yamamura and Tawara extrapolate two formulas, one for heavy ions and another for light ions. In addition to this formula, Yamamura and Ishida have developed a Monte Carlo code–ACAT–which calculates the sputtering yield using the approximation of binary collisions. If we consider an incident particle with atomic mass **M1** and atomic number **Z1**, a target material composed of atoms with atomic mass **M2** and atomic number **Z2**, the sputtering yield for normal incidence **Y(E)** givenYamamuraetal.is written **[1][4]**

$$Y(E) = 0.042 \frac{Q(Z_2)\alpha^*\left(\frac{M1}{M2}\right)}{U_s} \frac{S_n(\epsilon)}{1+\Gamma K_e \epsilon^{0.3}} \left[1 - \sqrt{\frac{E_{th}}{E}}\right] \quad (6)$$

With energy **E** in **eV**, **ϵ** is the reduced energy

$$\epsilon = \frac{0.03255}{Z_1 Z_2 \left(Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}}\right)} \times \frac{M_2}{M_1 + M_2} E, \quad (7)$$

$S_n(\epsilon)$and **k_e $\epsilon^{0.3}$** represent, respectively, the electronic and nuclear stopping powers, **Us** is the sublimation.

$$\Gamma = \frac{W(Z_2)}{1+\left(\frac{M_1}{7}\right)3}, \quad (8)$$

and **α*** depends on the masses report $\frac{\mathbf{M1}}{\mathbf{M2}}$ and represents the collisional inelastic phenomena. It has been tabulated for a large number of ions/target pairs allowing Yamamura obtain a formula for this coefficient:

$$\alpha^* = 0.249 \times \left(\frac{M_2}{M_1}\right)^{0.56} + 0.0035 \times \left(\frac{M_2}{M_1}\right)^{1.5} \quad when\ M_1 \geq M_2 \quad (9)$$

And

$$\alpha^* = 0.0875 \times \left(\frac{M_2}{M_1}\right)^{-0.15} + 0.165 \times \left(\frac{M_2}{M_1}\right) \quad when\ M_1 \leq M_2 \qquad (10)$$

Threshold sputtering **E_{th}** has also been tabulated from experimental data. Yamamura gave a general expression in which this coefficient depends on the binding energy and mass of ions and target:

$$\frac{E_{th}}{U_s} = \frac{0.7}{\gamma} \quad for\ M_1 \geq M_2 \qquad (11)$$

And

$$\frac{E_{th}}{U_s} = \frac{1+5.7\times\left(\frac{M_1}{M_2}\right)}{\gamma} \quad for\ M_1 \leq M_2 \qquad (12)$$

With

$$\gamma = \frac{4M_1M_2}{(M_1+M_2)^2} \qquad (13)$$

3.Various Sputtering Regimes

3.1 Single Knock-On

The initial ion-surface collision sets target atoms in motion. If enough energy is transferred, binding forces can be overcome. Typical threshold energies are in the 10 - 30 eV range. **[31]**

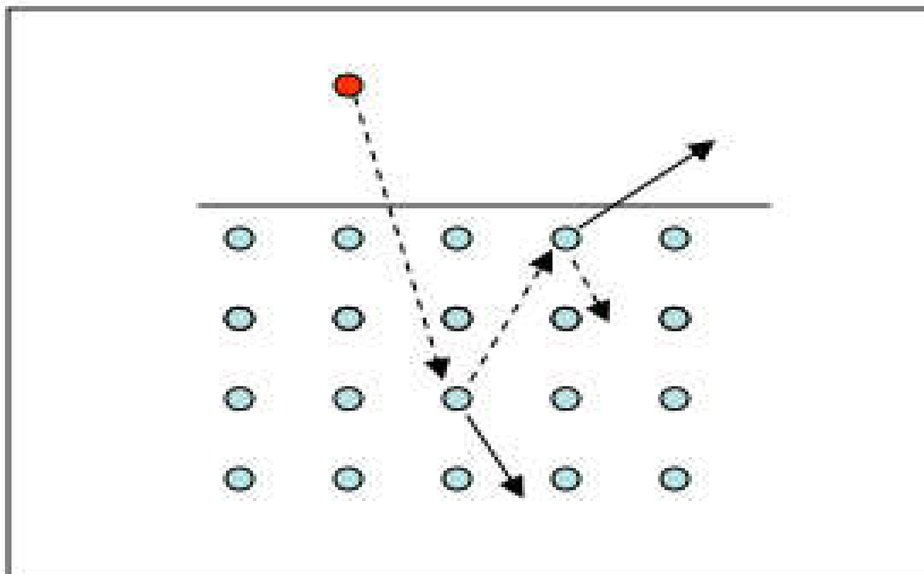

Figure 2.3 Schematic representation of Single Knock-On

3.2 Linear Collision Cascade

At higher ion energies (100 eV-10 keV) recoil is minimal and a cascading effect produces sputtering. **[31]**

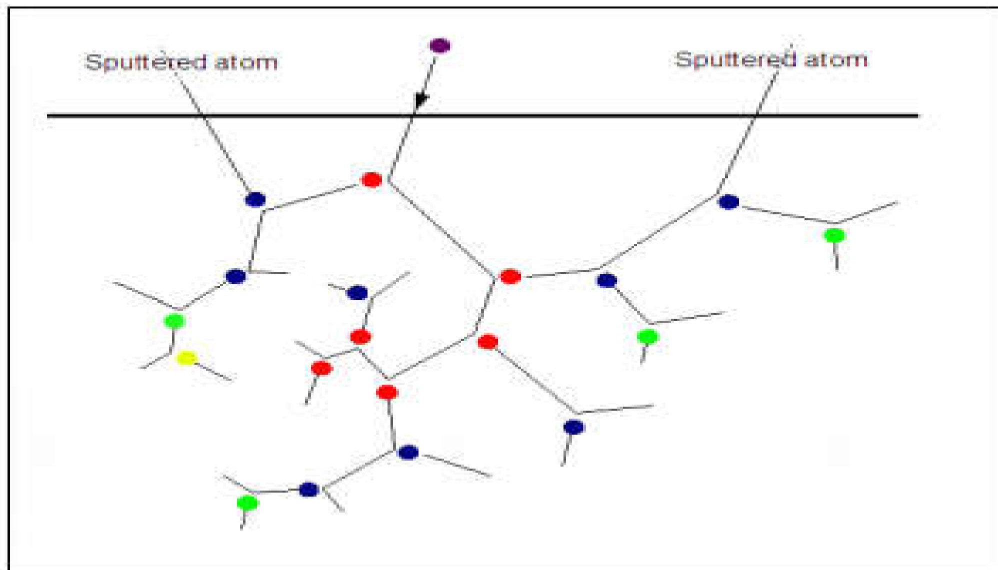

Figure 2.4 Schematic representation of linear collision cascade

4.General sputtering methodology

4.1 Reactive sputtering

Reactive Sputtering is the process of adding a gas to the vacuum chamber that undergoes a chemical reaction before coming into contact with the materials to be coated. Gases like Nitrogen or Oxygen which are normally stable and inert under normal circumstances become ionized and reactive in the plasma environment as a result of the high energy collisions. When this happens, the gas can react chemically with the target material cloud and create a molecular compound which then becomes the thin film coating. For example, a silicon target reactively sputtered with oxygen gas can produce a silicon oxide film, or with nitrogen can produce a silicon nitride film which are at the heart of the semiconductor industry. **[32]**

4.2 RF (radio frequency) sputter deposition

RF or Radio Frequency Sputtering is the technique involved in alternating the electrical potential of the current in the vacuum environment at radio frequencies to avoid a charge building up on certain types of sputtering target materials, which over time can result in arcing into the plasma that spews droplets creating quality control issues on the thin films – and can even lead to the complete cessation of the sputtering of atoms terminating the process.

In RF sputtering there are a cathode (the target) and a anode, in series with a blocking capacitor (C). The capacitor is part of an impedance-matching network that proves the power transfer from the RF source to the plasma discharge. The power supply is a high voltage RF source often fixed at 13.56 MHz. The blocking capacitor C is placed in the circuit to develop the all-important DC self-bias, and a matching network is utilized to optimize power transfer from the RF source to the plasma. RF-sputtering offers advantages over DC; in particular sputtering of an electrically insulating target become possible. **[32]**

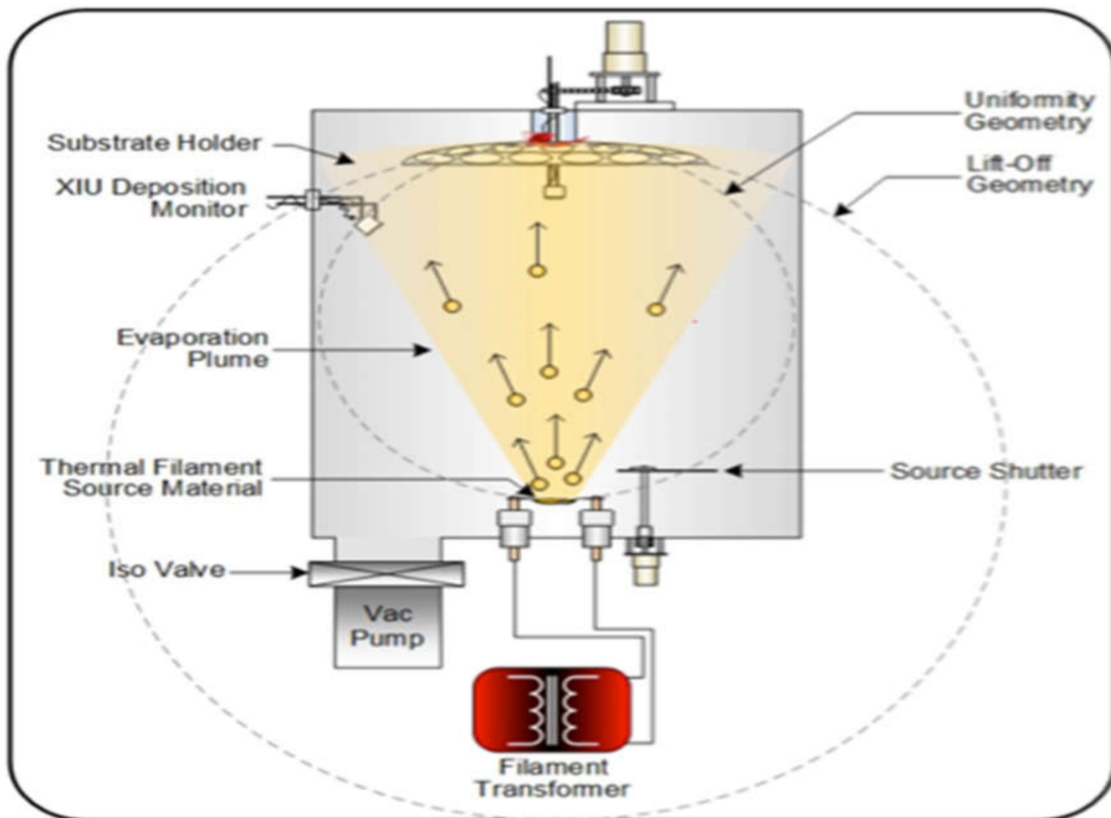

Figure 2.5 Diagram of the RF Sputtering Process

4.3. Magnetron sputtering

The "diode sputtering" example given above has proven to be a useful technique in the deposition of thin films when the cathode is covered with source material ("sputtering target"). Diode sputtering however has two major problems - the deposition rate is slow and the electron bombardment of the substrate is extensive and can cause overheating and structural damage.

