



OVERVIEW OF THIN FILM DEPOSITION TECHNIQUES

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ABSTRACT:

The surface properties of a material can affect the performance and behavior of the material while in service. Modification and tuning of these surface properties to meet specific demands for better performance is feasible and has been widely used in different aspects of life. This can be achieved by coating the surface by depositing a thin film. This study provides a review of the existing literature on various deposition techniques used for surface modification and coating. Two major areas of physical and chemical vapor deposition techniques are discussed and areas of application of surface coatings are briefly highlighted in this report.

KEYWORDS: accumulation of chemical vapors; physical vapor deposition; surface coating; thin layer.

INTRODUCTION

Most material selection processes may be based on texture, aesthetics, and color, but functional engineering materials depend not only on physical appearance and bulk properties, but also on the design of surface features, especially in areas where surface contact occurs. Behavior is the highest priority. In addition, external factors should also be thoroughly investigated while using these components. A functional engineer component must be able to efficiently and successfully accomplish desired objectives while in service in a hostile environment under numerous conditions, without malfunctioning or incurring a catastrophic disaster. The performance of a material is highly dependent on the surface properties of the material. Surface modifications can be revealed using various techniques of material surface engineering. The surfaces of metallic materials are composed of a matrix of individual discrete grains varying in size and bond strength. Surface engineered materials provide enhanced and improved performance, added functionality, reduced cost, improved material use efficiency and performance that would not be possible with bulk materials.

Surface engineering is a branch of science that focuses on techniques for obtaining desired surface finishes and near-surface properties for engineering components that make them suitable for various in-service applications. Surface engineering techniques are now effectively applied in a wide range of engineering industries. Industries include aerospace, biomedical, power, military, machine tools etc. including but not limited to industries related to improving wear resistance and corrosion behavior. Surface engineering has also found application in design companies for coating surfaces. They are also being used to modify surface properties such as magnetic, chemical, electrical, electronic, physical and mechanical properties of advanced functional materials that are difficult to achieve with bulk materials alone. With the versatile nature of the process, virtually all types of materials can be deposited on the same or different materials depending on the desired properties and can be modified to meet specific demands. It is also possible to coat advanced materials with films (e.g. matte glass, polymers, superlattices, photocatalysts), hierarchical deposits, metamaterials and multicomponent deposits.

Surface engineering includes coating processes, surface modification techniques and surface coating techniques. In the coating process which is sometimes referred to as hard facing, a protective material with excellent physical and chemical properties is deposited on the surface of the substrate and the underlying material (substrate) is covered and not visible on the surface resulting in a thick and solid film... This process involves applying one or more metals with specific characters to the base metal to improve desirable properties or restore the original dimensions of the component. Unlike normal welding, in which two pieces of material are joined together, weld overlay applies a corrosion-resistant or hard-facing layer to the parent material to extend its life. Laser cladding, laser additive manufacturing and weld cladding are methods used for cladding processes. Surface modification techniques modify the chemistry of the surface properties while maintaining the bulk properties of the substrate material. Examples are heat treating, implanting, carburizing, nitriding etc. Surface coating techniques require the deposition of a thin film layer on a surface, which changes the surface properties. Examples of surface coating techniques are vapor phase process deposition (physical and chemical vapor deposition), solution phase process and fusion process. This process can be achieved by thin film processing, plasma enhancement, ion bombardment, self-assembly, nanomachining, chemical treatment. The term thin film is generally applied to surface deposition layers that are 2-dimensional and have a thickness below 1 micron (10^{-6} m), and layers thicker than the 1 micron range are called coatings or sometimes thick films. The resulting thin film can range from single crystal to amorphous, fully dense to less than fully dense, pure to impure, and thin to thick. Thin films offer great potential due to the following reasons:

- Conservation of rare materials,
- Production of nanostructured coatings and nanocomposites,
- Ecological considerations – reducing current output and power consumption,
- Improved functionality of existing products,
- Solving previously unsolved engineering problems and,
- Creation of completely new and revolutionary products.

The area of review interest is on thin film deposition; Therefore, this review has been carefully chosen to focus more on surface coating techniques used for the deposition and growth of thin films below tens of micrometers in thickness.

