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Review Paper

Advances in Thin-Film Deposition Technologies: From Physical and Chemical Vapor Deposition to Computational Modeling

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ABSTRACT
Because of their many uses in microelectronics, optoelectronics, energy systems, biomedical devices, protective coatings, and surface engineering, thin-film deposition technologies are essential to contemporary materials science and engineering. The structural, mechanical, electrical, and optical characteristics of thin films are largely dependent on the choice of a suitable deposition method. The main thin-film deposition techniques, such as molecular beam epitaxy (MBE), chemical vapor deposition (CVD), physical vapor deposition (PVD), and computational simulation techniques, are thoroughly covered in this review. The operating principles, benefits, drawbacks, and common uses of both traditional and cutting-edge PVD methods—such as thermal evaporation, electron beam evaporation, sputtering, pulsed laser deposition, ion plating, activated reactive evaporation, and ionized cluster beam deposition—are covered in this review. Additionally, it highlights the deposition mechanisms and process features of the major CVD processes, including conventional CVD, plasma-enhanced CVD, and laser-assisted CVD. Additionally, the contribution of molecular beam epitaxy to the production of superior epitaxial thin films is discussed. Furthermore, recent advances in computational modeling are reviewed as useful tools for comprehending film growth mechanisms, optimizing deposition parameters, and enhancing coating performance. These include molecular dynamics, Monte Carlo methods, multiscale modeling, and predictive control techniques. Lastly, the review highlights the suitability of various materials and industrial applications by contrasting the capabilities of physical, chemical, and simulation-based approaches. For researchers and engineers interested in thin-film deposition technologies and their future development, this work offers a succinct and current reference

KEYWORDS: coating; chemical vapor deposition; thin film preparation; physical vapor deposition

1-INTRODUCTION

Most materials are selected on the basis of texture, color, and aesthetics, but for functionally engineered materials, surface composition and characteristics must be considered in addition to bulk properties and physical appearance, especially in applications where surface contact behavior is crucial. It is also important to carefully consider the external factors when using these components. Functionally engineered components must be able to perform their intended tasks in a variety of challenging conditions and hostile environments without degrading or failing catastrophically [1]. A material's surface characteristics have a big impact on how well it performs. Surfaces can be modified through a variety of surface engineering techniques. The surfaces of metallic materials are made up of a matrix of distinct individual grains with different sizes and levels of bonding. Surface-engineered materials are more functional, perform better, are less expensive, and use material more efficiently than bulk materials [2].

The goal of surface engineering is to develop methods for near-surface region properties and surface finishing that will enable engineering components to be used in a variety of service applications [1, 3, 4].
Nowadays, Numerous engineering disciplines successfully employ surface engineering techniques. The aerospace, biomedical, power, military, machine tool, and other industries are among those that work on altering corrosion behavior and wear resistance. Design firms have also used surface engineering for surface coating. In order to provide services that are challenging to provide using only the bulk material, they are also used to modify the surface properties of advanced functional materials, such as magnetic, chemical, electrical,

electronic, physical, and mechanical properties. The process is adaptable enough to be changed to satisfy specific needs, and nearly any kind of material (ceramics, metals, polymers, and composites) can be composited onto materials that are similar or different, depending on the desired qualities. It is also likely that a film will be applied to graded deposits, metamaterials, multicomponent deposits, met glass, polymers, superlattices, and photocatalysts [5-7].

Surface engineering encompasses surface modification, surface coating, and overlay techniques. A thick, solid film is produced when a protective substance with better physical and chemical qualities is applied using an overlay process, covering the substrate and making it invisible on the surface [8].

While maintaining the general properties of the substrate materials, a surface modification technique modifies the chemistry of the surface. Examples include nitriding, implanting, carburizing, and heat treatment [8-10].

Through the application of thin film layers, the surface coating technique modifies the surface's properties. Surface coatings can be applied using a variety of techniques, including vapor phase (including chemical and physical vapor depositing), fusion, and solution state. This process can be carried out in a number of ways, including thin-layer deposition, ion bombardment, chemical treatments, and plasma enhancement [11-15].

Two-dimensional surface deposition layers with a thickness range of less than 1 micron (10^{-6} m) are frequently called thin films, whereas layers thicker than this range are occasionally called coatings or thick films [5, 10, 16].

and because the subject of interest is thin film deposition. The focus of this review is primarily on surface coating techniques that are employed to deposit and grow thin films with thicknesses less than 10^{-6} m [17].

1. Deposition methods:

Physical processes (physical vapor deposition) and chemical processes (chemical vapor deposition and chemical solvent deposition) make up the majority of the broad category of thin-film techniques and procedures. This review describes the processes of physical vapor deposition (PVD) and chemical vapor deposition (CVD).

2. Physical deposition techniques:

Physical vapor deposition, or PVD, refers to the deposition procedures where material particles are heated to the vapor phase and then deposit as condensed thin films on the substrate. As a result, these procedures can divide into three categories based on the mechanism of deposition which summarized in table 1.

Table 1: PVD classifications [10, 18, 19].

Classification Basis	Category	Main Techniques	Description
1. By Deposition Mechanism	Evaporation-based PVD	Resistive evaporation, Electron beam evaporation	Material is thermally vaporized in vacuum and condensed on substrate
	Sputtering-based PVD	DC sputtering, RF sputtering, Magnetron sputtering	Atoms are ejected from target via ion (Ar^+) bombardment in plasma
2. By Energy Source	Thermal energy	Resistive evaporation	Joule heating via resistive filament or boat
	Electron beam energy	Electron beam evaporation	Localized heating using focused high-energy electron beam
	Laser energy	Pulsed Laser Deposition (PLD)	Laser ablation creates plasma plume from target
	Plasma / ion-assisted processes	Ion plating, Activated Reactive Evaporation (ARE)	Evaporation combined with plasma or ion bombardment
	Ion/cluster beam	Ionized Cluster Beam Deposition (ICBD)	Deposition using ionized atomic clusters for dense films
3. Advanced Hybrid PVD Techniques	Plasma / ion / laser hybrid methods	Ion plating, ARE, ICBD, PLD	Combine evaporation with plasma, ion or laser activation to enhance film properties

3. By mechanism

there are two types of physical vapor deposition based on the deposition techniques which are evaporation and sputtering based.