The development of magnetron sputtering deals with both of these issues simultaneously. By using magnets behind the cathode to trap the free electrons in a magnetic field directly above the target surface, these electrons are not free to bombard the substrate to the same extent as with diode

sputtering. At the same time the extensive, circuitous path carved by these same electrons when trapped in the magnetic field, enhances their probability of ionizing a neutral gas molecule by several orders of magnitude. This increase in available ions significantly increases the rate at which target material is eroded and subsequently deposited onto the substrate. **[31]**

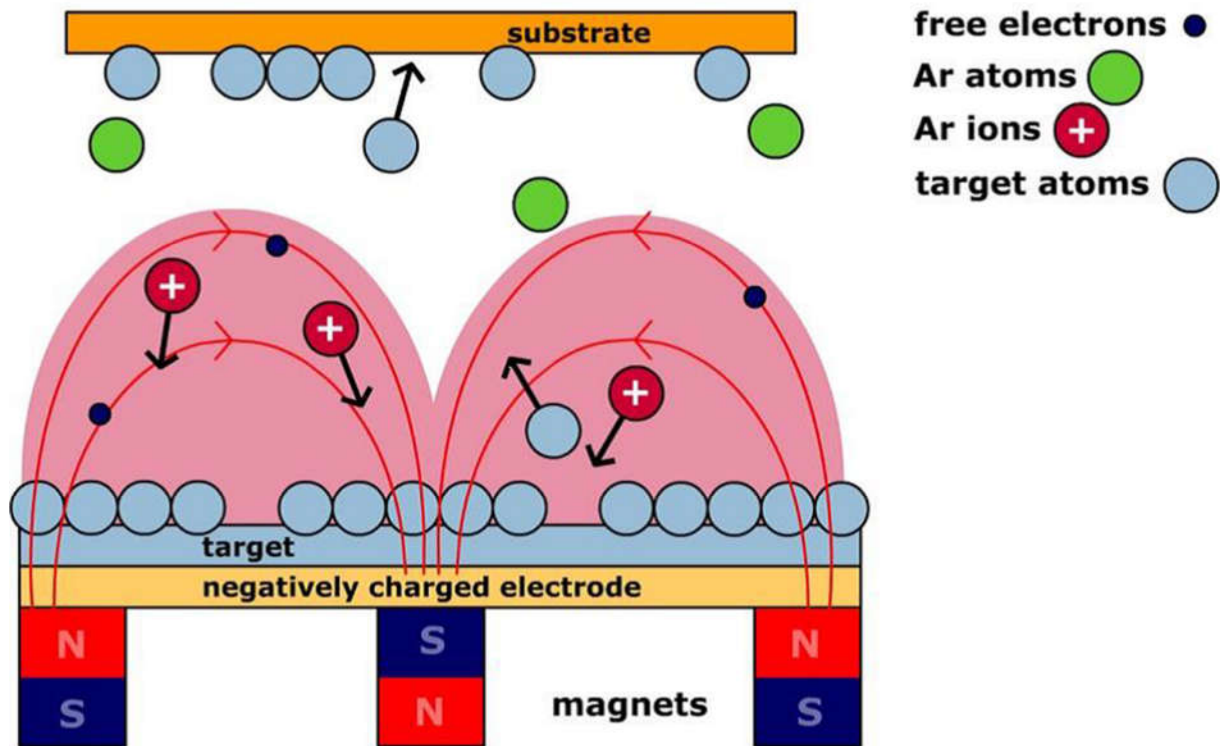

Figure 2.6 Schematic representation of Magnetron sputtering system

4.4. Direct sputtering (DC sputtering)

DC or Direct Current Sputtering is a Thin Film Physical Vapor Deposition (PVD) Coating technique where a target material to be used as the coating is bombarded with ionized gas molecules causing atoms to be “Sputtered” off into the plasma. These vaporized atoms are then deposited when they condense as a thin film on the substrate to be coated. It is the most basic and inexpensive type of sputtering for PVD metal deposition and electrically conductive target coating materials. Two major advantages of DC as a power source for this process is that it is easy to control and is a low cost option if you are doing metal deposition for coating. it is used extensively in the semiconductor industry creating microchip circuitry on the molecular level. It is used for gold sputter coatings of jewelry, watches and other decorative finishes, for non-reflective coatings on glass and optical components, as well as for metalized packaging plastics. The basic configuration of a DC Sputtering coating system is the target material to be used as a coating is placed in a vacuum chamber parallel to the substrate to be coated. **[31]**

A direct sputtering system configuration is when the substrate is positioned or moving directly in front of and parallel to the magnetron sputtering source targets. As a rule, target diameters (or "lengths" as in the case of rectangular magnetron sputtering sources) should be about 20% to 30% larger than the substrate to achieve reasonable uniformity. For example a 100 mm wafer would require a 150 mm sputter target to achieve +/- 5% deposition uniformity. Although this configuration is much less flexible and generally more expensive than con-focal sputtering, it has its place in production applications which require maximum deposition rates (semiconductor wafer metallization), applications which utilize large substrates (e.g. flat panel displays) and a few techniques that demand "line-of-sight deposition"

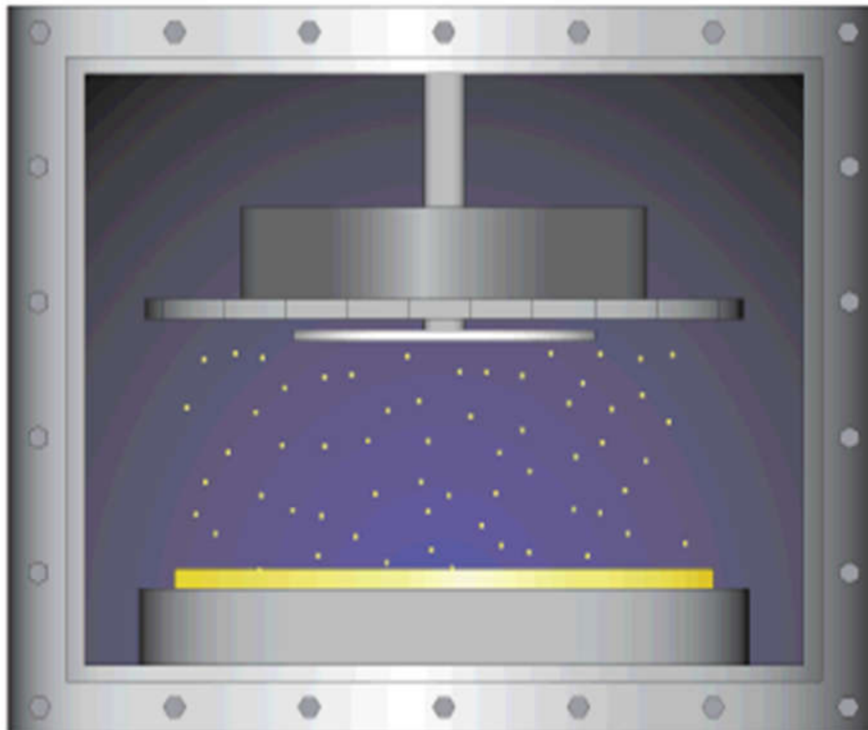

Figure 2.7 Direct sputtering (DC sputtering)

4.5. Confocal sputtering

Confocal sputtering is the technique of arranging magnetrons within a vacuum chamber in such a way that multiple materials can be applied onto the substrate without breaking vacuum. Confocal sputtering also allows the user to co-sputter, or to create a film of two or more materials at once. This method is popular for research and development tools and for small scale batch productions. it is based on changing the angle of the cathode target with respect to the substrate in order to create a more uniform deposition process. Confocal sputtering requires that the cathode be mounted at an angle (θ) relative to the vertical (y) axis. **[33]**

4.6. Co-Sputtering

Co-Sputtering is where two or more target materials are sputtered at once in the vacuum chamber and is often used with Reactive Sputtering to produce thin films that are compounds such as alloys or composites. It is widely used in the optical and architectural glass industries. By utilizing Reactive Co-Sputtering of two target materials such as Silicon and Titanium with dual Magnetron Sputtering, the refractive index or shading effect of the glass can be carefully and precisely controlled on applications ranging from large scale surfaces such as skyscraper architectural glass to sunglasses. It is also widely used producing solar panels. **[33]**

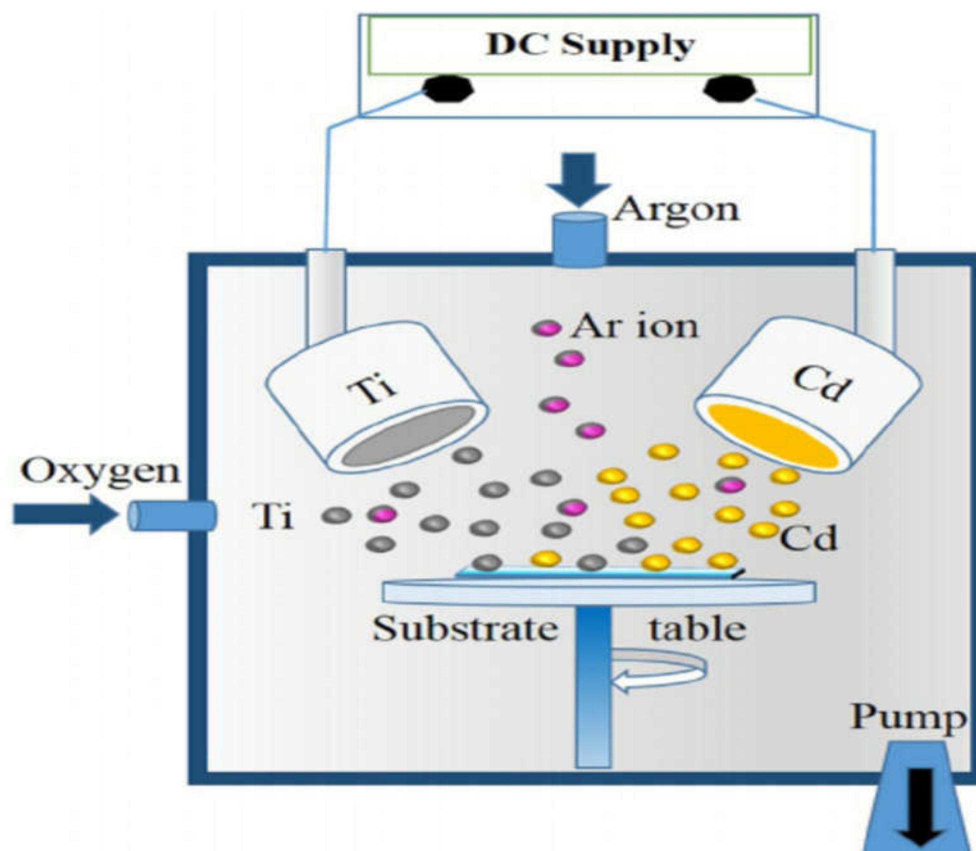

Figure 2.8 Schematic diagram of dc magnetron co-sputtering system

4.6. Pulsed DC Sputtering

Pulsed DC Sputtering is a physical vapor deposition technique with a wide range of applications in the semiconductor, optical and industrial coating industries. Pulsed DC Sputtering is particularly effective for the sputtering of metals and dielectric coating – coatings which are insulating non-conducting materials that can acquire a charge. It is most often used with Reactive Sputtering where there is a chemical reaction occurring in the plasma between the vaporized target material and ionized gases like Oxygen to form deposition molecules such as silicon oxides. Pulsed DC Sputtering has revolutionized the Reactive Sputtering of “difficult” dielectric materials like Alumina, Titania and

Silica with high deposition rates that are impossible with straight DC Sputtering alone. Compared to conventional DC Sputtering, arcing can be greatly decreased or even eliminated by pulsing the DC voltage in the 10–350 kHz range with duty cycles in the 50–90% range. A Pulsed DC electrical current typically in the few hundreds of volts range is applied to the target coating material. the voltage is either turned off or reversed with a low voltage short duration cycle to "cleanse" the target of any charge buildup. **[33]**