1. Deposition techniques

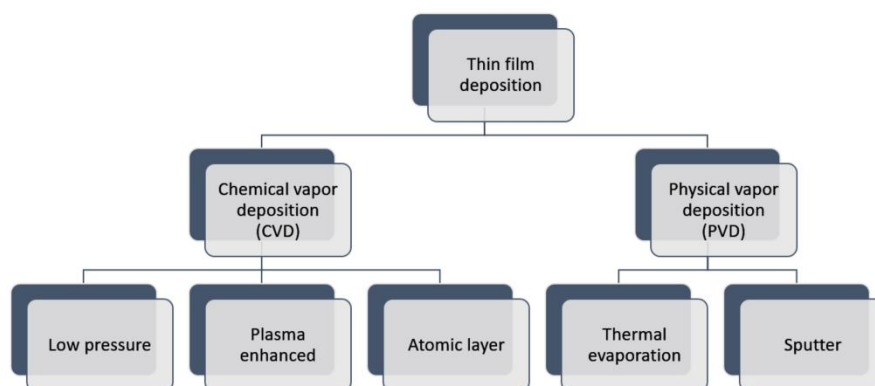
Thin films have distinct advantages over bulk materials because most deposition techniques used to produce thin films are non-equilibrium in nature, so thin film formation is not constrained by the metallurgical phase diagram. Thin film deposition techniques are considered an integral key to the creation of new materials to meet the ever-increasing demand from industries for versatile and multi-dynamics materials. Deposition techniques determine virtually all properties of thin films and can also be used to modify existing properties. Deposition techniques need to be carefully considered according to the application area because not all deposition techniques result in the same properties such as microstructure, surface morphology, tribological, electrical, biocompatibility, optical, corrosion and hardness. The same material can be used for different applications and properties can be tailored to meet optimal requirements using different deposition techniques. A combination of different techniques can also be used to create a hybrid deposition process with each contributing to the thin film result. Most deposition techniques follow three major sequences:

- Synthesis of Deposition Species,
- Transport from source to substrate,
- Deposition and adhesion of the source to the substrate and subsequent film growth.

There are many types of deposition techniques, but since the focus of this review is on thin films deposition to produce layers below one micron, priority will be given to the two major deposition

techniques used for thin films. The major subsets of deposition techniques are physical vapor deposition (PVD) and chemical vapor deposition (CVD). The distinguishing feature between PVD and CVD is vapor. In PVD, the vapor is composed of atoms and molecules that simply condense on the substrate, and for CVD, the vapor chemically reacts with the substrate to form a thin film. Following figure shows the types of thin film deposition which are fully gaseous state, solution state and molten or semi-molten state.

Image 1.1 Variants of thin film deposition techniques



2. Physical vapour deposition (PVD) process

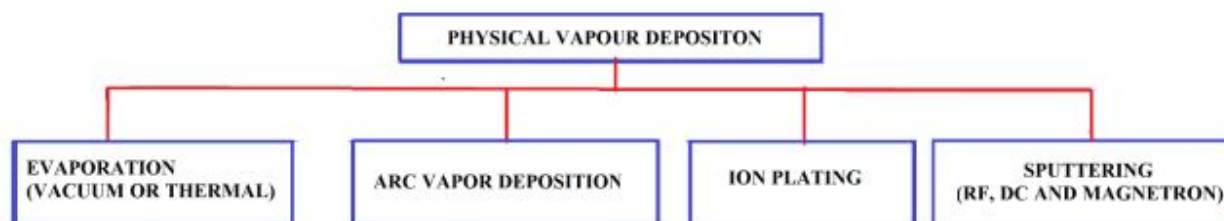
Physical vapor deposition (PVD) is a general term used to quantify thin film deposition processes that require the condensation of a vaporized solid above the solid surface under partial vacuum conditions. PVD is an atomistic deposition process that involves the physical discharge of atoms or molecules and the condensation and nucleation of these atoms on a substrate by means of a vacuum or a low-pressure gas or plasma atmosphere. Plasma or ions are usually vapor phase components. Sometimes, the reactive gas can enter the vapor during the deposition process and this is called reactive deposition. Atoms or molecules are delivered to the surface of the substrate to condense as vapors through a vacuum or low pressure gas or plasma atmosphere. Typically, PVD processes are used to deposit thin films with thicknesses in the range of a few nanometers to thousandths of nanometers. They can also be applied in hybrid form with multilayer deposition coating, graded composition deposition, very thick deposit, free-standing structure and other deposition techniques.

Each PVD process can be attributed to three basic steps that they all follow.

- Formation of vapor-phase species. This requires the conversion of the material to be deposited from the solid state to the vapor state by evaporation, sputtering, or ion bombardment.
- Movement or transport from source to substrate. Atoms or molecules ejected from the target will be carried away by molecular flow conditions and thermal scattering processes. Also, if the partial pressure of the metal vapor or gaseous species in the vapor phase is high enough to cause ionization of some of the species, there will be significant collisions in the vapor phase as they move through the substrate.
- Film growth on the surface. The transported atoms or molecules begin to nucleate around the substrate and grow by several processes. The initial growth of the film determines the type of interface formation between the substrate and the atoms or molecules. The composition and microstructure of thin films can be altered by bombarding the growing film with ions in the vapor phase, resulting in sputtering, recondensation, and nucleation of film atoms and enhanced surface movement of atoms around the film surface.

The major forms of PVD are listed in following figure, but the three basic processes of PVD are vacuum or thermal evaporation, ion plating, and sputtering.

Figure 2. Variants of Physical Vapour Deposition



During the evaporation process, thermal effects cause atoms to escape from the source, while for the ion plating process, the growing film is exposed to concurrent ion bombardment. During sputtering, atoms are ejected from the surface of the solid target by the impact of gas ions and then deposited on the surface of the substrate.