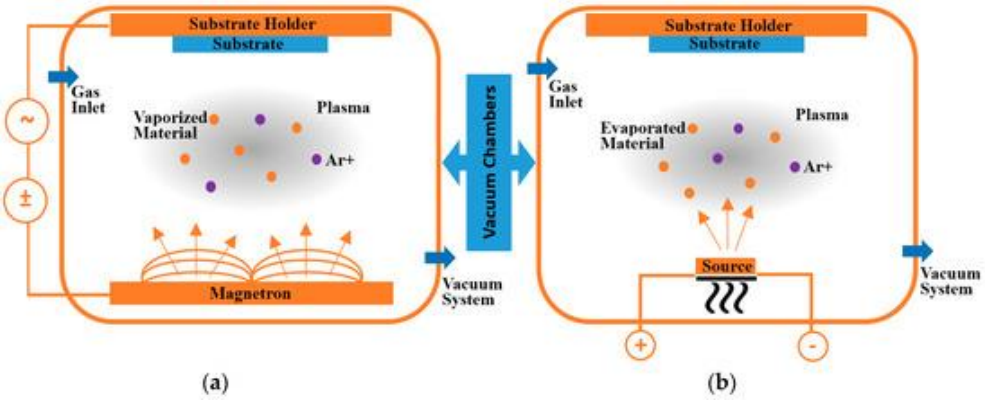

Figure 1: shows a schematic of two traditional PVD processes: (a) sputtering and (b) evaporating with ionized argon (Ar+) gas [20].

4.1 evaporation

There are two main types of evaporation, which are essentially similar but differ in their method of operation.

4.1.1 Resistive evaporation and electron beam evaporation:

The vacuum evaporation procedure typically consists of two steps: First, materials that need to be deposited must be evaporated in a vacuum chamber within a pressure lower than 10^{-6} torr. The second is when materials that have evaporated condense on a substrate.[21]

Resistive heating, which is the most frequently used heating source for thin-film deposition, is used to evaporate materials through a filament, a boat, or a refractory crucible. Notably, these filaments are typically constructed from refractory metals like Ta, Mo, and W with or without a ceramic coating. In this approach, as shown in figure 1, the effectiveness of the procedure depends on two key factors: Due to surface tension, it is first and foremost necessary for the evaporated materials to condense into droplets that stick to the filament. Second, it is crucial that the materials' ability to react with the filament or form alloys is negligible. It should be noted that the first and second cases are quite different from one another. When defining this issue, it can be said that materials that adhere to the filament properly have a greater propensity to become alloyed with the filament. The ability of metals to chemically react with the filament is generally limited; alkali metals are the exceptions (i.e., potassium, sodium, etc.). It is impossible to evaporate refractory metals by a typical resistive heating source, so an indirect heating method called an electron beam source is used to vaporize these metals. In this case, indirect heating is typically accomplished using crucibles made of graphite, quartz, beryllia, alumina, nitride, boron, or zirconia. Additionally, there are two significant distinctions between resistive heating sources and electron beam sources: First, unlike resistive heating, thermal energy is provided in the uppermost portion of the materials to be deposited using a high-current electron beam's significant kinetic energy. Second, the materials to be deposited are put in a cavity or crucible that is being cooled by water in electron beam evaporation.[22, 23]

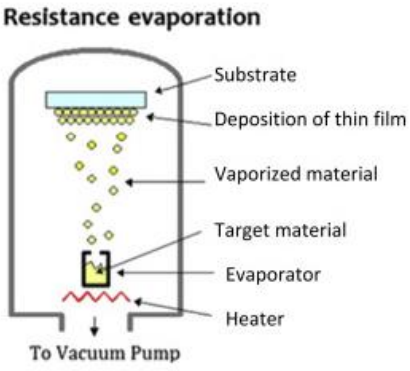

Figure 1: Diagrammatic representation of the "Resistance Evaporation" method of thermal evaporation.[24]

4.2 The sputtering techniques

The basic sputtering process involves bombarding a target (or cathode) plate with energetic ions produced in a glow discharge plasma that is placed in front of the target. Target atoms are removed during the bombardment process, or "sputtering," and may subsequently condense as a thin film on a substrate [25]. The ion bombardment also causes the target surface to release secondary electrons, which are crucial for preserving the plasma. Many materials have been successfully deposited using the fundamental sputtering process, which has been understood for many years [26, 27]. However, the process is limited by low deposition rates, low ionization efficiencies in the plasma, and high substrate heating effects.

4.2.1 DC sputtering

By sputtering elemental or alloyed targets in a working gas that contains a reactive gas component, reactive D.C. sputtering as shown in figure 2 produces films of chemical compounds. In this case, the reactive gas flow rate and the power density on the target are competing parameters. The impact ratio of the metal particles ~M in the vapor stream to the reactive gas atoms ~ determines the defined stoichiometry of the deposit under constant excitation conditions. At every point on the substrate surface, the particle densities of the plasma, reactive gas flow, and vapor stream must be maintained as constant as possible [28].

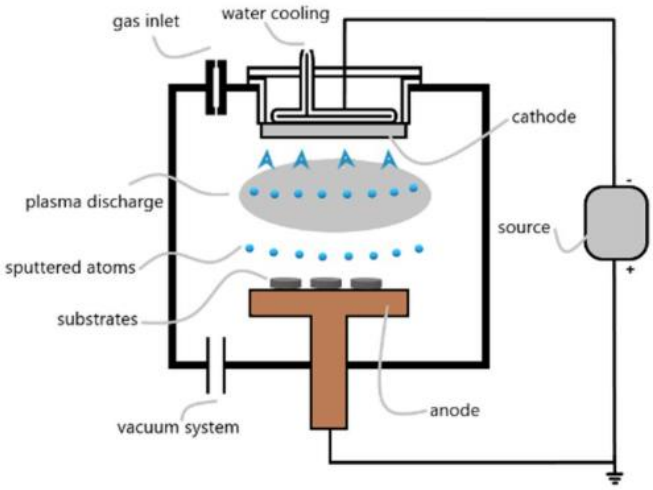

Figure 2: DC sputtering technique. [29]

4.2.2 Magnetron sputtering

Magnetrons exploit the ability of a magnetic field oriented parallel to the target surface to limit secondary electron motion to the target's vicinity. One pole of the magnets is placed at the target's central axis, and the second pole is created by a ring of magnets surrounding the target's outer edge. This kind of electron trapping significantly raises the likelihood of an ionizing electron-atom collision. A magnetron's higher ionization efficiency produces a dense plasma in the target area. Higher sputtering rates and, consequently, higher deposition rates at the substrate result from increased ion bombardment of the target. Furthermore, compared to the basic sputtering mode, the magnetron mode's higher ionization efficiency enables the discharge to be maintained at lower operating pressures (usually 10−3 mbar, as opposed to 10−2 mbar) and lower operating voltages (usually −500V, as opposed to −2 to −3 kV) [19] as shown in figure 3.