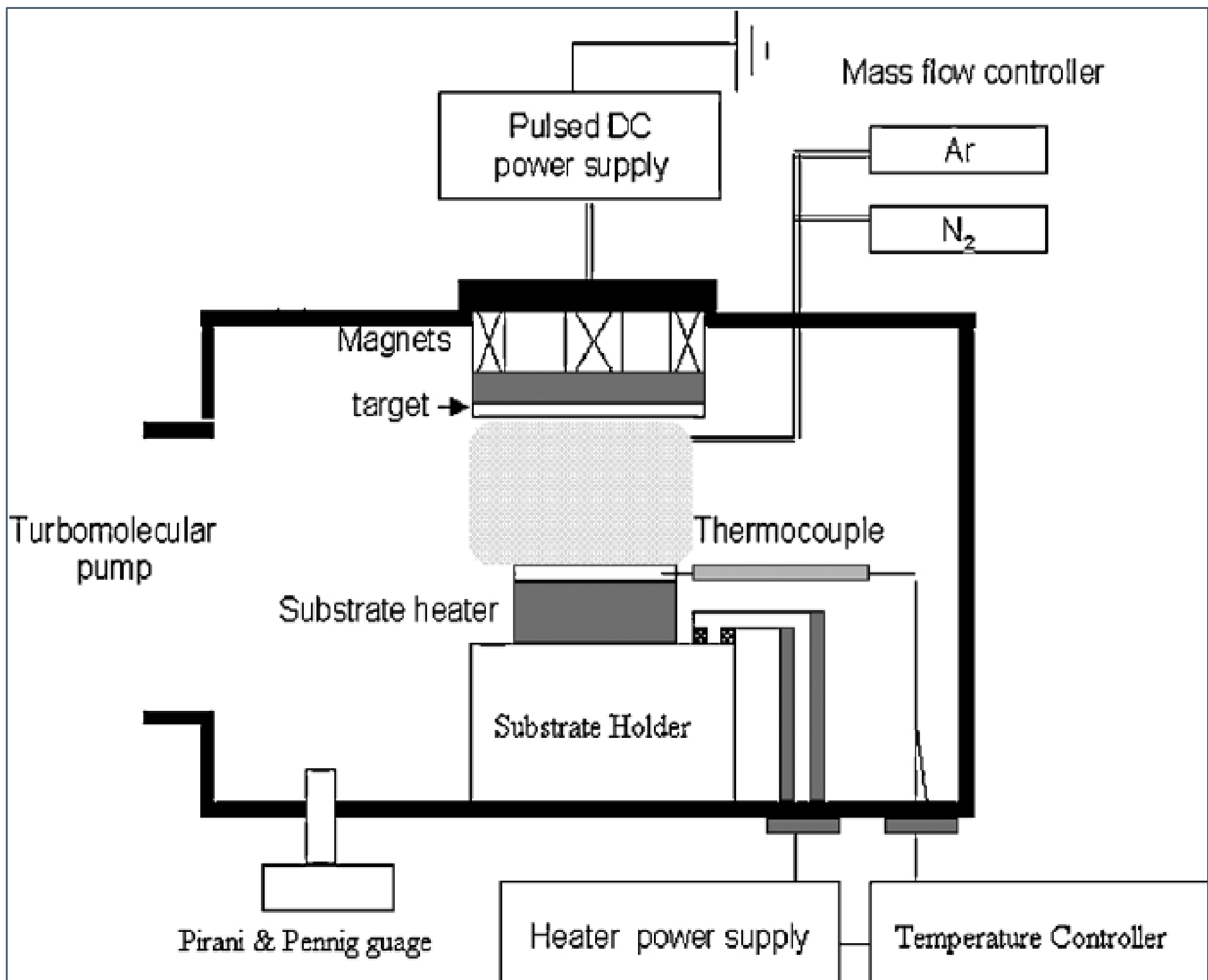

Figure 2.9 Schematic diagram of Pulsed DC sputtering system

4.7. Ion Beam Sputtering

Basics Ion beam sputtering utilizes an ion source to generate a relatively focused ion beam directed at the target to be sputtered. The ion source consists of a cathode and anode with a common central axis. Applying a high voltage field of 2-10 kV to the anode creates an electrostatic field inside the ion source, confining electrons around a saddle point in the center of the source. When argon gas is injected into the ion source, the high electric field causes the gas to ionize, creating a plasma inside

the source region. The ions are then accelerated from the anode region to the exit aperture (cathode) creating a "collimated" ion beam. The resulting ion beam impinges upon a target material and, via momentum transfer between the ion and the target, sputters this material onto the sample. **[33]**

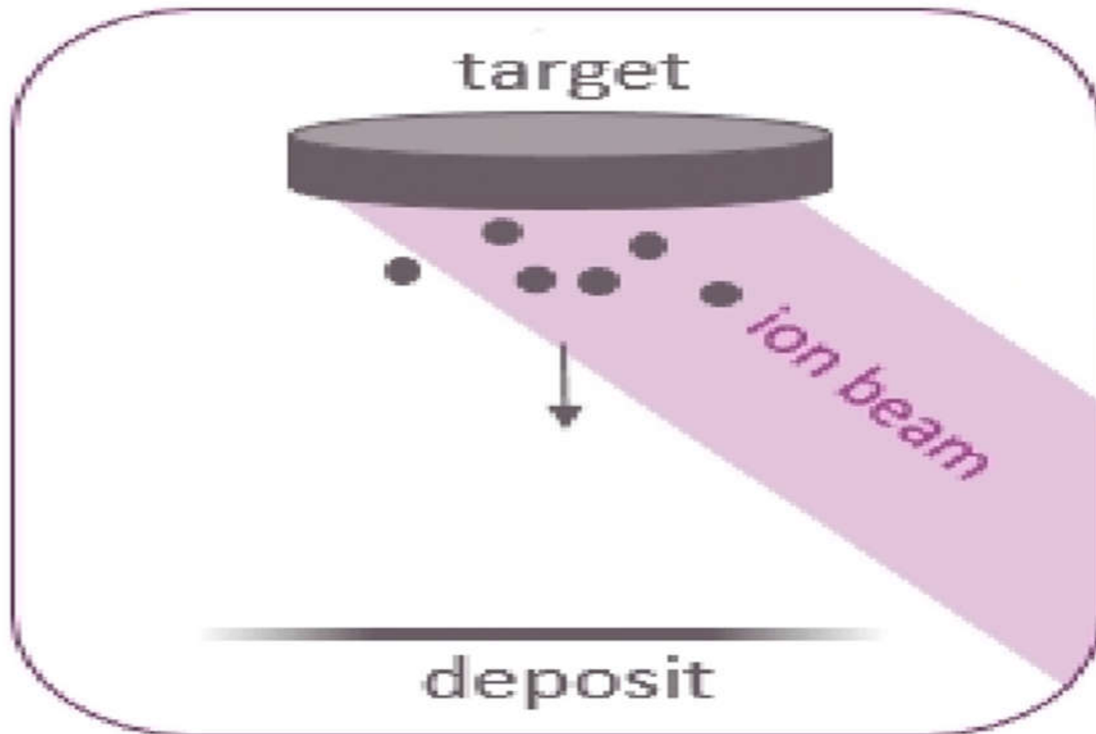

Figure 2.10 Schematic representation of ion beam sputtering system

5. Vacuum chamber

A vacuum chamber is a rigid enclosure from which air and other gases are removed by a vacuum pump. This results in a low-pressure environment within the chamber, commonly referred to as a vacuum. A vacuum environment allows researchers to conduct physical experiments or to test mechanical devices which must operate in outer space (for example) or for processes such as vacuum drying or vacuum coating. Chambers are typically made of metals which may or may not shield applied external magnetic fields depending on wall thickness, frequency, resistivity, and permeability of the material used. Only some materials are suitable for vacuum use.

Chambers often have multiple ports, covered with vacuum flanges, to allow instruments or windows to be installed in the walls of the chamber. In low to medium-vacuum applications, these are sealed with elastomer o-rings. In higher vacuum applications, the flanges have hardened steel knives welded onto them, which cut into a copper gasket when the flange is bolted on.

A type of vacuum chamber frequently used in the field of spacecraft engineering is a thermal vacuum chamber, which provides a thermal environment representing what a spacecraft would experience in space. **[30]**

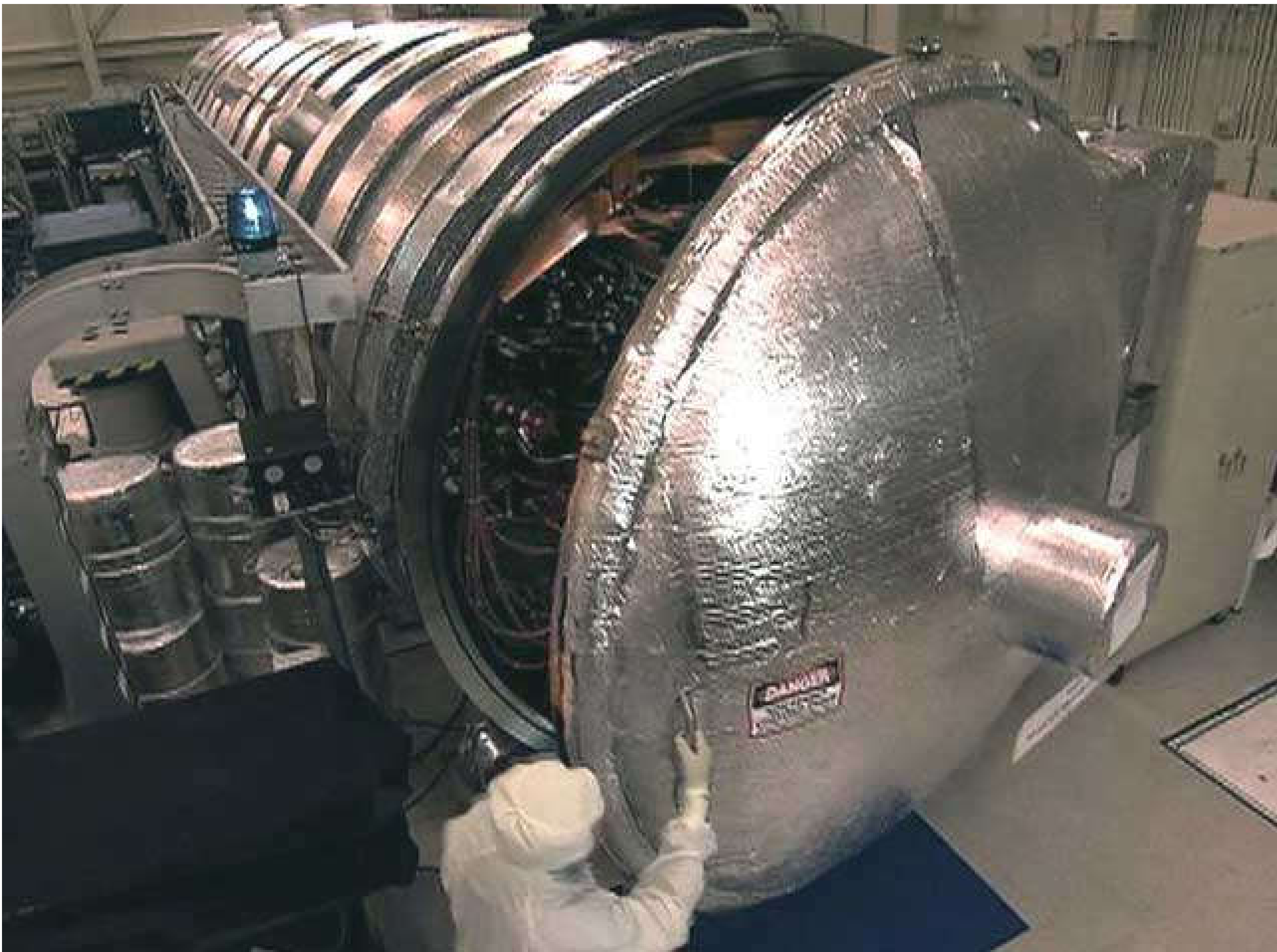

Figure 2.11 A large vacuum chamber.