3.1 Thermal (or vacuum) evaporation

- Thermal (or vacuum) evaporation is an old deposition process used for the formation and growth of thin films on the surface of solids. This process is still beneficial in contemporary environments and is widely applied in laboratories and industry for thin film deposition. The basic sequential steps for thermal or vacuum evaporation are given below:
- Steam is produced by sublimating or boiling the target material to very high temperatures,
- The vapor extracted from the target material is transported by vacuum to the substrate,
- Condensation of the vapor occurs to form a solid thin film on the substrate surface and further repetition of the deposition cycle leads to growth and nucleation of the thin film.

During the thermal evaporation process, the target material vaporized from the thermal process sources is incorporated into the substrate material with minimal interference. The process is often performed at high vacuum pressure (HV) and the path to the target material substrate is a straight path called line of sight. A vapor stream is created by heating the surface of the source material to a sufficiently elevated temperature in a vacuum. The flux can then condense on the surface of the substrate material to form a thin film. The vacuum environment creates a safe zone that allows gaseous contaminants to accumulate to acceptable and minimal levels and allows for essentially collisionless transport of vaporized atoms from the source to the substrate. The gas pressure range is typically between 0.0013 Pa and 1.3×10^{-9} Pa depending on the degree of contamination in the deposition system, with a mean free path (MFP, mean distance between collisions between species) of no less than 5 mm. Thermal evaporation rates can be very high compared to other PVD processes. Tungsten wire coils are commonly used as a source of thermal heat or to heat a target material to a high temperature using a high energy electron beam.

Evaporation processes have been reported to be carried out using different configurations. These are molecular beam epitaxy, reactive evaporation and active reactive evaporation. Molecular beam epitaxy (MBE) was developed by JR. Arthur and Alfred Y. Discovered by Cho in the 1960s at Bell Telephone Laboratories. MBE is used to promote epitaxy through the active interaction of discrete or numerous atomic or molecular beams on the surface of a heated crystalline substrate material. . Evaporation takes place in an ultra-high vacuum to deposit a controlled composition of uniform thickness of thin film from a specific deposition rate. This process has been applied in the fabrication of semiconductor devices such as cellular phones, transistor conductors, and Wi-Fi. Reactive evaporation involves the evaporation of metal atoms from a target material in a chamber with the presence of a reactive gas at partial pressure. During the evaporation process, the atoms react chemically with the gas to form a compound thin film on the surface of the substrate. Reactive vapors can form stoichiometric oxides, alloys. Another type of evaporation technique is active reactive evaporation (ARE). ARE occurs by

atomic evaporation from the surface of the target material in the presence of plasma and reacts with the reactive gas in the chamber to form compounds with faster deposition rates and improved adhesion properties. The plasma improves the rate of reaction between the target and the substrate, ionization of both coatings of metal and gas atoms in the vapor phase and high conversion of neutral atoms to ions or energetic neutrals thus increasing the reaction potential and the rate for deposition of refractory compounds. ARE process If the substrate is held at negative bias voltage, it is biased active reactive evaporation.

3.2 Sputtering

Sputtering is an important and key process in PVD processes. It is a non-thermal evaporation process whereby individual atoms escape from the target surface due to atomic collision cascades through appropriate high energy ion bombardment. Unlike evaporation, the source is no longer produced thermally but by ion impact on the target. Also, the target substrate gap is shorter and, in many cases, outperforms other PVD processes with greater performance and efficiency, such as improved adhesion and thicker films. During the sputtering process, atoms are removed from the surface of the target material by transferring sustainable momentum from the plasma to the accelerated gas ions from the atom-sized energetic bombarding particles. Sputtering deposition can be achieved in vacuum at low pressure plasmas of <0.67 Pa where the sputtered particles are in the line of sight, and can also be performed at high plasma pressures of 0.67 to 4 Pa, where energetic particles are sputtered or reflected from the sputtering target. They are thermalized by gas phase collisions before reaching the substrate surface. Sputtering is used for surface cleaning and patterning of solids due to its ability to eject atoms from electrode surfaces.

Sputtering deposition has become a generic name for a variety of sputtering processes. These processes are named based on their source and process orientation. Types of sputtering are diode sputtering (cathode or radio frequency), reactive sputtering, bias sputtering, magnetron sputtering and ion-beam sputtering.

Sputtering deposition techniques use various sources of power and vary the working pressure depending on the power configuration. DC sputtering consists of a pair of planar electrodes (called cold cathode and anode). The target material for deposition is placed on the cathode and the substrate is placed on the anode. The working gas in the deposition chamber is usually argon gas due to its larger mass compared to neon and helium because the higher mass is associated with more energetic collisions with the target material and lower costs compared to xenon and krypton. A DC voltage is supplied between the cathode (target material) and the anode (substrate) to sustain the glow discharge. The gas ions produced by the continuous glow discharge rapidly grow towards the target material and are sputtered which causes a thin film to be deposited on the surface of the substrate material. In DC sputtering systems, the target is made of a metallic conductive material as a glow discharge (current flow) is maintained between the metallic electrodes.