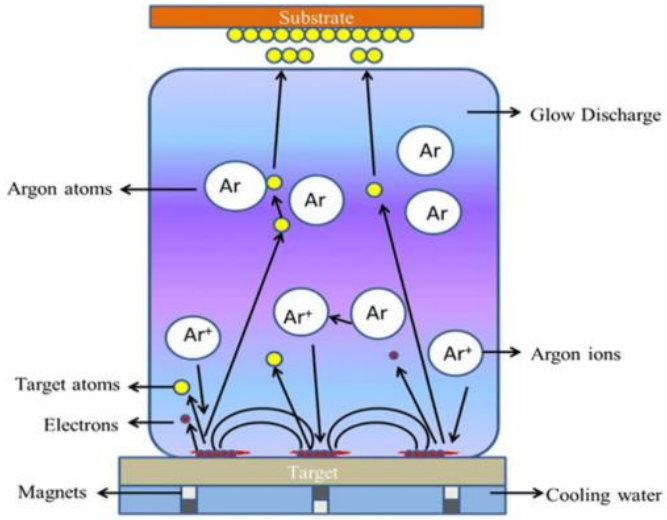

Figure 3: schematic diagram of magnetron sputtering technique [30].

4.2.3 RF sputtering

When your target is an electrical insulator, you employ radio frequency sputtering, or RF sputtering. RF sputtering uses an alternating current at 13.56 MHz to neutralize the target surface with each cycle, in contrast to DC sputtering, which fails on insulators due to charge buildup.[31]

High-quality films can be produced by RF sputtering, but the deposition rates are very low (usually in the μm/h range). Furthermore, it is challenging to scale up RF sputtering systems for commercial use due to their complexity [19]. as shown in figure 4

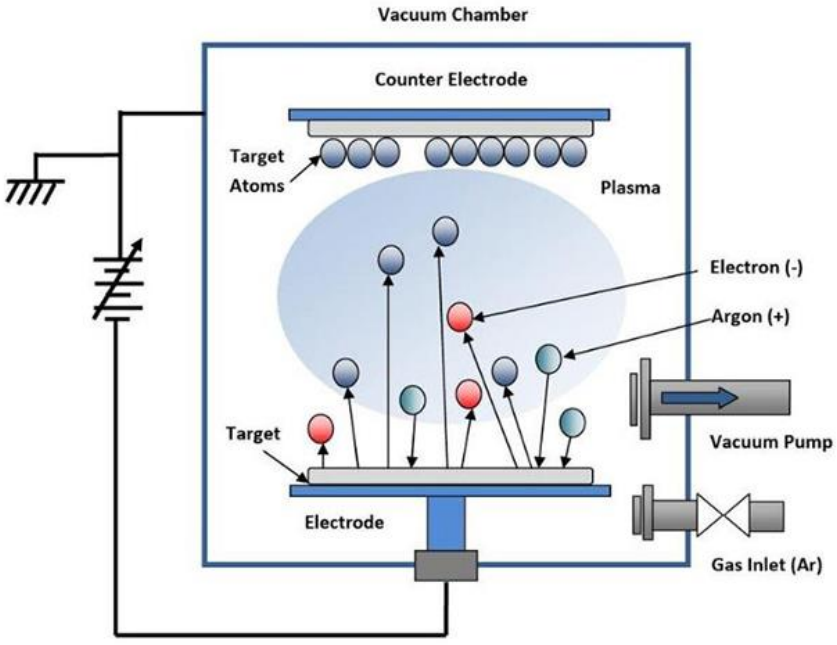

Figure 4: schematic diagram of RF sputtering technique. [31]

4. by energy source

A variety of thin-film deposition methods are included in Physical Vapor Deposition (PVD), which is based on the idea of moving material from a solid source to a substrate through the vapor phase under vacuum. While PVD techniques are often categorized based on the deposition mechanism (e.g., evaporation or

sputtering), another popular method is to categorize them based on the main energy source that produces the vaporized or activated species.
In this classification, the process by which atoms, molecules, or clusters are released and moved in the direction of the substrate is determined by the energy applied to the source material. Conventional resistive evaporation uses thermal energy to raise the source material to its evaporation temperature through Joule heating. Materials with high melting points can benefit from electron beam evaporation, which uses a concentrated beam of high-energy electrons to produce localized heating and vaporization. Pulsed Laser Deposition (PLD) creates a highly energetic plasma plume by ablating material from a target using laser energy. In order to improve film growth and alter coating properties, plasma- and ion-assisted methods like Ion Plating and Activated Reactive Evaporation (ARE) rely on energetic ions and plasma species. [10]
The relationship between the deposition energy, the depositing species' transport mechanism, and the final film properties is highlighted by this energy-source-based classification. As a result, it offers a helpful framework for comprehending the potential, benefits, and drawbacks of different PVD methods utilized in contemporary thin-film technology.[32]

5.1 Ion plating

Early in the 1960s, Donald M. Mattox introduced the vacuum-based deposition method known as "ion plating". It uses a deposition source such as thermal evaporation, electron beam evaporation, cathodic arc evaporation, sputtering, or chemical vapor precursor. The characteristics of a growing film, such as its adhesion, density, morphology, index of refraction, residual stress, etc., can be changed using this technique by continuously or repeatedly bombarding the film's surface with inert or reactive particles. As a result, two methods of bombardment are possible: ion plating based on plasma and ion plating based on vacuum. In the first scenario, plasma produced in the deposition chamber is used to accelerate ions toward the substrate. In the latter scenario, an ion source produces ions. Surface preparation, nucleation and interface formation, and film growth are the three main stages of ion plating [33].
Sputter cleaning during the surface preparation stage largely eliminates contamination at the substrate surface. In this regard, sputter cleaning takes place during deposition in the ion plating method and is an integral part of the procedure. Cleaning therefore stops the substrate from becoming recontaminated during growth; however, this may result in gas atoms becoming trapped in the developing film. Therefore, by heating the substrate during deposition, the effects of the aforementioned issue can be reduced. Lattice defects, which can be particularly problematic for semiconductor processing because they can act as electron traps close to the interface, can also be produced as a result of the bombardment of the surface. It is also noteworthy that a surface that is bombarded has a higher nucleation density than a surface that is not bombarded because of things like a clean surface, surface flaws, surface heating, and recoil implantation.[34, 35]