6. Sputter deposition advantages

6.1 Advantages

- Able to deposit a wide variety of metals, insulators, alloys and composites.
- Replication of target composition in the deposited films.
- Capable of in-situ cleaning prior to film deposition by reversing the potential on the electrodes .
- Better film quality and step coverage than evaporation.
- This is partly because atoms are more energetic, and film is ‘densified’ by in-situ ion bombardment, and it is easier to heat up to high T than evaporation that is in vacuum.
- More reproducible deposition control – same deposition rate for same process parameters (not true for evaporation), so easy film thickness control via time.

- Can use large area targets for uniform thickness over large substrates.
- Sufficient target material for many depositions.
- No x-ray damage.

6.2. Disadvantages

- Substrate damage due to ion bombardment or UV generated by plasma.
- Higher pressures 1 –100 mtorr (< 10^{-5} torr in evaporation), more contaminations unless using ultra clean gasses and ultra clean targets.
- Deposition rate of some materials quite low.
- Some materials (e.g., organics) degrade due to ionic bombardment.
- Most of the energy incident on the target becomes heat, which must be removed.

7. Sputtering system applications

Aerospace and Defence

- Head-upcockpit displays.
- Jet turbines engines.
- Mirror for optical and x-ray telescopes .
- Night vision equipement.

Wear and Coatings

- Anti-corrosion coatings.
- Anti-seize coatings.
- Dies and molds.
- Sweing needles.
- Touls and drill bit harding.

Automotive

- Auto head lights and tail-light.
- Auto drim component.
- Wheels and rims.

Optics

- Anti-reflectives /Anti glare coating.
- Cable communication.
- Laser lenses.
- Optical filters for achromatic lenses.
- Spectroscopy.

CHAPTER III

Results And Discussion

1. Monte Carlo method

1.1.Introduction

In general terms, the Monte Carlo method (or Monte Carlo simulation) can be used to describe any technique that approximates solutions to quantitative problems through statistical sampling. As used here, 'Monte Carlo simulation' is more specifically used to describe a method for propagating (translating) uncertainties in model inputs into uncertainties in model outputs (results). Hence, it is a type of simulation that explicitly and quantitatively represents uncertainties. Monte Carlo simulation relies on the process of explicitly representing uncertainties by specifying inputs as probability distributions. If the inputs describing a system are uncertain, the prediction of future performance is necessarily uncertain. That is, the result of any analysis based on inputs represented by probability distributions is itself a probability distribution. Whereas the result of a single simulation of an uncertain system is a *qualified statement* ("if we build the dam, the salmon population could go extinct"), the result of a probabilistic (Monte Carlo) simulation is a *quantified probability* ("if we build the dam, there is a 20% chance that the salmon population will go extinct"). Such a result (in this case, quantifying the risk of extinction) is typically much more useful to decision-makers who utilize the simulation results. In order to compute the probability distribution of predicted performance, it is necessary to propagate (translate) the input uncertainties into uncertainties in the results. A variety of methods exist for propagating uncertainty. Monte Carlo simulation is perhaps the most common technique for propagating the uncertainty in the various aspects of a system to the predicted performance.

1.2. History

Monte Carlo simulation was named after the city in Monaco (famous for its casino) where games of chance (e.g., roulette) involve repetitive events with known probabilities. Although there were a number of isolated and undeveloped applications of Monte Carlo simulation principles at earlier dates, modern application of Monte Carlo methods date from the 1940s during work on the atomic bomb. Mathematician Stanislaw Ulam is credited with recognizing how computers could make Monte Carlo simulation of complex systems feasible:

The first thoughts and attempts I made to practice [the Monte Carlo Method] were suggested by a question which occurred to me in 1946 as I was convalescing from an illness and playing solitaires. The question was what are the chances that a Canfield solitaire laid out with 52 cards will come out successfully? After spending a lot of time trying to estimate them by pure combinatorial calculations, I wondered whether a more practical method than “abstract thinking” might not be to lay it out say one hundred times and simply observe and count

the number of successful plays. This was already possible to envisage with the beginning of the new era of fast computers, and I immediately thought of problems of neutron diffusion and other questions of mathematical physics, and more generally how to change processes described by certain differential equations into an equivalent form interpretable as a succession of random operations. Later … [in 1946, I] described the idea to John von Neumann, and we began to plan actual calculations. **[34]**

1.3. Generality

The Monte Carlo method, also called Monte Carlo analysis, is a means of statistical evaluation of mathematical function s using random samples. This requires a good source of random numbers . There is always some error involved with this scheme, but the larger the number of random samples taken, the more accurate the result. In its pure mathematical form, the Monte Carlo method consists of finding the definite integral of a function by choosing a large number of independent-variable samples at random from within an interval or region, averaging the resulting dependent-variable values, and then dividing by the span of the interval or the size of the region over which the random samples were chosen. This differs from the classical method of approximating a definite integral, in which independent-variable samples are selected at equally-spaced points within an interval or region. The Monte Carlo method is most famous for its use during the Second World War in the design of the atomic bomb. It has also been used in diverse applications, such as the analysis of traffic flow on superhighways, the development of models for the evolution of stars, and attempts to predict fluctuations in the stock market. The scheme also finds applications in integrated circuit (IC) design, quantum mechanics , and communications engineering.**[34]**

2. Monte Carlo Simulation

The Monte Carlo simulation is a tool to investigate the transport of sputtered atoms and to assist engineers to optimize a given deposition setup. The model is based on numerical Monte Carlo simulations which are statistical methods that allow one to link a physical value to a random number. Every test is calculated independently of all the others. Final results are the average of the simulations. The Monte Carlo method can provide various kinds of information on properties of sputtered particle flows being deposited on the substrate, and allows a considerable contribution in understanding details of the sputtered atom transport in low-pressure gas as well as energy exchanges between sputtered atoms and gas molecules. The method is very useful for examining the design of real sputtering systems, which have a complex geometry. [1]

3. SRIM 2013 (TRIM)

3.1. Generality

To estimate the energy distribution of sputtered atoms and ions reflected, we used simulation software called SRIM – "Stopping and Range of Ions in Matter" developed by Ziegler and al. We chose this program because it is easily reachable on the web. This software consists of several modules that can calculate the path of the ions in matter. Among these modules, one that has been used is the TRIM module '– 'Transport of Ions in Matter". It allows considering complex targets: targets or alloys composed of eight different films. It considers all kinetic phenomena related to the energy losses of sputtering ions ionization, producing phonons. It can also determining the collisions cascades which take place in the target, and thus indicate the atoms that reach the surface with their respectively energy. The method of calculation used is based on Monte Carlo code that simulates the transport and interaction of an ion beam to the surface of a target material and which also determines the sputtering yield. The model has several input parameters (motion energy, lattice binding energy) but more importantly, for sputtering portion is the binding energy of target material: other parameters affect less the results. **[4]**

4.Part one

4.1.Results found by SRIM simulation

For this study, we have configured the TRIM module to handle in a specific way the sputtering of a target. This mode is called "Surface Sputtering/Monolayer Collision steps" in this software.

4.1.1. Variation of the ions sputtering yield for different metals

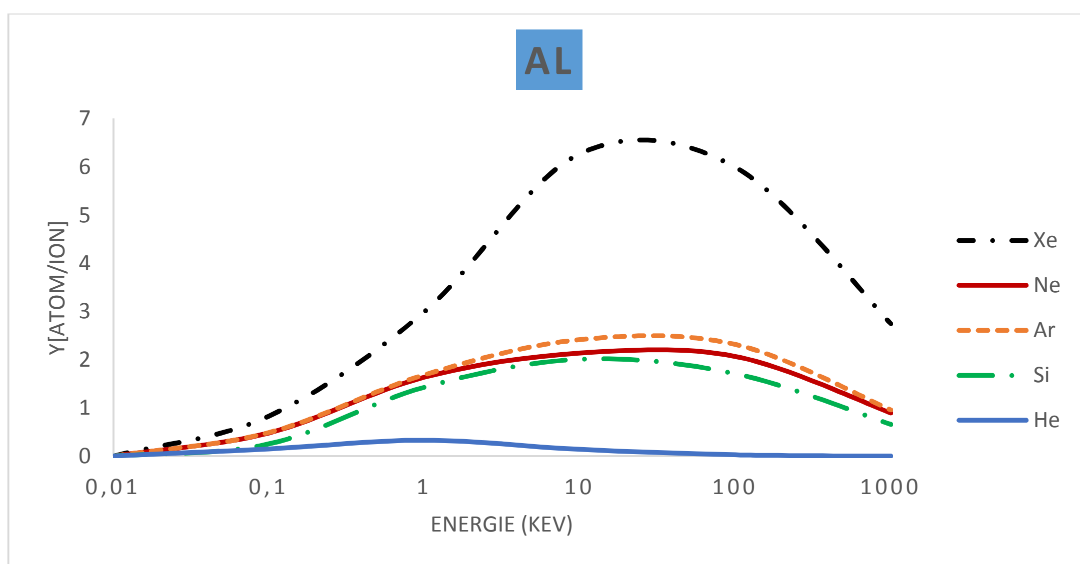

Figure 3.1 Variation of sputtering yield of Aluminum for different ions found by SRIM simulation.

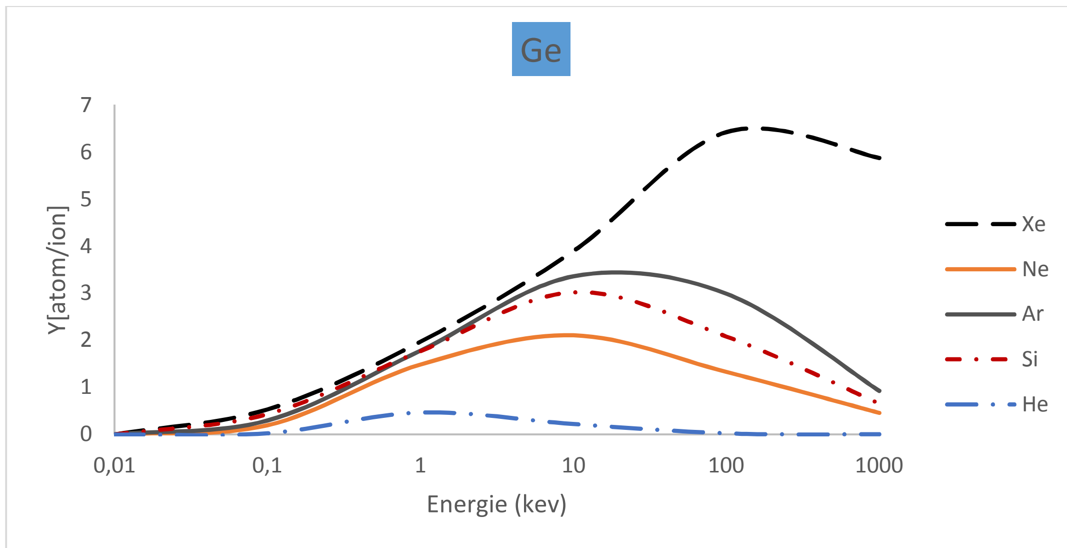

Figure 3.2 Variation of sputtering yield of Germanium for different ions found by SRIM simulation.