Radio frequency (RF) sputtering is another form of sputtering that involves changing the electrical potential of a vacuum environment at radio frequency to prevent charging of certain types of sputtering target material. In RF sputtering, a cathode (target) which forms a thin film coating and an anode are connected in series with a blocking capacitor across it. The capacitor is part of the impedance-matching network that provides power transfer from the RF source to the plasma discharge. The cathode is bombarded with a high voltage in a vacuum chamber which causes high energy ions to eject from the atoms as a thin film covering the substrate at a fixed frequency of 13.56 MHz. The essence of the capacitor is to develop DC self-bias and enhance the optimization of power transfer to the target material in the created plasma. RF sputtering offers numerous advantages such as the possibility of deposition on insulating materials, the ability to maintain the plasma at low pressures of 0.13 to 2 Pa,

diffusion of the RF plasma throughout the chamber, and reduced formation of race track erosion on the target surface. Ability to clean target material after each cycle from buildup charge to reduce arcing effect.

During the sputtering process, secondary electrons are emitted from the target surface as a result of ion bombardment, and magnetron sputtering uses a magnetic field to restrict the movement of secondary electrons around the target material. The configuration and strength of the magnetic field array determines the flow rate of the ionization efficiency onto the target material resulting in a high deposition rate in the substrate. The increased ionization efficiency observed during magnetron sputtering allows the sputtering process to continue at a lower pressure of 100 Pa and a lower voltage of -500 V compared to 10 Pa and -2 kV to 3 kV for conventional sputtering processes. The two major configurations for magnetron sputtering are conventional (balanced) and unbalanced magnetron sputtering. In the balanced configuration, the plasma is confined to the target area while for the unbalanced configuration, not all the magnetic field lines are closed but some are directed towards the substrate while others follow the closed field path. Further reading on this can be found in. Conductive materials can be deposited using a direct current (DC) power supply, and insulators can be deposited using a radio frequency (RF) power supply. Magnetic arrays in magnetron sputtering configurations can vary in position without tempering with the electromagnet.

Reactive sputter deposition is used to produce compound thin films. During sputtering, a reactive gas such as nitrogen or oxygen is introduced into the deposition chamber and the gas reacts with the target material to form a compound thin film on the surface of the substrate. This process is called reactive sputtering. The addition of a reactive gas causes the topmost layer of the target material to change from a single phase to a compound phase, often leading to changes in properties such as conductivity, e.g. Conductive surfaces become non-conductive and vice versa. The inert gas commonly used for this process is argon, and it is possible to combine the inert gas with an ionized non-inert gas (reactive gas) or to introduce ionized non-inert gas (reactive gas) into the chamber alone. The percentage of reactive gas added to the chamber can be controlled to produce a specific stoichiometric ratio of compounds. Argon is the main gas in most cases and the amount of reactive gas entering the process chamber is controlled either to achieve a certain amount of doping or to produce a fully reactive compound. The resulting deposited thin film is different from the target.

Recently, another type of magnetron sputtering was discovered, which is considered as an emerging technology called pulsed magnetron sputtering PMS. This technique provides solutions to challenging problems with other magnetron techniques such as the low deposition rate experienced with RF magnetron sputtering and target poisoning and arc events associated with reactive magnetron sputtering. The PMS concept is based on short or intermittent pulses in the medium frequency range of 10-200 kHz of the magnetron discharge for tens of microseconds at low duty cycles. The two modes for operating PMS are unipolar PM where the target material voltage is pulsed between ground and standard operating voltage and bipolar pulsed sputtering where the target material voltage is reversed and turns positive during the pulse-off period. The pulsation process produces super-dense plasma with superior properties leading to more uniform thin films and the possibility of obtaining smooth surface coatings with complex and irregularly shaped substrate materials. Due to the limitations of the sputtering process, a new method of sputtering deposition is now being used as duplex sputtering where two or more deposition techniques are used to produce functionally graded materials with wide area and improved properties.

3.3 Ion plating

The first to report the ion plating technique in 1960 by Mattox. It uses continuous or intermittent bombardment in an inert gas discharge system for film deposition by energetic particles of atomic size

to modify and regulate the properties of the deposited film. Plasma is produced in a hollow cathode discharge source. The substrate material is bombarded by high energy flux ions sufficient to spatter the substrate surface prior to and during thin film growth. The deposition material may be vaporized by other physical vapor deposition techniques such as evaporation, sputtering, arc erosion, or decomposition of the chemical vapor precursor, but the vaporized atoms pass through a gaseous glow discharge on their way to the substrate, resulting in some vaporized atoms. Ionizing ion bombardment during film growth helps to form a solid film with a high material density and thus makes it suitable for hard-thin film deposition on the compound material. The gas pressure for the ion plating process ranges from 1 to 0.1 Pa. This pressure is sufficient to disperse the vapor particles in all directions through numerous collisions to sustain the glow discharge as well as improve the overall coverage of the substrate during film growth. A reactive gas can be added to form a compound surface coating and the process is known as reactive ion plating.