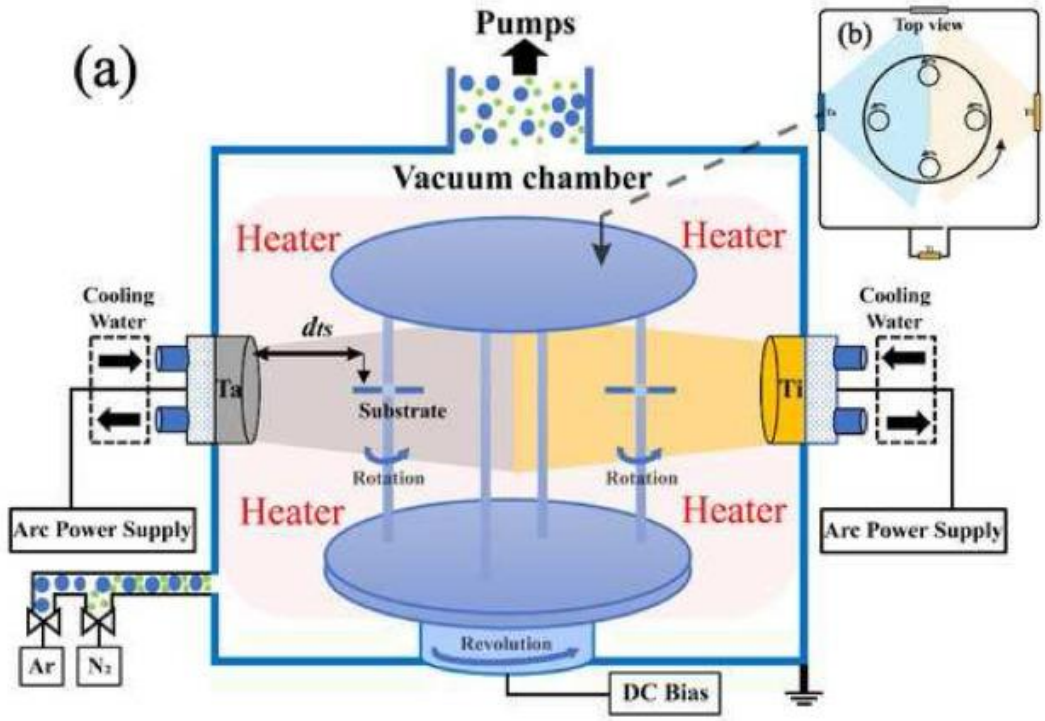

Figure 4: (a) front view of the multi-arc ion-plating system schematic diagram. (b) top view [36].

5.2 Activated reactive evaporation (ARE)

is a thin-film deposition method that was initially put forth by Bunshah and is used to deposit metal carbides, nitrides, and oxides. Metals and alloys evaporate during the ARE process, which also involves the presence of plasma from a reactive gas. Growing TiC and TiN films by evaporating titanium in the presence of C2H2 and N2 is one example of this process. As a result, the main roles of plasma are to start the chemical reactions needed to create compound materials and to adjust the growth kinetics to fit the shape and structure of films.

In the ARE method, the evaporation process uses a thermal source, such as an electron beam or cathodic arc. The rate of evaporation in the ARE process does not depend heavily on the plasma and increases as the target surface temperature and the target material's vapor pressure do. As a result, this process's evaporation rate is largely independent of the plasma. The interaction of the thermal source with the plasma during the ARE process does not significantly affect how quickly compound layers are deposited. As a result, especially when cathodic arc or a beam of electrons is used as the thermal source, the compounds formed on the surface of the metallic target are likely dissociated due to the extreme temperature at the target area [37].

Since different reactions can occur when the evaporated material interacts with the plasma, only a few of these reactions—electron-impact dissociation, ionization, and excitation—are important in the ARE process. It is also well known that when a glow discharge is present, the substrate is bombarded by electrons, ions, and neutrals; the energy and species bombarding depend on the process parameters and the substrate's geometrical location within the system. Consequently, the bombardment has a substantial impact and can change the substrate's surface chemistry, increase substrate temperature, re-sputter deposits, add gas to the film, and change, among other things, grain size, morphology, and crystal orientation [22, 38, 39].

5.3 Ionized cluster beam deposition (ICBD)

invented by Takagi in the seventeenth of twenty century, is a technique that evolved from the ion plating technique figure 5. This method's deposition procedure consists of the following four steps: A nozzle is used to first evaporate atoms from a closed source. After cooling through expansion in the nozzle, the atoms form clusters; the number of atoms in each cluster can range from a few hundred to a thousand. Third, the formed clusters are ionized after passing through a plasma region. The ionized clusters are then accelerated in the direction of the substrate.

In this regard, even though the accelerated clusters can have energy in the range of kilo-electron volts, the average energy of the atoms in these clusters is between 0.2 and several electron volts. It is therefore unlikely that the adatoms will cause damage to the substrate surface because of their comparatively low energy [22].
Examining the characteristics of the films produced by ion-assisted deposition techniques like ion plating and ion beam sputtering is complicated in general. However, because films are deposited in a region with a relatively high vacuum, it is simple to estimate the impact of deposition parameters on film formation when using the ionized-cluster beam deposition method. Practically, there are some key elements that have a significant impact on the films' caliber: The substrate temperature, the impinging rate of the depositing particles, the ambient gas or reactive gas pressure, and the substrate surface condition are all factors, the kinetic energy of deposition particles, and the number of ions present in all of the depositing particles.[40, 41]

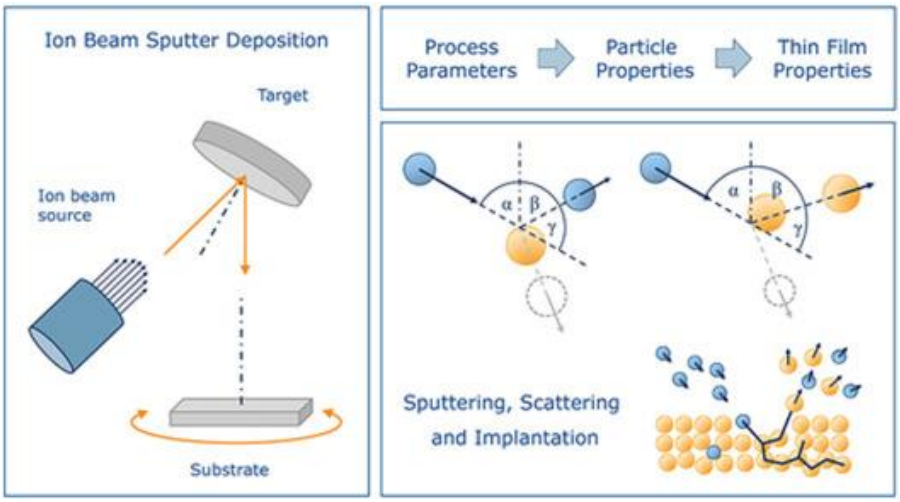

Figure 5: Ion beam sputter deposition schematic view [42].