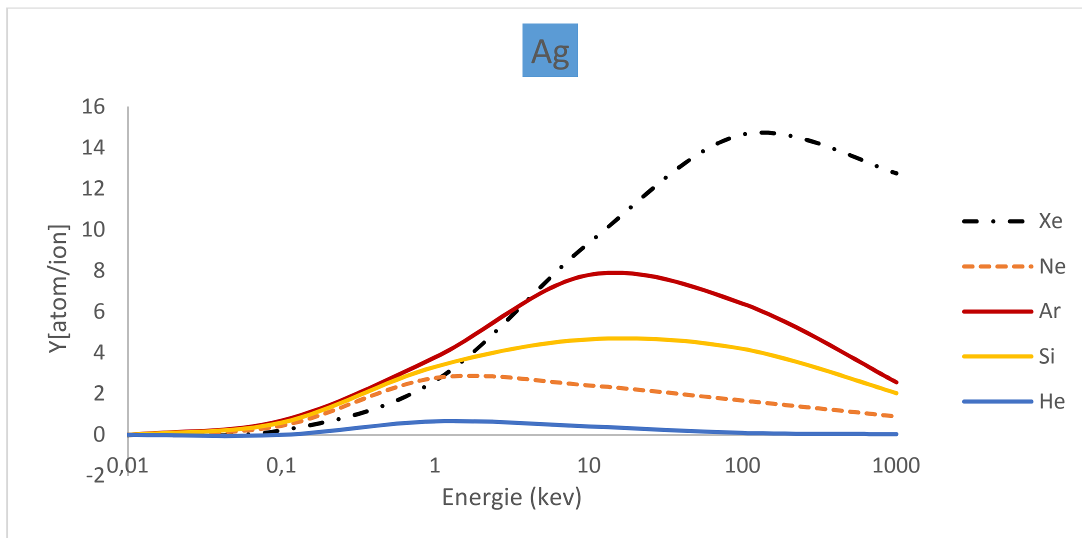

Figure 3.3 Variation of sputtering yield of silver for different ions found by SRIM simulation.

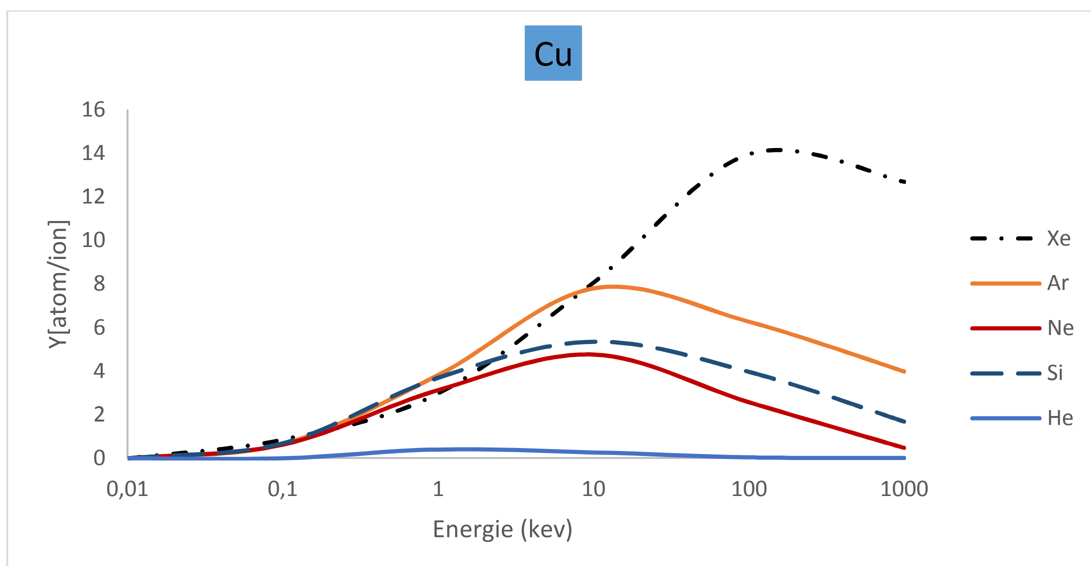

Figure 3.4 Variation of sputtering yield of copper for different ions found by SRIM simulation.

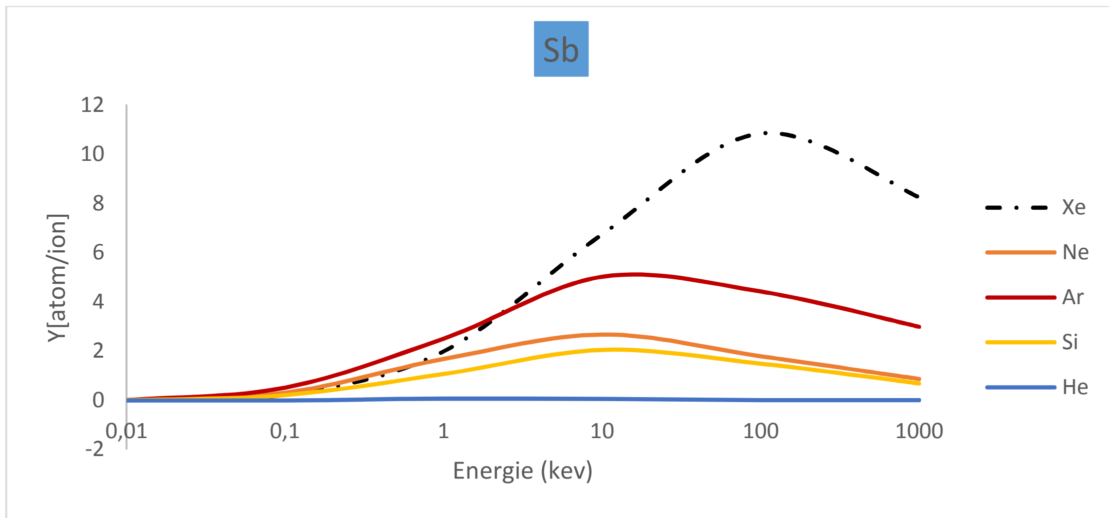

Figure 3.5 Variation of sputtering yield of Antimony for different ions found by SRIM simulation.

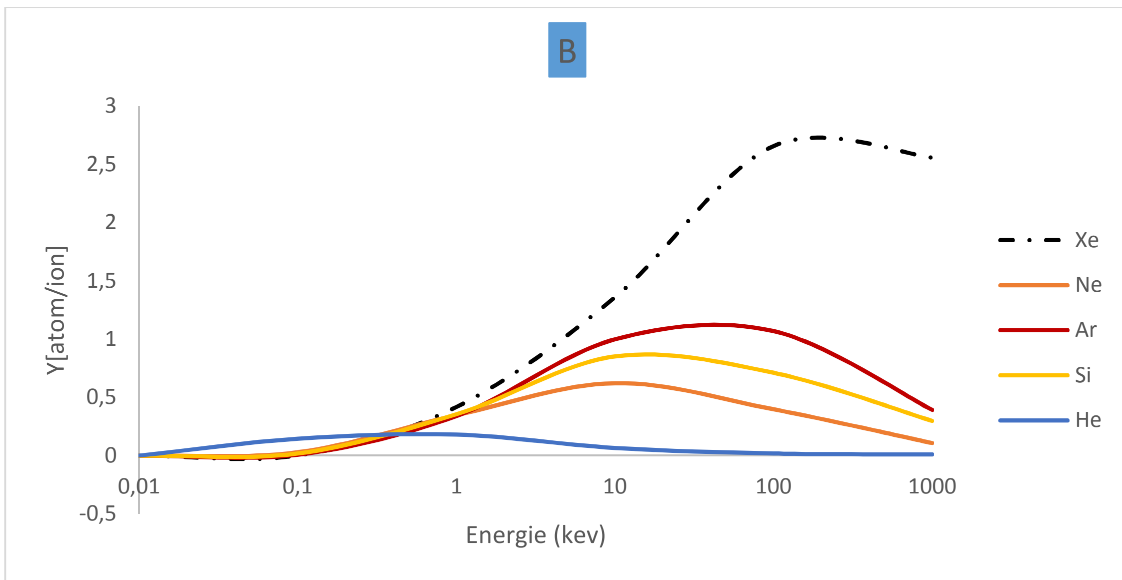

Figure 3.6 Variation of sputtering yield of Boron for different ions found by SRIM simulation.

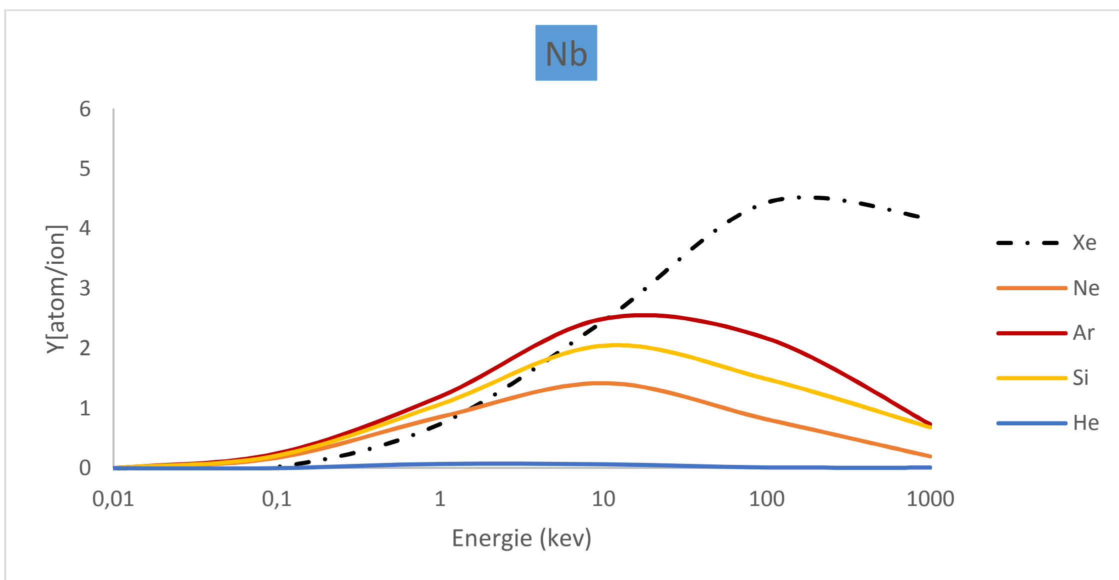

Figure 3.7 Variation of sputtering yield of Niobium for different ions found by SRIM simulation.