3.4 Arc vapour deposition

Arc vapor deposition is a deposition process that uses an electric arc at high current and low voltage to vaporize the cathodic electrode (cathodic arc) or anodic electrode (anodic arc) and deposit the vaporized material on the substrate. The layer is usually biased so that the film ions are brought to the surface faster and the evaporated material is highly ionized. The flux is generated by creating an arc that passes over the target surface. An arc strike causes atoms to eject from the target material and condense on the substrate in the form of a thin film coating. Most of the metal atoms are ionized and separated by vacuum or thermal evaporation. This significant number of ionized atoms makes it reliable for producing thick coatings and can be used for hard decorative surface-coating operations.

4. Chemical vapour deposition (CVD) process

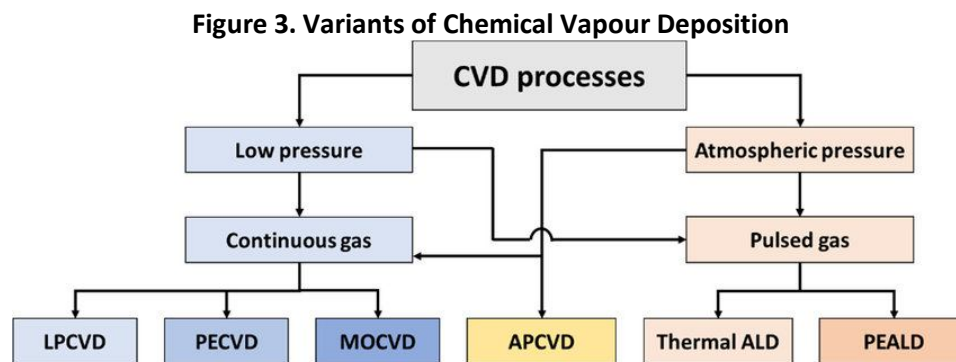
CVD is a general term for deposition of thin film series by chemical reaction. The process of physical synthesis occurs when a target component in the vapor phase reacts near the surface or on the surface of the substrate through a chemical process, leading to the growth of a thin film. Note that the mechanism behind CVD is very different from the PVD process. In PVD, a thin film is formed by condensation of atoms or molecules on the surface of the substrate due to evaporation, ion bombardment or sputtering. On the other hand, CVD is a thermodynamically complex process that involves chemical reactions under specific conditions such as temperature, pressure, reaction rate and speed, mass and energy transport. Many process factors and chemical reactions between the reactants and the substrate are responsible for the quality of the films formed during CVD, and film quality can be controlled and improved by using the appropriate combination of process parameters such as flow rate, pressure, temperature, concentration. Chemical species, reactor geometry etc.. The main characteristics of chemical vapor deposition are its resourcefulness, excellent throwing power, and the production of coatings of uniform thickness, to form both simple and complex compounds with relative ease, usually at low temperatures. CVD coating growth rate is higher than the ease of epitaxial film growth and offers better reproducible coatings with the same or nearly the same mechanical, optical, chemical and physical properties. In addition, CVD has the ability to deposit materials that are problematic to evaporate with low porosity onto substrates of complex shapes that are difficult to fabricate by other deposition techniques. During CVD, the chemical structure of the reaction and material structure can be tailored by monitoring and regulating the chemical reaction and deposition process parameters such as temperature, input concentration, pressure, gas flow rate, and reactor geometry. CVD essentials cover an interdisciplinary range of gas phase reaction chemistry, thermodynamics, kinetic and transport mechanisms, film nucleation phenomena, and reactor engineering. It should be noted that not all chemical reactions are desirable in all types of CVD processes. A variety of chemical reactions are

possible during CVD. Possible CVD reaction types are pyrolysis, reduction, oxidation, compound formation, disproportionation and reversible transfer. The chemical reaction that takes place depends on the reactant (precursor) gas and the by-products. In addition, the reaction must be thermodynamically predictable, that is, sufficient energy must be available for the reaction to occur and the Gibbs free energy (total available energy) must be minimized to allow for temperature and pressure. reaction to change. This process involves the reaction of one or more volatile precursors transported through the vapor phase to form a non-volatile solid that atomizes onto a substrate suitably placed within the confines of the reaction chamber. The basic sequential steps involved in each CVD process are mentioned below:

A reaction or diffusion movement in the gas phase in a reaction chamber,

- Chemical and gas phase reactions that produce reactive species and by-products,
- Transport of reactants from the boundary layer to the substrate surface,
- Chemical and physical adsorption of reactants on the substrate surface,
- Solid film formation due to heterogeneous surface reactions,
- Absorption of volatile by-products into the main gas stream by diffusion through the boundary layer,
- Removal of gaseous by-products from the reactor by convection and diffusion processes.

CVD processes are usually characterized by volatile reactions of by-products and unused precursor species. Many CVD reaction by-products are very hazardous volatile by-products such as H_2 , Cl_2 , HCl, HF or water vapor. Proper safety precautions must be taken when using CVD. The CVD process requires venting, scrubbing of by-products and unreacted compounds. CVD can be classified based on the energy used to drive the chemical reaction. The energy source can be either photons, lasers or temperature (thermal). Figure 3 illustrates the types of CVD processes.



CVD covers a wide range of reactor and process types. The application determines the choice of process/reactor based on substrate material and coating material, surface morphology, film thickness and uniformity, availability of precursors and cost.