5. Advanced Hybrid PVD Techniques

To get around the drawbacks of traditional evaporation and sputtering processes, advanced hybrid physical vapor deposition (PVD) techniques have been developed. In order to improve the quality and functionality of deposited thin films, hybrid techniques combine two or more physical processes, such as thermal evaporation, plasma activation, ion bombardment, and laser ablation, whereas traditional PVD methods mainly rely on a single deposition mechanism. Greater control over the kinetic energy of depositing species is made possible by the integration of multiple energy sources, which improves film adhesion, density, microstructure, and compositional uniformity.[7]
These cutting-edge methods are especially useful in applications like microelectronics, optical devices, biomedical implants, aerospace components, and protective surface engineering that call for high-performance coatings. Hybrid PVD techniques can create coatings with better mechanical, electrical, optical, and tribological properties than those made with traditional deposition techniques by introducing energetic ions, reactive plasma species, or laser-generated plumes into the deposition process.[43]
Pulsed Laser Deposition (PLD), Ion Plating, Activated Reactive Evaporation (ARE), and Ionized Cluster Beam Deposition (ICBD) are some of the most significant advanced hybrid PVD methods. To customize thin-film growth and maximize coating performance for particular technological applications, each technique uses a different combination of vapor generation and energetic particle assistance. As a result, these techniques are now crucial instruments in cutting-edge materials research and thin-film engineering.[44]

6.1 Pulsed laser deposition (PLD)

a method developed from thermal processes, was first used by Smith and Turner for the thin-film deposition of alloy/compound thin films. In this regard, a quartz lens and a high-power pulsed laser (like the KrF excimer) are two essential parts of the method. The laser's function is to irradiate a target, and the quartz lens' function is to magnify the laser power over the target's surface. Atoms of the target are deposited on a nearby substrate using this technique, which involves reaching a vapor phase through ablation or evaporation; the image depicts a typical system. Additionally, this process may include plasma processes in addition to thermal

processes. The target is primarily evaporated locally by the laser in the absence of air. The high-power laser pulse could, however, cause photo-emitted electrons, which would create a plasma plume [45].
One benefit of this technique is that it can work with a variety of target forms and has a simple design as shown in figure 6 (e.g., single crystal, powder, sintered components, etc.). However, there are some restrictions at the moment, including the relatively small area where the film is uniform and the potential for the deposition of particles or micro-sized globules. One can position the substrate off-axis to get around the latter restriction.[22]

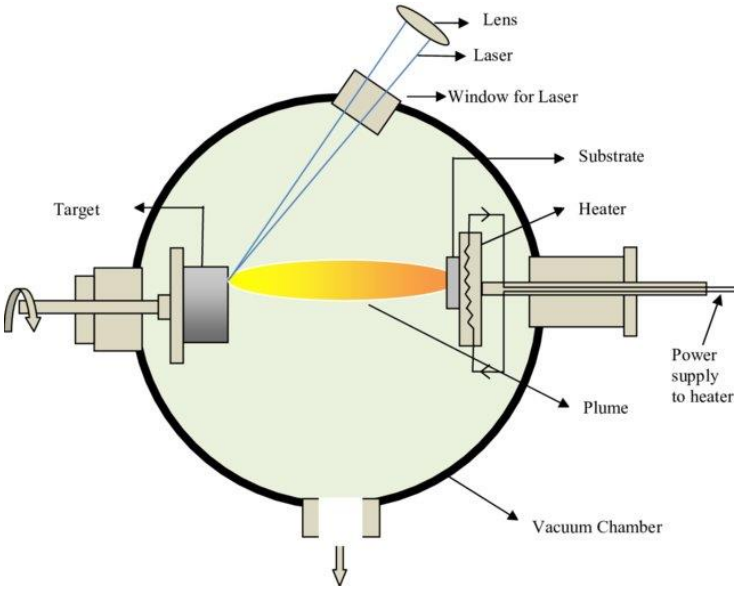

Figure 6: shows a schematic of the setup for pulsed laser deposition [46].

6. CVD processes:

These procedures are defined by two primary steps: The vapor phase is where a volatile substance that must be deposited first appears. Second, when heat sources are present, the vaporized compound disintegrates into atoms and molecules and creates thin films by interacting with nearby gases, vapors, and liquids [47].
In this sense, most CVD processes operate in the range of a few Torr to a pressure higher than the atmospheric pressure of the reactants. Some modified CVD processes, such as plasma-enhanced chemical vapor deposition (PECVD) and plasma-assisted chemical vapor deposition (PACVD), only require a lower operating temperature than these processes, which also require a high temperature of roughly 1000°C. Generally speaking, CVD processes fall into three categories:

5.1 (CVD) Chemical vapor deposition:

Atoms, molecules, or a mix of the two are commonly used as depositing species in the thin-film chemical vapor deposition process. It is described as a chemical reaction in the vapor phase that results in the deposition of a solid film on a heated surface. Usually, there are three steps involved in this process:

1. One of the substance's volatile components evaporates.
2. The vapor either thermally breaks down into atoms and molecules or chemically combines with other liquids, vapors, and gases at the substrate.
3. Nonvolatile reaction products are deposited onto the substrate.

In this regard, relatively high temperatures (around 1000°C) and reactant pressures ranging from a few torr to above atmospheric pressure are typically necessary in this process.
As a thin-film method, CVD has a number of benefits that occasionally make it preferred to PVD methods. First off, CVD is not constrained by a line-of-sight deposition, in contrast to other physical vapor deposition (PVD) processes like evaporation and sputtering. The technique can comparatively easily coat holes, deep crannies, and other unusual concavities and convexities thanks to its high throwing power. Second, the technique can produce thick coatings and has high deposition rates, making it more cost-effective than PVD processes occasionally. Third, a high vacuum is not typically needed for CVD.