4.1.2. Variation of the ions sputtering yield for different gas

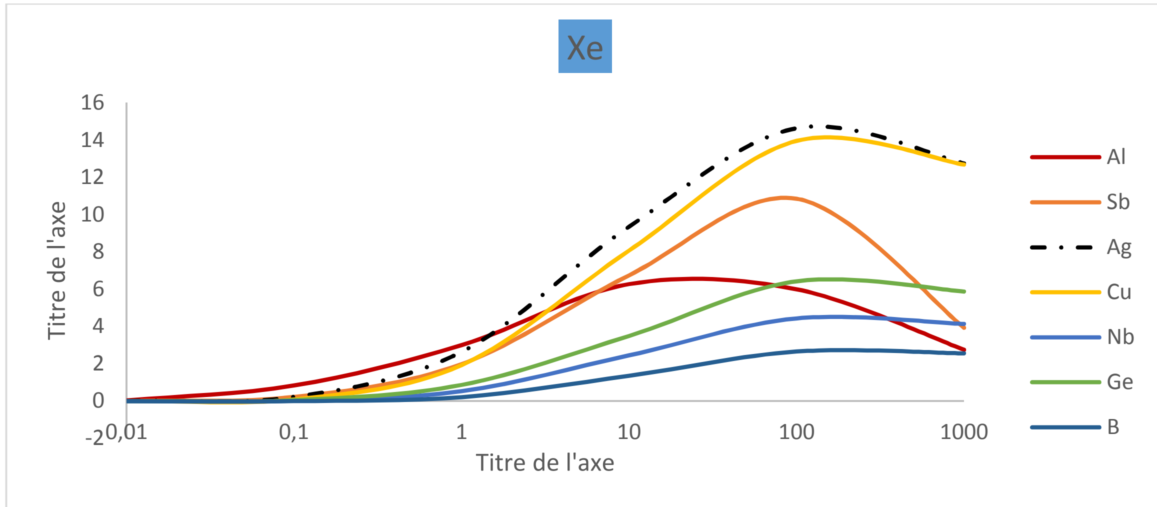

Figure 3.8 Sputtering yield of silver, aluminum, Germanium, Boron, Niobium, Antimony and copper for an xenon ion beam at normal incidence calculating

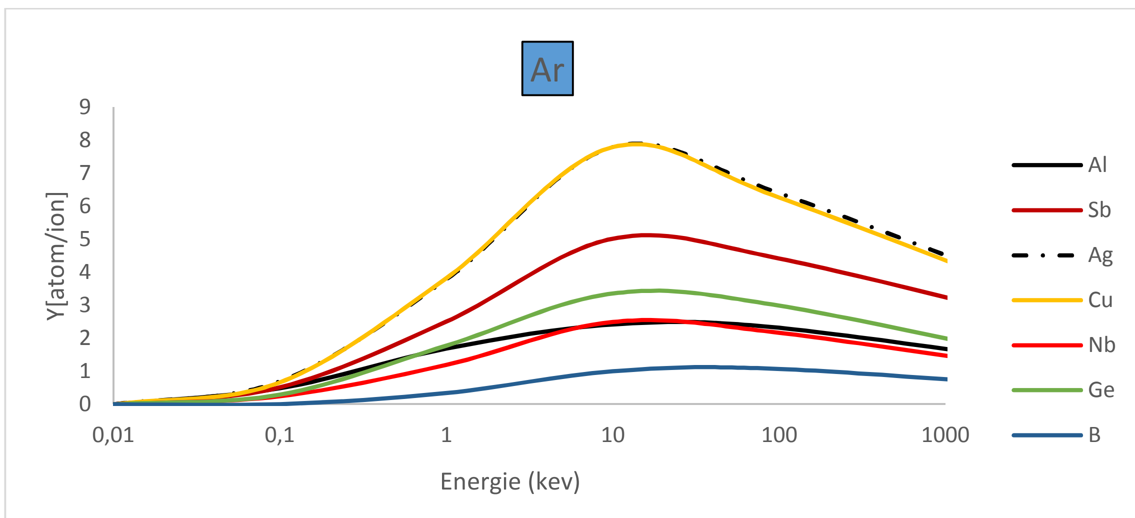

Figure 3.9 Sputtering yield of silver, aluminum, Germanium, Boron, Niobium, Antimony and copper for an Argon ion beam at normal incidence calculating

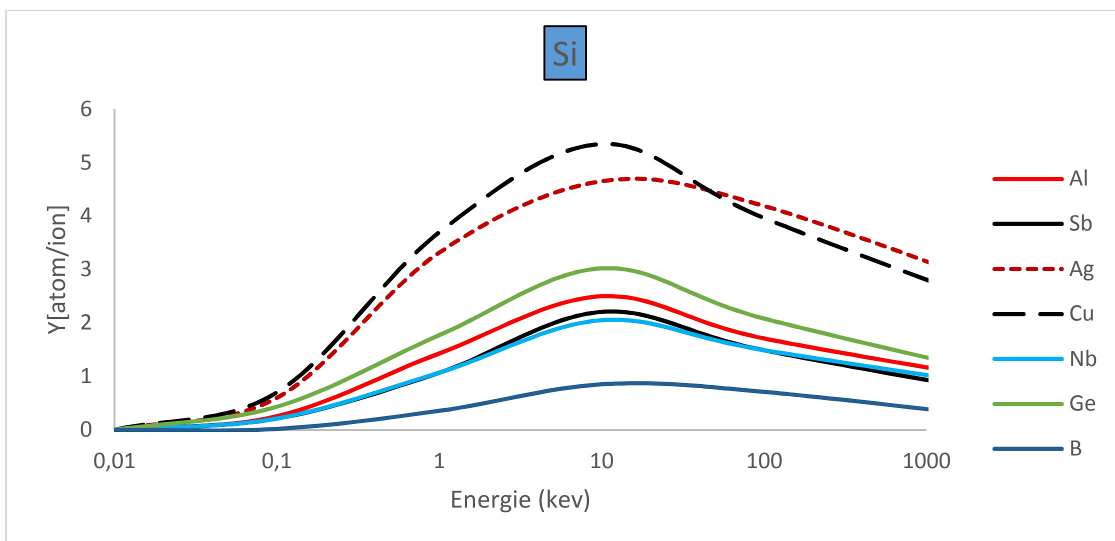

Figure 3.10 Sputtering yield of silver, aluminum, Germanium, Boron, Niobium, Antimony and copper for an Silicon ion beam at normal incidence calculating

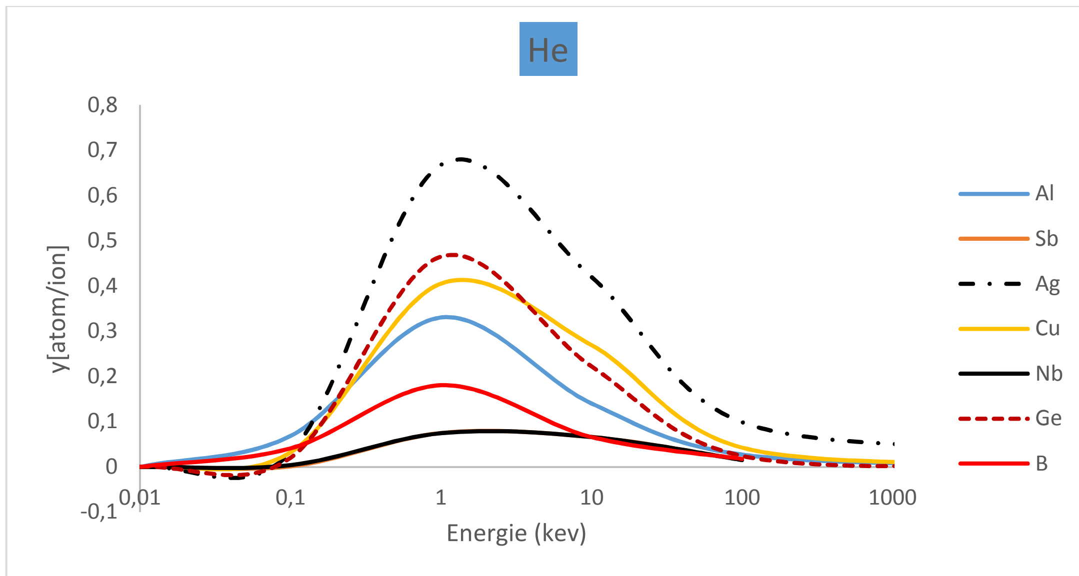

Figure 3.11 Sputtering yield of silver, aluminum, Germanium, Boron, Niobium, Antimony and copper for an Helium ion beam at normal incidence calculating

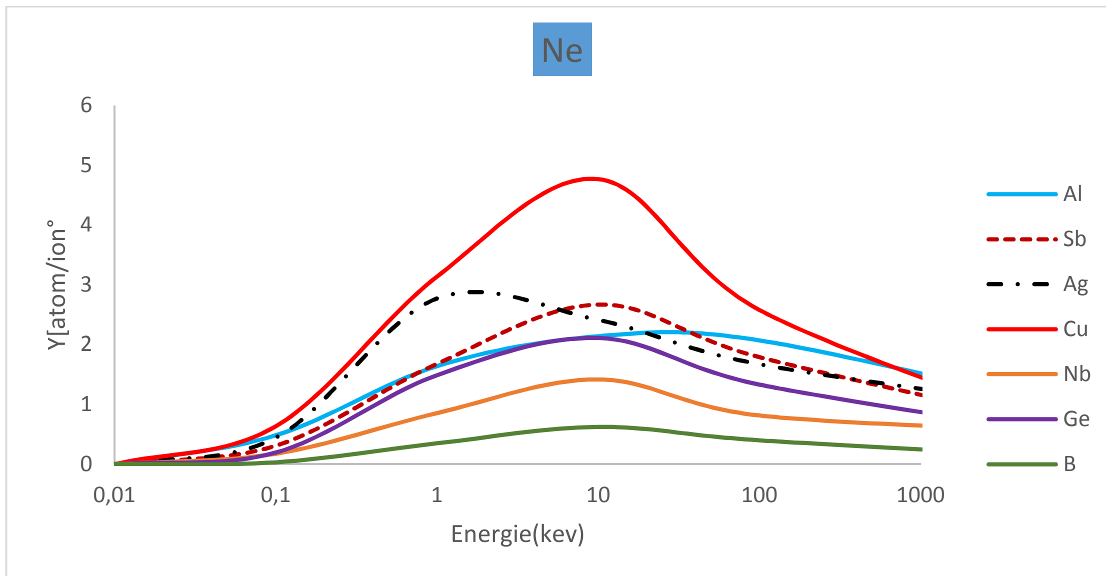

Figure 3.12 Sputtering yield of silver, aluminum, Germanium, Boron, Niobium, Antimony and copper for an Neon ion beam at normal incidence calculating

When the ion energy is less than 100 eV, sufficient energy is transferred to eject target atoms but too low to produce cascade collision. This mechanism is called the single collision scheme. For ions having energy between 100 eV and up, the target atoms acquire enough energy to be in collisions with their neighbors: the collisional cascade regime. If the energy exceeds 1 keV, there is a major movement of atoms located in the interaction area of the incident ion.

5. Effects of Incidence Angle

The yield increases with the incident angle and shows a maximum at angles between 60° and 75°, while it decreases rapidly for larger angles. The angular distributions of sputtered atoms for the normal incidence ion bombardment were studied in maximum ranges of incident ion energy.

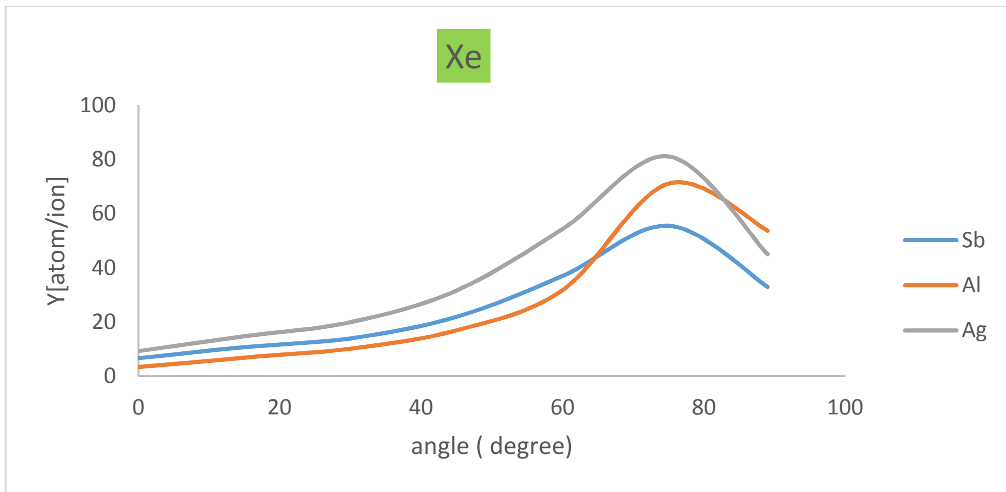

Figure 3.13 Variation of sputtering yield of Xenon for different angle found by SRIM simulation.