4.1 Thermal CVD

Thermal CVD is a CVD process for thin film deposition on various materials. This process uses heating lamps or other methods to rapidly heat the substrate and activate the energy necessary for the reaction to occur. The growing film surface is exposed to thermal energy from a condensing atom or substrate heater to form a thin film. This thermal surface energy is responsible for bringing the atoms together to form a thin film with uniform thickness and good surface coverage and finishing. Since the thermal surface energy depends on the operating temperature, an increase in temperature also improves the distribution of the thin film on the substrate surface. Surface chemistry and surface atom dynamics are aided only by substrate temperature.

4.2 Laser CVD (LCVD)

LCVD is also a variant of the CVD process. It involves exposing a focused laser beam to locally heat a layer of one or more volatile precursors that react on the surface to form a thin film deposition. A laser generated by generating a coherent, monochromatic high-energy beam of thermal energy photons can be effectively used to drive a CVD reactor for the deposition of thin films.

4.3 Photon CVD

Photon CVD is another form of CVD. The chemical reaction is driven by photons, usually ultraviolet (UV) radiation that have the energy necessary to break the chemical bonds between reactant molecules to deposit a thin film.

4.4 Plasma-enhanced CVD (PECVD)

PECVD is a type of CVD that is used to deposit a thin film from a gaseous state to a solid state on a substrate. The chemical reaction occurs after plasma is formed in the reactor chamber and then a thin film is deposited on the surface of the substrate. PECVD uses an electrical source of energy to generate the plasma and sustain the reaction process, rather than thermal energy for the majority of CVD processes. Electrical energy is used to initiate homogeneous reactions to produce chemically active ions and radicals that can participate in heterogeneous reactions, thereby forming layers on the substrate. The main advantage of PECVD over thermal CVD processes is the possibility of deposition at very low temperatures close to ambient temperature and allows working on materials that are sensitive to temperature changes. The use of plasma to activate gas phase chemistry opens up many new reaction pathways for deposition at significantly lower temperatures.

4.5 Pulsed CVD

Pulsed CVD was also known as Atomic Layer Deposition (ALD) or Atomic Layer Epitaxy (ALE). Its origin can be traced to two different places. ALD was first developed in Russia in the 1960s by Aleskovsky as a promising coating technology on inorganic materials and referred to as molecular layering. This became a major innovation in the 1970s when Suntola developed the atomic layer epitaxy technique to deposit ZnS for electroluminescent displays. ALD is based on a self-limiting reaction between two gaseous precursors and allows thin films to be deposited in a layer-by-layer fashion. The ability to deposit conformal films on high aspect ratio structures at (relatively) low temperatures and moderate pressures, as well as excellent thickness control is beyond the reach of other thin film technologies such as physical vapor deposition. and ALD has become the technique of choice for chemical vapor deposition and fabrication of ultrathin films. It uses only surface chemical reactions to produce ultrathin films with the ability to achieve highly precise control of thin film thickness down to the atomic level. ALD allows for large-scale deposition and is also seen as an alternative method to explore more surface-based growth mechanisms to create new hybrid nanostructures. It has been widely used for nanofabrication processes for microelectronic applications. ALD became commercially important in the early 2000s when the semiconductor industry began adopting ALD to produce high-performance complementary metal-oxide-semiconductor (CMOS) transistors. Both Intel and IBM have used ALD to create high-k dielectric layers in CMOS since 2007. Recently, Intel stated that the use of ALD was a key factor in the successful development of high-k metal gate transistors that allowed further downscaling. Size of integrated circuit chips. Nowadays, ALD is already entering multiple application domains such as magnetic recording heads, optics, demanding protective coatings and micro-electromechanical systems.

5. Thin film

A thin film can be labeled as a layer of thin material from a fraction of a nanometer to a micron (10^{-6} m) thick. The most important difference between thin film and thick coating deposition is the thickness of the deposited layers. Thin film deposition involves the deposition of individual atoms or molecules on a surface while thick coating is associated with particle deposition. It is being used to improve the physical and chemical properties and surface morphology of materials without changing the bulk material properties. A thin film can be individualized as a homogeneous structure, single layer, crystalline phase structure and microstructure, or an inhomogeneous multilayer or composite structure depending on the desired properties and the field of application. The structure of the multilayer can be periodic, have a set pattern or be completely random. Almost all thin films deposition techniques have four or five basic chronological steps. The steps for overall properties of thin films are unique and are listed below :

- The source of pure material to be deposited is selected. This source of material will serve as a target during the deposition process,
- The target is transported by a medium into the prepared substrate. This medium can be either a liquid or a vacuum, depending on the materials used and the deposition technique.
- The target is deposited on the substrate, forming a thin film on the substrate surface,
- Depending on whether this is necessary to achieve the desired film properties, the thin film may be subjected to annealing or other heat treatment processes,
- Film properties are analyzed. If necessary, analysis results can be incorporated to modify the deposition process.