Despite this, CVD has some serious disadvantages. First off, many substrates are not thermally stable at the high temperatures at which it frequently operates. It also needs highly volatile chemical precursors, which can be extremely toxic and hazardous. Third, because neutralizing the toxic and corrosive by-products of CVD can be an expensive process occasionally.[22, 48]

5.2 PECVD/PACVD

Plasma-enhanced chemical vapor deposition (PECVD) figure 7, also referred to as plasma-assisted chemical vapor deposition (PACVD), is one of the modified CVD processes. It was developed partly to increase the effectiveness of chemical reactions at lower temperatures. In PECVD systems, the electric power necessary for the generation of the plasma can be supplied using either diode glow-discharge electrodes or an induction coil placed outside of the chamber. PECVD systems frequently use plasma with an ionization degree of just 10-4, which results in the gas in the reactor being primarily neutrals. These systems operate in working pressure ranges of 10 to 100 Pa.

The electric field of the plasma gives electrons and ions energy as they move around the chamber. The electrons in the plasma have mean electron energies of 2 to 8 eV and temperatures ranging from 23000 to 92800 K. However, because they could not get enough coupling energy from the electric field, the energy of heavy, relatively immobile ions in the plasma was marginally higher than that of neutrals at room temperature. Consequently, the ion temperature of the plasma is mostly 500 K [49].

Because electrons have a far greater temperature compared to the gas during PECVD processes, thermal equilibrium between neutrals and electrons cannot be maintained. Thus, the glow discharge may be thought of as cold plasma that contains hot electrons and high-temperature electrons along with room-temperature gas molecules. After taking into account the previously mentioned facts, one can state with confidence that these hot electrons improve the chemical reactions occurring in the plasma, leading to a reduction in the temperature needed for reactions.

To date, a number of improvements have been put forth to create PECVD processes. One example of these developments is the use of microwave-based plasmas to lower the working pressure. In order to produce an electron cyclotron resonance (ECR) condition—that is, a resonance between the applied electric field and the electron cyclotron frequency—a magnetic field can also be added to the system.[22, 50]

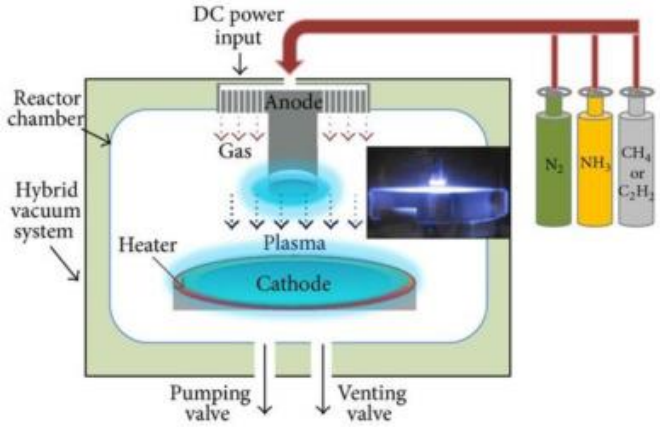

Figure 7: Diagrammatic depiction of the guiding concepts for plasma-enhanced CVD [51].

5.3 Laser chemical vapor deposition (LCVD)

One modified CVD method for depositing thin films is laser chemical vapor deposition (LCVD). An LCVD device consists of a chamber with inlets for reagent gases. As a result, reagent gases can break down into metallic or ceramic films when heated by a concentrated laser beam. By shifting the focused laser beam in relation to the substrate, an LCVD device with a local laser heating system can make writing and patterning easier. A thin solid film and a by-product are produced at the end of the process, which primarily involves inserting two reagent gases into the chamber.

Generally, there are two subdivisions of an LCVD process:

1. Photolytic LCVD: In this process, reagent gases absorb the energy from the focused laser beam, causing the gas molecules to break down and a thin solid layer to form on the substrate. Furthermore, because gas molecules absorb energy during the photolytic LCVD process, laser wavelengths should be specifically selected to depend on the materials. UV lasers like Ar+, ArF, and KrF are frequently employed in the process.

2. Pyrolytic LCVD: This technique focuses the laser beam on the desired deposit locations. Consequently, when the temperature locally rises on the substrate until it reaches the required threshold, a thin solid film is deposited on the substrate. Continuous-wave infrared lasers with Nd:YAG and CO2 wavelengths are commonly employed in the process.

In the photolytic LCVD process shown in figure 8, resolution is lost and thickness and width are increased when laser absorption extends along the laser beam instead of staying inside the beam focal point. Better resolution (up to 5 m) is possible with the pyrolytic LCVD process, though, due to its more localized heating.[22, 52]

