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PVD Processes for Sustainability – an Approach through Smart Designs

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ABSTRACT

Material and energy efficiency is a major focus when designing and optimizing a PVD production process. The goal of sustainability compels us to seek designs that possess high vapor-collection efficiency, optimal thickness uniformity, high deposition rates and low energy consumption. In practice, it is crucial to be able to quantify these fundamental tradeoffs in PVD engineering. A set of numerical modeling tools (Tin Model LLC's V-Grade 5S Pro suite) are found suitable for assessing these aspects of PVD processes and thus enabling engineering choices that simultaneously achieve qualities of deposited materials and minimize environmental footprints. A real-world example is discussed.

INTRODUCTION

As with all major manufacturing methods, physical vapor deposition (PVD) processes must be assessed on their efficiencies: how efficiently they utilize raw materials and consume energy. Such assessments are important not only for the cost of manufacturing but also for gauging their environmental impacts, a growing awareness of which can be felt in our industry [1]. Throughout the history of PVD, however, processes have seldom been analyzed or compared from this perspective. A difficulty lies in the lack of quantitative accounts for some of the fundamental characteristics as vapor capture. For obvious reasons, analyses of this kind are the most beneficial and impactful if they are conducted when a manufacturing process is at its conception and design stages.

For assessments of this kind, numerical modeling is probably the only practical approach: constructing of a physical and functioning model is cost prohibitive in most cases. Although numerical modeling has been associated with PVD engineering throughout the past decades [2-5], it remains uncommon for a study to provide a comprehensive set of information that enables comparative appraisals of various choices from the view point of efficiency and sustainability. Specifically, a comprehensive set should include these 3 basic measures of a PVD process: vapor capture, deposition rate under a given power and thickness distribution.

In this work we show that numerical modeling can not only provide the information but also stimulate innovations that lead to better PVD processes. In addition, the modeling allows us to propose a metric that may be employed to objectively compare processes in regard to their overall efficiency, both intramodal and intermodal.

METHOD OF NUMERICAL MODELING

1. Modeling Approach

In a typical PVD process, a substrate moves with respect to the atomic plume (vapor plume) of a source. These movements can be as simple as a linear transportation or as complex as triple rotations with three independent axes. In rare cases, a substrate undergoes a combination of different motion types or subscribes to an uncommon trajectory. On the other hand, the work pieces (substrates) to be coated can be as simple as a flat disc or as complex as having arbitrary surface types and shapes. As for vapor sources, they can also have any physical construction and face any direction (orientation) in the space. Furthermore, there can also be a number of vapor-obstruction elements, such as correction masks, room dividers and chimneys.

In constructing our modeling program, flexibility is a major emphasis: all the above-mentions elements can be handled seamlessly. The program follows a number of sampling points (1 to several thousand) on the substrate for computation, which, in essence, is a numerical integral that covers the entire trajectories of the sampled points. A user can define a suitable step size depending on the complexity of the substrate motion for speed and precision.

A realistic model must take into account the varying types of vapor plumes produced by various materials and sources types. In our modeling the vapor plume emanated by a source point is characterized by a three-term polynomial of the cosine:

$$\text{Flux} = C_1 cos^{\varepsilon1}\alpha + C_2 cos^{\varepsilon2}\alpha + C_3 cos^{\varepsilon3}\alpha. \qquad (1)$$

This plume function encompasses nearly all the observed vapor plumes from practical devices. The overall vapor plume is a summation of the elemental emissions from an ensemble of source points. An erosion track of a magnetron sputtering source is typically represented by several hundred points of weighted emission. Each of the emission points can have their own symmetry axis from which angle α in Eq. (1) is measured: this allows for modeling of such vapor sources as cylindrical magnetrons and ion-beam sputtering.

2. Determination of Vapor Plume

While it is common to assume a generic and simple plume function for a given PVD source, a more nuanced and accurate plume characterization can significantly improve the realism of the modeling. To facilitate this, we created a tool that extracts the plume function, namely, the six parameters in Eq. (1), from experimentally measured thickness distribution on a substrate or a substrate carrier. The method of extraction is based on a least-square fitting of the experimental data. If the plume function of a source is already known, users can simply enter the parameters in the program.