5.1 Thin film growth and nucleation

Often, the properties of thin films are influenced by the inherent properties of the substrate and can vary greatly depending on the thickness of the film and the deposition techniques used for deposition. Three major steps are required in thin film growth and nucleation. The first step involves the preparation of the deposition species, i.e., the substrate and the target material, followed by transport from the target to the substrate using any deposition technique, and the final step involves the growth of the target on the substrate. thin layer. Target atoms impinge on the substrate, where they can either immediately reflect off the substrate, evaporate into the gas phase after a certain residence time, or condense on the substrate surface. This process is affected by many factors including activation energy, binding energy between target and substrate, adhesion coefficient, etc. The ratio of condensing atoms to impinging atoms is called the sticking coefficient. During this process, the atoms lose energy and may not immediately react with the substrate.

Before condensation occurs, their surface will have some mobility and these moving atoms are called adatoms which is a portmanteau for adsorbed atoms. The energy lost during surface atom condensation can be either chemical reactions with substrate atoms, collisions of dispersed surface atoms, preferential nucleation sites, or collisions of adsorbed surface species. If the surface mobility is low and the atom-to-atom interaction is strong, each atom can act as a nucleation site for growth but when the adatom-surface interaction is weak, the surface mobility of the condensing adatom will be high and result in preferential condensation. Nucleation sites where there is strong bonding due to an increase in coordination number or a change in basic or electronic chemistry. Condensing atoms react with surface atoms and form atom-to-atom chemical bonds. The chemical bonds formed can be of any of the following types: electrostatic attraction (van der Waals forces) due to the polarization of atoms, metallic (homopolar) bonding where atoms share orbital electrons, or electrostatic (Coulombic heteropolar) where ions are. An electron is formed due to loss or gain. If the bond formed by the reaction between the condensed atom and the surface atom is very strong, the atom is said to have

undergone chemisorption. These adatoms were transformed into nuclei by the aggregation of several adatoms, resulting in a continuous thin film.

Due to the nature of the deposition, the resulting nuclei formed at an early stage are often thermodynamically unstable and may adsorb over time depending on the deposition parameters used. After some time, the clustered nuclei reach a critical safe size and are thermodynamically stable and are said to have overcome the nucleation challenge. This process involving the transition from a thermodynamically unstable state to a thermodynamically stable state where a stable, critical-sized nucleus is formed is called the nucleation stage. As the deposition process continues, stable critical nuclei increase in number and size until a saturated nucleation density is reached. The nucleation density and average nucleus ratio depend on a number of deposition parameters such as substrate temperature, working pressure, adhesion properties, binding energy between target and substrate, energy of impinging species, activation energy of adsorption, segregation, thermal diffusion, Influence of substrate, topography and rate of chemical formation.

The nucleus can grow in two modes, parallel and perpendicular, depending on the configuration of the substrate and target, and the two conditions can be experienced in a single deposition. Surface diffusion of adsorbed atoms leads to parallel growth on the substrate while perpendicular growth occurs due to direct impact of the species. However, at this point the rate of parallel growth, sometimes called lateral growth, is greater than that of perpendicular growth, and the enlarged nuclei are called islands. In the coalescence stage, small islands on the surface of the substrate begin to coalesce with each other so that the surface area of the substrate is reduced and replaced by a thin film coating. This formed a large island and this process is called agglomeration. Increasing the surface mobility of adatoms increases the aggregation process and growth density of nucleation sites, i.e., by increasing the surface temperature of the substrate. In some reactions, the formation of new nuclei may also occur at newly exposed regions due to aggregation. Large islands grow together, leaving channels and pores of the substrate open between the islands, and a continuous film is formed on the surface of the substrate to form porous defects on the surface. The channels and pores formed by the further growth of large islands continuously coalesce and fill.

Studies of evaporated films by Lewis and Anderson classified the nucleation mechanism of thin film growth into three major types depending on the interaction between the deposited atoms of the target and the surface of the substrate. These are:

- Van der Merwe or island growth mechanism. This increase is observed when the atom-to-atom adhesion is greater than the bond between the substrate and the adatoms. A group of stable adatoms accumulates and aggregates on a surface and grows in three dimensions to form an island,
- Volmer weber or layer system. This occurs when the adhesion between the atoms and the surface is high. The film grows layer by layer on the surface of the substrate and can be used for dense coating,
- Stronsky-Krastanov (S-K) mechanism. The SK mechanism combines both island and growth mechanisms. After the initial layer grows, adatoms begin to accumulate and form islands.

6. Simulation techniques used for thin film

Computer simulation involves designing a model of a real or theoretical physical system, executing the model on a digital computer, and analyzing the execution output. In engineering, computer simulation is widely used in the fields of thermal transport, fluid flow and stress analysis. Computer simulations act as a bridge between microscopic length and time scales (theory) and the macroscopic world of the laboratory (experiment). Simulations are used to understand the properties of assemblies of molecules, their conformational behavior and the microscopic interactions between them. It serves as a complement to traditional experiments, enabling us to learn about processes and