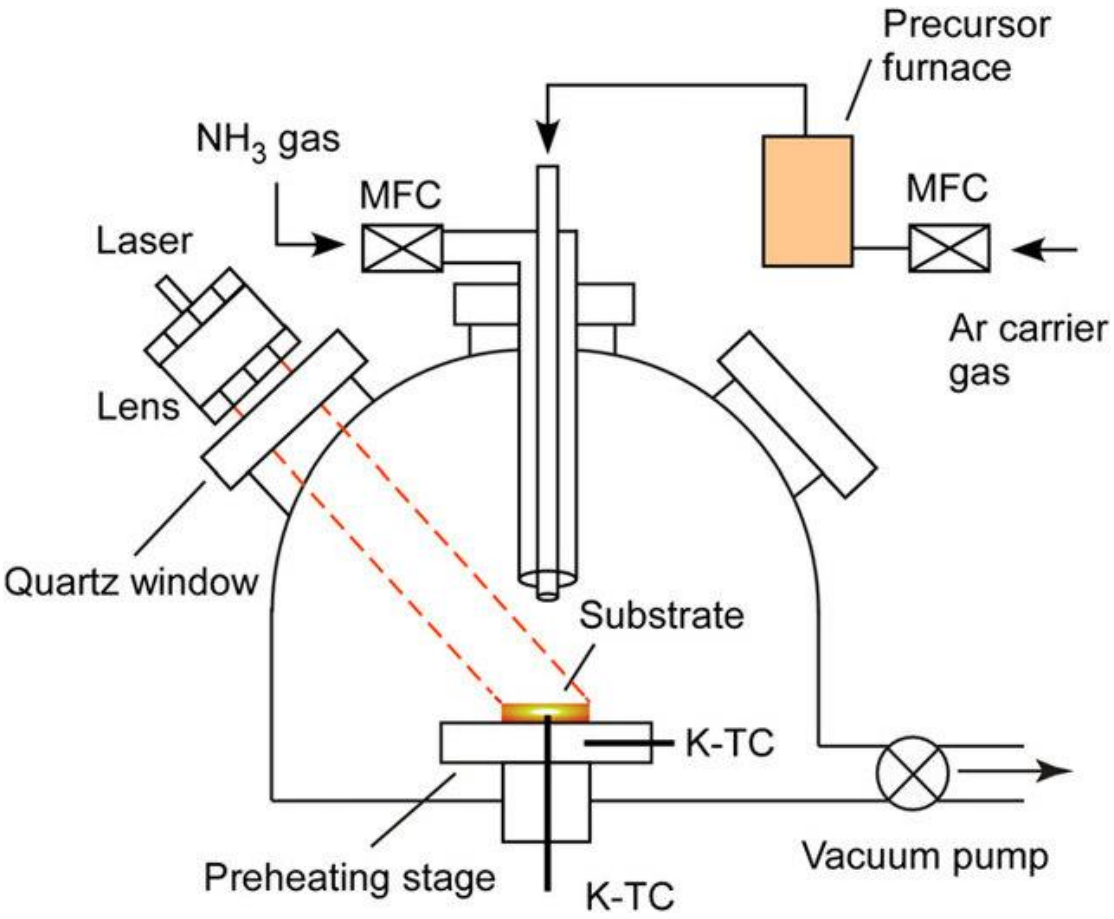

Figure 8: Diagram of the laser chemical vapor deposition system [53]

7. Molecular beam epitaxy

One of the most dependable thermal evaporation-based thin film deposition techniques is molecular beam epitaxy (MBE). However, because of its work in ultra-high vacuum (UHV) regenerating highly atomic or stimulating beams that precisely target crystalline tumor growth, MBE is frequently presented as a distinct branch under PVD from an academic standpoint. This controllable system, which has a computerized process control unit, can regulate how quickly materials in the source evaporate. A growth chamber, sample chamber, and an analysis chamber make up a typical MBE system in this regard. These days, this method is frequently used for the carefully regulated deposition of compounds and alloys. For instance, the technique can be used to create superlattice structures of GaAs/GaAlAs.

The presence of the ultra-high vacuum (For example, residual gas pressures below 10^{-7} N/m².) near the effusion cells (i.e., crucibles consisting of source material and a heating source) and the substrate is of enormous significance for the deposition of high-quality materials, among other factors that should be taken into account in an MBE process. Notably, the residual gas pressure needed to deposit high-purity Si or GaAs is considerably lower than the pressure experienced in an ultra-high vacuum (less than 10^{-9} Pa).

Therefore, the vacuum bake-out process—which uses heat and vacuum to remove volatile compounds from objects—and a titanium sublimation pump—which uses highly reactive titanium atoms to react with residual gas in ultra-high vacuum systems—are typically used in MBE systems. An MBE system as shown in figure 9,

has three chambers, as was previously mentioned: To allow for substrate degasification, the substrate is positioned in the first chamber. The installation of analysis tools, X-ray photoelectron spectroscopy and Auger electron spectroscopy, for example, are performed in the second chamber, also known as the analysis chamber. To prevent external contaminants from entering the third chamber, the second chamber acts as a partition between it and the first. The third chamber is where the deposition process is conducted [22, 54].

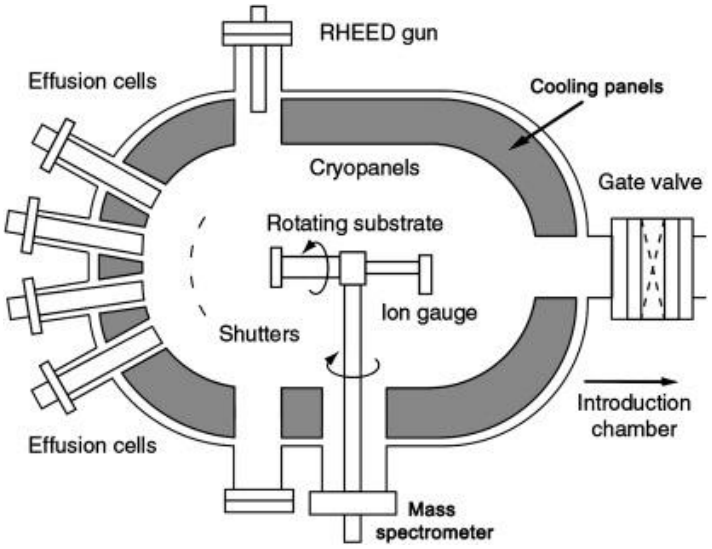

Figure 9: An illustration diagram of the molecular beam epitaxy system [55].

Table 2 provides a summary of the deposition principles, operating conditions, deposition rates, major advantages, limitations, typical applications, and relative costs of the thin-film deposition techniques covered in this review. This comparison offers a useful guideline for choosing the best deposition method based on material specifications and application demands.

Table 2: Detailed comparison of thin-film deposition methods.

Deposition Technique	Deposition Principle	Typical Operating Conditions	Deposition Rate	Main Advantages	Main Limitations	Typical Applications	Relative Cost
Resistive Evaporation	Thermal evaporation by resistive heating	High vacuum (10^{-6}–10^{-7} Torr); low substrate temperature	High	Simple equipment, low cost, high deposition rate	Limited to low melting-point materials; possible contamination from filament	Metal coatings, optical films, laboratory research	Low
Electron Beam Evaporation	Localized heating using high-energy electron beam	High vacuum (10^{-7}–10^{-9} Torr)	High	High-purity films; suitable for refractory materials; excellent thickness control	High equipment cost; complex operation	Semiconductor devices, optical coatings, high-purity thin films	High
DC Sputtering	Ion bombardment of conductive target	Ar plasma; 1–10 mTorr	Moderate	Good adhesion; dense films; uniform coatings	Limited to conductive targets	Metallic coatings, MEMS, electronics	Medium
RF Sputtering	Radio-frequency plasma sputtering	Ar plasma; 5–20 mTorr	Low–Moderate	Deposits insulating materials; high film quality	Lower deposition rate; higher system complexity	Ceramic coatings, dielectric layers	High