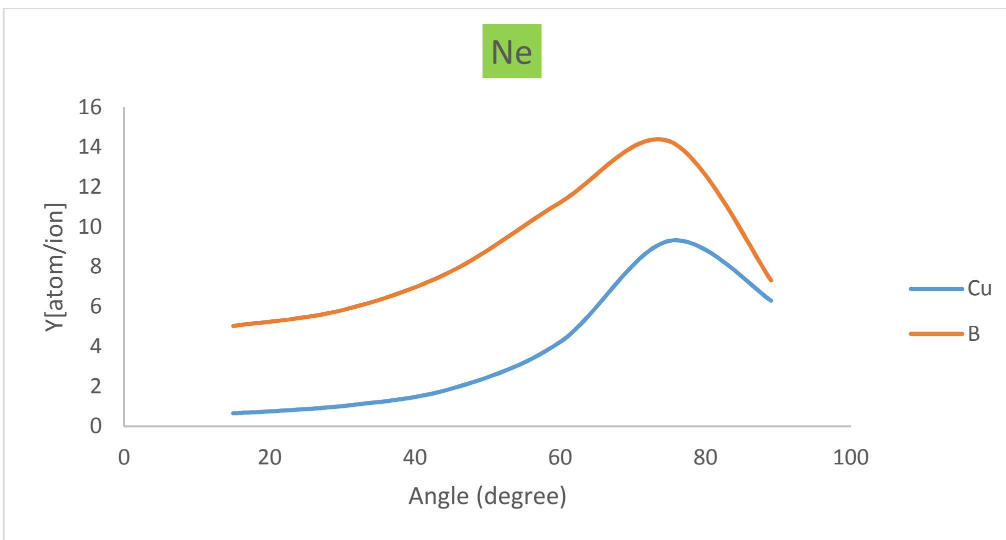

Figure 3.14 Variation of sputtering yield of Neon for different angle found by SRIM simulation.

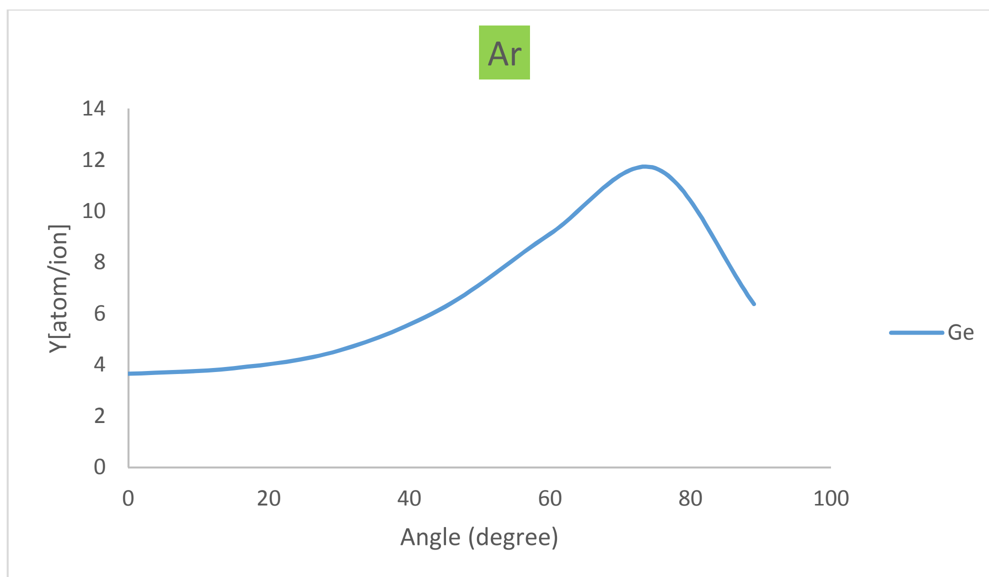

Figure 3.15 Variation of sputtering yield of Argon for different angle found by SRIM simulation.

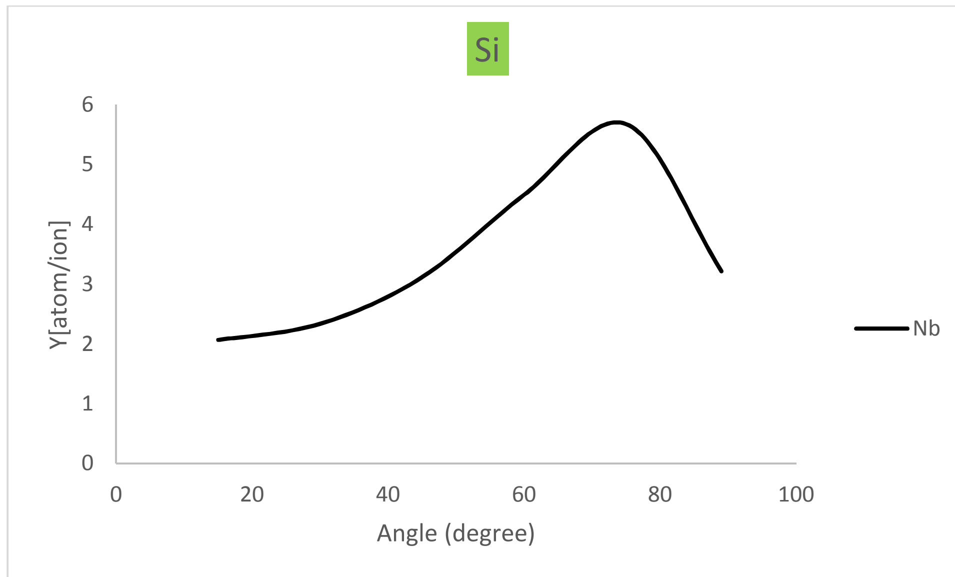

Figure 3.16 Variation of sputtering yield of Silicon for different angle found by SRIM simulation.

6. Part tow

6.1.SIMTRA (SImulation of Metal TRAnsport)

The program SIMTRA is designed as a tool to simulate the transport of energetic neutral particles through a low density background gas, specifically for the case of magnetron sputter deposition. Currently the background gas is considered homogeneous and in thermal equilibrium. And for now only elastic collisions of the transported particles with the background gas atoms are taken into account. SIMTRA is a test particle Monte Carlo code. It can be used to simulate deposition characteristics in complex magnetron deposition systems. To this end there is the possibility to create arbitrary chamber configuration consisting of a set of basic surface elements. Both planar and cylindrical targets can be added in as large a number as requested. However at this point no interaction between the magnetrons is considered.

6.2 Influence of divers parameters on the number of sputtered atoms arriving at the substrate and their energy

6.2.1 Variation of chamber temperature

Figures (3.17), (3.18), (3.19), (3.20), (3.21) and (3.22) show, respectively, the simulation results of the sputtered metals and semiconductors atoms (Cu, Al. Ge, B, Si and Ag) arriving at the substrate for different chamber vacuum pressures. The energy of the Ar+ ions, the angle and the pressures are again fixed at 100 eV, 60°/75° and 0.5 Pa, respectively.

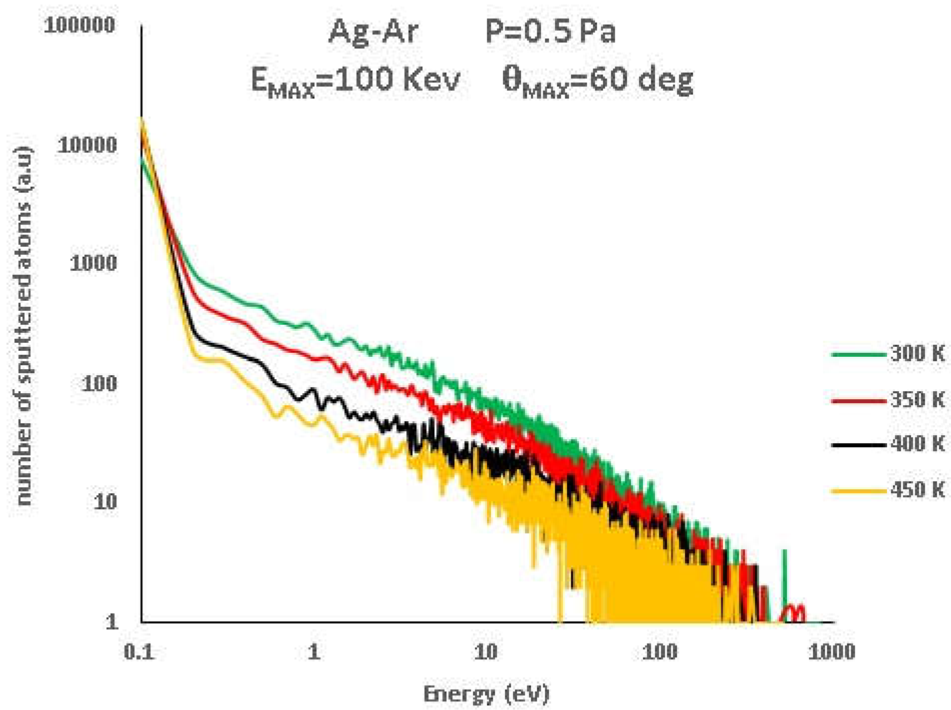

Figure 3.17 (Color online) The energy distribution for arriving Ag atoms as a function of temperature

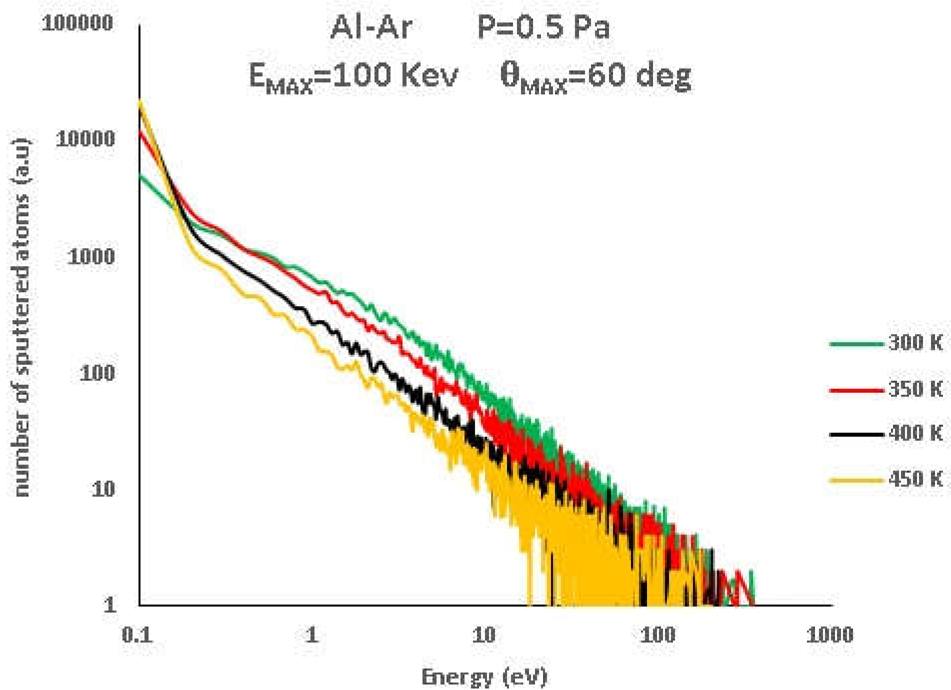

Figure 3.18 (Color online) The energy distribution for arriving Al atoms as a function of temperature