behaviors that are difficult to analyze with experimental techniques. This enables us to solve complex theoretical models beyond specific approximations, provides a hint to experimentalists for further investigation, and optimizes process development time. Typical simulation techniques used to study the evolution of thin films are the continuum method, density functional theory (DFT) model, molecular dynamics (MD) method, and Monte Carlo (MC) method. However, molecular dynamics (MD) and Monte Carlo (MC) methods are two typical modeling techniques. MD simulations are used to predict time-dependent (transport) properties at the atomic level, for example, thermal conductivity, viscosity and diffusivity coefficients, while MC methods are applied to predict equilibrium properties, for example, potential energy calculations, adsorption studies, phase equilibrium studies. Although these simulations help improve the understanding of thin film deposition concepts, they come with important limitations such as expensive computational costs, high operating times, challenges in accurately analyzing microphysics, and challenges in analyzing bond formation and breakage phenomena at the atomic scale. These limitations were addressed with the development of hybrid and multiscale methods. These methods combine features of different simulation techniques for optimization and control schemes. This helps to improve the quality of thin films, reduce the deposition cost and efficiently simulate the surface growth of the thin film deposition process. Multiscale processes consider both linear and nonlinear relationships between process parameters and optimize them to produce accurate feedback. Despite the development and progress in multiscale modeling, the process still faces challenges and limitations. Simulation of multiscale models is not trivial because of the numerical complexity that arises when coupling modeling methods with different features. Also, the computational demands required to simulate phenomena on microscopic length and time scales impose additional constraints. Therefore, most current applications in multiscale modeling couple phenomena occurring at two different length and time scales, that is, they simply couple two different modeling methods. To overcome this limitation, the Kinetic Monte Carlo (KMC) model can be used to create a hybrid model with multiscale modeling and prevent challenges. The Kinetic Monte Carlo (KMC) method is often suitable for describing phenomena at different length and time scales. Because of its versatility, this stochastic method is preferred for modeling phenomena occurring at the atomic, molecular, or nanoscopic scale. Thus, multiscale modeling formulations often combine the KMC model with a continuum model, which predicts the behavior of physical systems at the micro/macroscale. Consequently, simulation process improvement studies for thin film growth are most easily performed using multi-scale modeling techniques that capture the relevant molecular and bulk phenomena at the scales at which they occur. In recent years, improvements in our understanding of the physics and chemistry of films, surfaces, and interfaces have aided the creation and development of deposition techniques. However, it has also provided a platform for developing predictive models for thin-film growth that offer the ability to control film structure and properties. Multiscale simulation also offers the ability to estimate the effect of uncertainty allowing robust control of small-scale systems. Model predictive control (MPC) provides an effective framework that uses system models to predict control actions that optimize performance indices in the presence of constraints to improve the deposition process while reducing cost and time. Model predictive control is also capable of accurately predicting output feedback such as surface roughness statistical moment, growth rate, etch rate, surface morphology, dynamic behavior, film porosity and film thickness.

7. Application of thin film

Over time, the applications of thin films have grown exponentially and have become an integral part of industrial and research processes. By improving surface properties such as thin film deposition, wear, fatigue, corrosion, hardness and other surface-related phenomena, the material can be versatile

and used for a variety of applications. Applications of thin films can be grouped under the following general areas:

- **Electronic component and display.** Undoubtedly, thin films have enormous and vast applications in the fabrication of electronic components such as semiconductors, single and multilayer metal conductor films, and microelectronic integrated circuits. Thin film deposition has greatly benefited compound conductor films and metal refractory silicide conductors for semiconductor, dielectric and insulating materials. The fabrication of electronic displays requires conductive and transparent films, luminescent or fluorescent films as well as dielectric and insulating layers.
- **Solid surface coating and biomedical.** The tribology resistance and corrosion performance of the components can be improved by coating the surface of the components with thin film coatings of carbides, silicides, nitrides and borides, respectively. These coatings are used in manufacturing tools, bearings and areas with sliding friction such as machine parts. In recent times, diamond-like carbon films have received more attention and interest due to their ability to provide appreciable resistance to heat, hardness, electrical isolation, and high-temperature and high-energy radiation. It is also used for biomedical applications to enhance proper osteointegration and adhesion properties.
- **Optical coating and optical data storage devices.** Optical coating requires a thin film coating. It is used to filter the interference on the solar panel and acts as a reflection objective. Thin films with appropriate refractive index gradients are being used on optical fibers to improve refraction and absorption coefficient performance. Highly reflective coatings that can withstand very high radiation intensities without fading and failure during use are essential for laser optics, and thin films with excellent properties are obtained by metal reflective coating. Infrared reflective coatings are applied to filament lamps to increase the intensity of the luminous flux. Commercial demand for thin film coating is also increasing in optical data storage devices such as computer memory and storage disks. They act as a protective coating on the surface and protect against temperature rise. Thin films have also been widely used in window glass and mirror coatings to prevent heat.

CONCLUSION:

When considering the most appropriate thin film deposition method for your application, it is important to understand the available processes so you can choose the one that will maximize the quality and throughput of your coatings. With a 10 ms response time, an accuracy of 0.5% of reading, and the ability to easily fit into your existing setup, Alicat's MCE or MCV-Series mass flow controllers can be used to produce high-quality, repeatable coatings. Variety of deposition setups.

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