Deposition Technique	Deposition Principle	Typical Operating Conditions	Deposition Rate	Main Advantages	Main Limitations	Typical Applications	Relative Cost
Magnetron Sputtering	Magnetically enhanced plasma sputtering	Ar plasma; 1–5 mTorr	High	High deposition efficiency; excellent adhesion; scalable	Higher equipment complexity	Hard coatings, solar cells, microelectronics	High
Pulsed Laser Deposition (PLD)	Laser ablation of target material	High vacuum or controlled gas atmosphere	Low–Moderate	Excellent stoichiometric transfer; suitable for complex materials	Small deposition area; particle formation	Oxide films, superconductors, functional materials	High
Ion Plating	Evaporation combined with ion bombardment	Vacuum with plasma assistance	Moderate	Excellent adhesion; dense coatings; improved mechanical properties	More complex process control	Wear-resistant coatings, aerospace, cutting tools	High
Activated Reactive Evaporation (ARE)	Thermal evaporation in reactive plasma	Reactive gases (O_2, N_2, CH_4) with plasma	Moderate–High	Produces high-quality compound coatings; improved film density	Requires precise plasma and gas control	Oxides, nitrides, carbides, optical coatings	High
Ionized Cluster Beam Deposition (ICBD)	Deposition of ionized atomic clusters	Ultra-high vacuum	Low	Excellent microstructure control; minimal substrate damage	Very expensive; limited industrial implementation	Nanostructured films, advanced electronics	Very High
Chemical Vapor Deposition (CVD)	Chemical reaction of gaseous precursors	600–1100°C; low or atmospheric pressure	High	Excellent conformity; high-quality coatings; thick films possible	High temperature; hazardous precursors	Semiconductors, protective coatings, diffusion barriers	Medium–High
Plasma-Enhanced CVD (PECVD/PACVD)	Plasma-assisted chemical reactions	100–400°C; plasma environment	Moderate	Low deposition temperature; suitable for temperature-sensitive substrates	Plasma damage may occur; equipment complexity	Solar cells, dielectric layers, biomedical coatings	High
Laser Chemical Vapor Deposition (LCVD)	Laser-induced decomposition of gaseous precursors	Localized laser heating	Moderate	Localized deposition; high spatial resolution	Limited deposition area; high equipment cost	Microelectronics, sensors, microfabrication	Very High
Molecular Beam Epitaxy (MBE)	Atomic beam deposition under ultra-high vacuum	Ultra-high vacuum ($<10^{-9}$ Torr)	Very Low	Atomic-layer control; exceptional crystal quality	Extremely slow; very expensive	III–V semiconductors, quantum wells, optoelectronics	Very High

8. Thin film simulation programs

The process of creating a computer model of a hypothetical or actual physical system, running the model, and evaluating the results is known as computer simulation. In engineering domains like thermal energy transport, fluid flow, and stress analysis, computer simulations are widely used. The microscopic world of the lab (experiment) and microscopic time and length scaling (theory) are connected by a computer simulation. Simulations are frequently used to study molecular assemblies, offering insights into their microscopic interactions and structural features. In addition to standard experiments, this aids in our understanding of processes and behaviors that are challenging to study through experimental methods. It helps us solve complicated theoretical frameworks beyond certain approximations, expedites the process of developing processes, and gives experimentalists a hint for additional research. [56] Common computational techniques for examining the formation of thin films include the density functional theory (DFT) model, Monte Carlo (MC), continuum method, and molecular dynamics (MD). However, there are two different approaches for modeling at the atomistic scale: Molecular Dynamics (MD) and Monte Carlo (MC). While the MC method is used to compute equilibrium properties like potential energy calculation, absorption investigations, and phase equilibria studies, MD simulations are typically used to estimate time-dependent (transport) properties like heat conductivity and diffusivity coefficients at the atomistic level. These simulations have serious limitations even though they aid in our comprehension of thin-film coating principles. These include difficulties in accurately analyzing small physics, lengthy operating times, high computational costs, and difficulties in examining bond formation and breakage events at the atomic scale [57-59]. The creation of hybrid and multiscale approaches allowed for the resolution of these constraints. These approaches combine the best aspects of different simulation, control, and optimization techniques. It accomplishes this by accurately simulating the topological growth of thin film deposition processes, lowering deposition costs, and enhancing thin film performance overall. [60-62]. In order to generate precise feedback, multiscale approaches optimize process parameters by taking into consideration both the linear and nonlinear relationships between them. The multi-scale modeling process still has limitations and challenges in spite of its advancements and expansion. The mathematical complexity that arises when connecting modeling techniques with disparate characteristics makes simulating a multiscale system nontrivial. Additional limitations are imposed by the computational demands necessary to simulate phenomena at the fine length and time scales. As a result, the majority of multi-scale modeling applications currently in use only combine two different modeling approaches, i.e., phenomena that occur at two different time and length scales. Multiscale modeling and Kinetic Monte Carlo (KMC) designs can be combined to overcome this constraint and create a hybrid model that circumvents the problems. The Kinetic Monte Carlo (KMC) approach can be used to explain a wide range of phenomena at various length and temporal scales. This stochastic method has emerged as the go-to option for modeling atomic, molecular, or nanoscopic events due to its adaptability. Therefore, a continuum model that forecasts the behavior of a physical system at both the microscopic and macroscopic levels is frequently combined with a KMC model in a multiscale modeling formulation. The use of multiscale modeling techniques, which capture pertinent large quantities and molecular phenomena on the various scales at which they occur, is therefore most appropriate for simulation process enhancement research studies for thin film growth. The development and promotion of deposition techniques have been facilitated by recent advances in our knowledge of the physical and chemical characteristics of films, surfaces, and interfaces. But this also made it possible to create models for predicting thin-film growth, which allowed for the control of the structure and characteristics of the film. [63-65]. Furthermore, the multiscale simulation enables accurate control of small-scale systems by forecasting the impact of uncertainty. Model Predictive Control (MPC) provides an effective framework that leverages the system model to forecast the control actions that maximize a performance index in the presence of constraints, thereby improving the deposition process while reducing expenses and time. [66]. Furthermore, output feedback, including statistical moments for surface roughness, growth rate, etching rates, surface morphology, and dynamic behavior, can be precisely predicted using model predictive control. The film's thickness [67-70]

3-CONCLUSION

In summary, thin film deposition methods are essential to contemporary applied physics and materials science because they allow for the controlled creation of structures with specific chemical, electronic, and physical characteristics. Regarding film quality, uniformity, scalability, and cost-effectiveness, each technique—whether PVD, CVD, sputtering, ALD (atomic layer deposition), or solution-based approaches—offers unique

benefits and drawbacks. Therefore, the intended application, the desired material properties, and the compatibility with underlying substrates all play a significant role in choosing an appropriate technique.
The development of deposition technologies is still crucial as the needs for functional materials and device miniaturization grow. It is anticipated that future studies will concentrate on developing environmentally sustainable processes, increasing energy efficiency, and improving atomic-scale precision. High-performance thin film production may be made possible by combining conventional deposition techniques with cutting-edge strategies like hybrid or plasma-assisted techniques. In the end, developments in deposition science will propel advancements in energy storage, photonics, microelectronics, and biomedical applications, highlighting the critical role thin film engineering plays in influencing the next wave of technological breakthroughs.

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