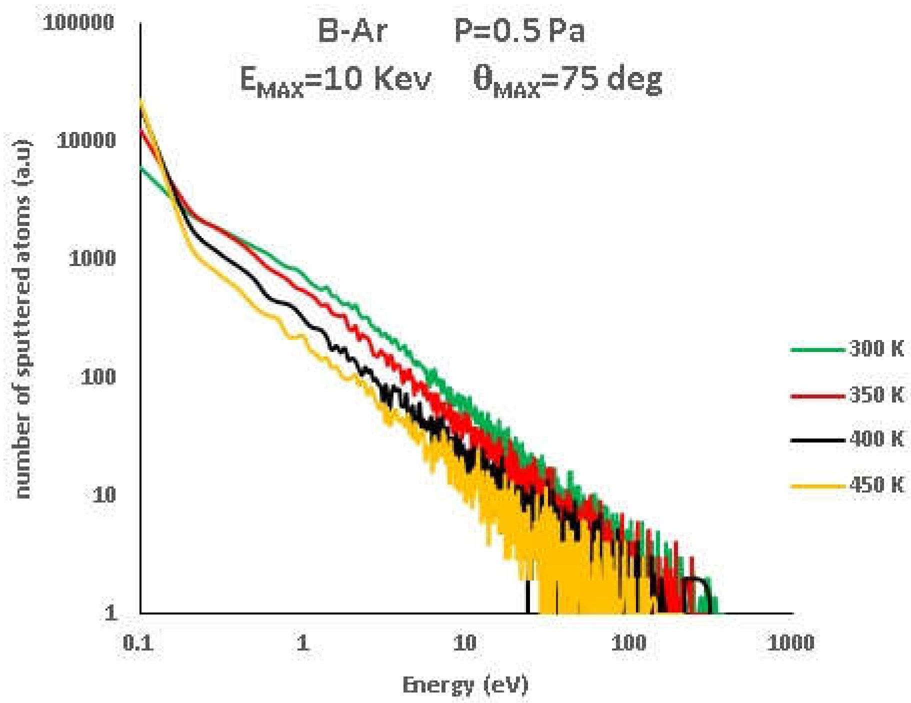

Figure 3.19 (Color online) The energy distribution for arriving B atoms as a function of temperature

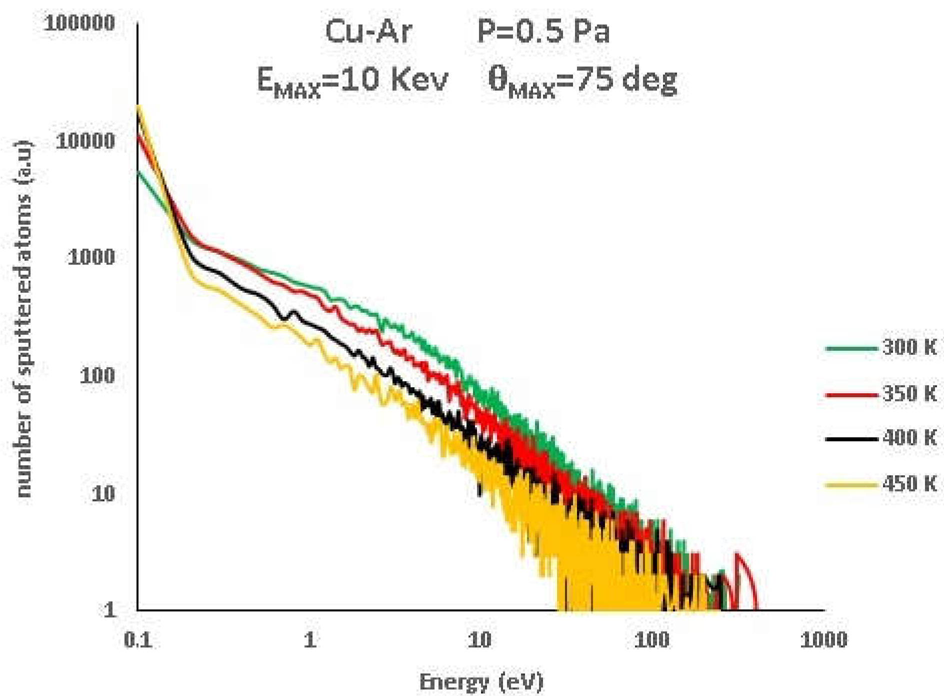

Figure 3.20 (Color online) The energy distribution for arriving Cu atoms as a function of temperature

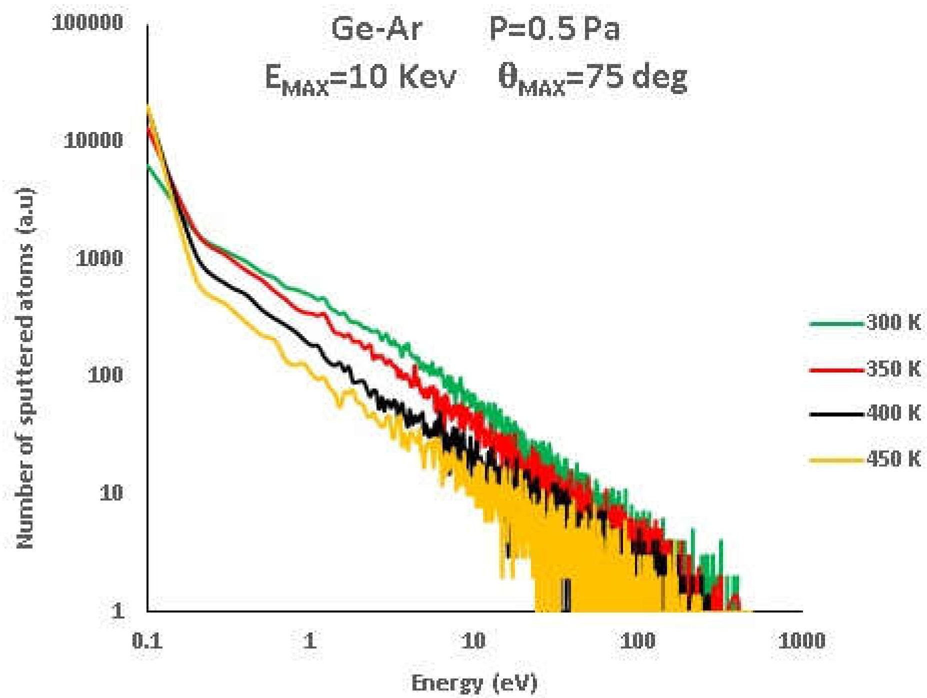

Figure 3.21 (Color online) The energy distribution for arriving Ge atoms as a function of temperature

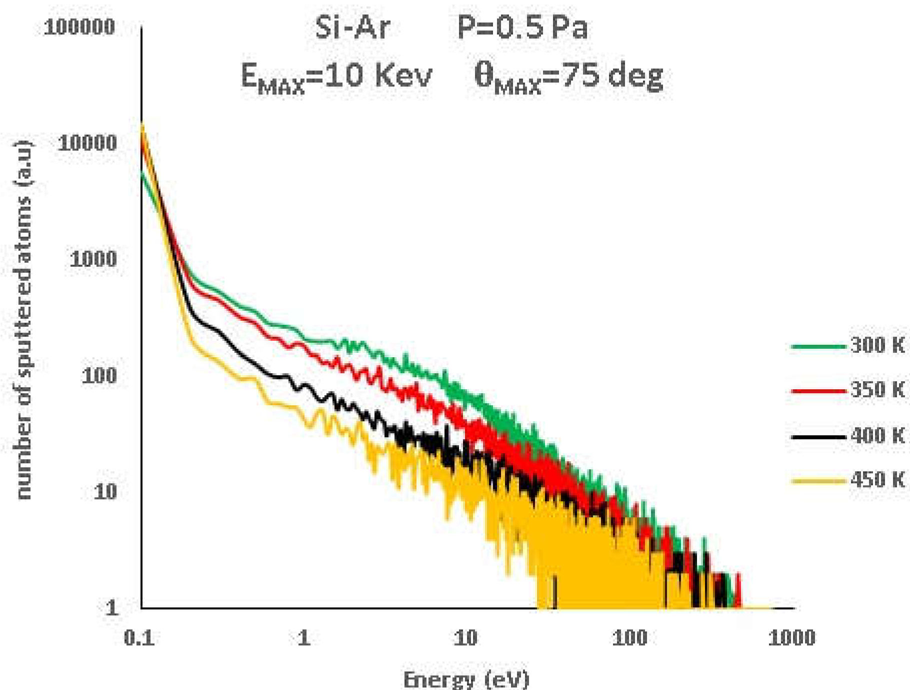

Figure 3.22 (Color online) The energy distribution for arriving Si atoms as a function of temperature

When 100 eV, 60°/75° and 0.5 Pa of energy, angle and pressures respectively is applied, the graphs show that with an increase in the sputtering temperature (300, 350, 400 and 450 K), the numbers of the sputtered metals and semiconductors atoms arriving at the substrate decrease (Al global sputtered atoms arriving at the substrate for 350 K of temperature. and this is similar for Ag,

Cu, Ge, B, Al and Si but with different amounts. Also, we can observe that increasing the temperature led to an increased number of collisions and also gradually losing an important amount of ions' kinetic energy in the transportation phase toward the substrate and also bands the energy distribution to lower values for both metals and semiconductors atoms.

General conclusion

With the development of smaller technologies, semiconductor layer depositions are used in several demanding applications such as integrated circuits, transistors, diodes and RF appliances used in very high-speed devices, and metal layer depositions are used in the manufacture of different kinds of transportation, jewelry and contacts and also in construction, household items and consumer electronics. The microstructures of these films have been the intention of our group in order to help people in industries by taking into account diverse parameters influencing the morphology of these films like the distance between the target and substrate, pressure and the temperature mentioned in this work.

The simulation with a Monte Carlo code has been applied in order to calculate the energy and the number of sputtered particles arriving at the substrate, which are both important parameters influencing the microstructure of the deposited thin film layers. It was shown that for temperature between 300 k and 450 K, global sputtered atoms arriving at the substrate for 350 K of temperature. Moreover, this work has also shown that the pressure and the distance between target and substrate are the two very important factors to modify the microstructure or crystallographic orientation of the deposited metal or semiconductor layers highly used in this ever-changing world and development processes.

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Abstract

this work is divided into two parts, in first part we calculate the sputtering yield of seven metals and semiconductors (Cu, Al, Ge, Nb, B, Si and Ag) using developed software called SRIM (Stopping and Range of Ions in Matter) with varied energy, then angle of incidence. In the second part we present the influence of temperature in the sputtering process of deposited layers of metals and semiconductors mentioned above The flux of the atoms and their energy arriving at the substrate have been simulated by Monte Carlo codes. A good agreement between previous works of other groups and our simulations for sputter temperature (300 K-450 K).

Résumé

Ce travail est divisé en deux parties, dans la première partie, nous calculons le rendement de sept métaux et semi-conducteurs (Cu, Al, Ge, Nb, B, Si et Ag) en utilisant un logiciel développé qui s'appelle SRIM (Stopping and Range of Ions in Matter) Avec une énergie variée, puis avec l'angle d'incidence. Dans la deuxième partie, nous présentons l'influence de la température dans le processus de pulvérisation des couches déposées de métaux et de semi-conducteurs mentionnés ci-dessus. Le flux des atomes et leur énergie arrivant au substrat, Ont été simulés par des codes Monte Carlo. Un bon accord entre les travaux antérieurs d'autres groupes et nos simulations pour la température de la pulvérisation cathodique (300 K-450 K).

ملخص

ينقسم هذا العمل إلى جزأين، في الجزء الأول تم حساب عائد الرش لسبعة المعادن وأشباه الموصلات (Cu, Al, Ge, Nb, B, Si ,Ag) باستعمال برنامج متطور يدعى SRIM (Stopping and Range of Ions in Matter) مع تغيير في الطاقة ا، ثم زاوية السقوط. في الجزء الثاني نقدم تأثير درجة الحرارة في عملية الرش من الطبقات المودعة من المعادن وأشباه الموصلات المذكورة أعلاه تدفق الذرات وطاقة التي تصل إلى الركيزة تم محاكاتها باستعمال رموز Monte Carlo . وهناك اتفاق جيد بين الأعمال السابقة من المجموعات الأخرى والمحاكاة لدينا لدرجة الحرارة ما بين (300 K-450K).