3. Obstruction of Vapor

Vapor obstruction, in the form of shadow masks, is frequently employed as means of achieving thickness uniformity or to obtain prescribed thickness gradients. In other cases, vapor obstruction accompanies devices intended for specific purposes such as collimation (in semiconductor manufacturing processes) and plasma confinement. In the modeling program, we allow a number of vapor-obstruction components to be placed in the vapor paths. These vapor-obstruction elements can be complex in shape, each definable by 56 anchor points which can be adjusted manually or automatically to achieve a desired outcome, such as a specified thickness uniformity. These obstruction elements can be stationary or rotating at a user-defined velocity.

4. Vapor Capture and Absolute Thickness

For the derivation of vapor capture efficiency, two quantities are computed: a) the amount of vapor intercepted by the substrate carrier; and b) the total vapor emitted by the source. The first quantity is an average of vapor intercept: in the case of a rotational fixture the average is calculated over a number of revolutions of the substrate carrier; in the case of a linear translation or a roll-to-roll coating the average covers the entire transit of the substrate in the vapor plume. (We must also take into account any obstruction between the source and the substrates.) Both of these quantities are dependent on the plume function, Eq. (1). Once these two quantities are known, their ratio gives the vapor capture coefficient in terms of percentage.

Knowledge of the vapor capture allows us to computer another important quantity of a PVD process: the absolute thickness (AbT) in unit of nm/gram, i.e., thickness in nanometers per gram of source materials vaporized. AbT is a standard output of our modeling programs.

5. Computation of Deposition Rates

To predict the deposition rate of a PVD process we must begin with a physical model that relates the vaporization rate of the material to the power applied to the source in use. Take ion-beam sputtering, for example, the vaporization rate is linearly proportional to the ion current but dependent on the ion energy in a nonlinear relationship; through some simplification we derived a formula that requires the input of only four physical quantities: molecular mass (of the target material), sputtering yield, ion energy and ion current. The first two quantities are wildly available in literature. Finally, with the knowledge of the vaporization rate, deposition rates in units of nm/minute can be calculated from AbT values.

In similar fashions, mathematical models are developed for magnetron sputtering sources and evaporation sources. All these models have withstood the tests and validation of a large number of experimental data.

FIGURE-OF-MERIT OF PVD PROCESSES

To objectively appraise a PVD processe, we propose a figure-of-merit: an index that is applicable to varied processes for a set of qualifications. We designate it as M with the following definition:

$$M = \frac{A \cdot R \cdot V \cdot (1 - U)}{W} \,,$$

Where A is the total area (of substrates or substrate carrier) in m^2; R is deposition rate in unit of *nm/minute*; V is the vapor capture (see previous section); U is the thickness nonuniformity (between 0 and 1, value 0 being the best); and W is the applied power in *kW*. This figure of merit can be employed for comparisons of PVD processes intermodal as well as intramodal. The higher the M value, the more efficient a process is in consumption of energy and the source material.

An intermodal comparison can tell us how one modality measures up to another when a manufacturing process is being designed. For example, when an electron-beam evaporation and a rotating cylindrical magnetron can both produce the same material for a product, a comparison of their respective M

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values can illuminate which one is more cost effective and environment friendly.

An intramodel comparison can help in optimizations of existing PVD equipment. Modifications to the fixtures, repositioning of a source, addition or subtraction of correction masks etc. affect not only the quality of the materials deposited but also the efficiency of a process, thus the cost of manufacturing. The figure of merit *M* can aid engineers in deriving the best outcome amongst many tradeoffs.

EXAMPLE OF COMPARATIVE STUDIES

We consider the deposition of a copper layer, by means of DC magnetron sputtering, on 16-inch-diameter substrates in the fabrication of an optoelectronic device. Assume that the production requires: 1) 6 substrates are coated in a single batch; 2) the thickness uniformity is better than 1%; and 3) the deposition rate is no less than 20 nm/min. In the below, we analyze two arrangements.

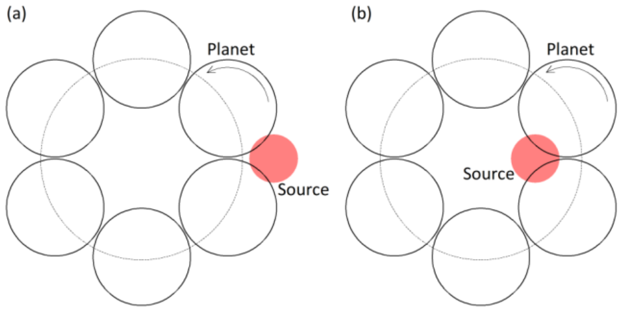

Figure 1. Top views of a magnetron source in a 6-planet coating system: In arrangement (a), the source is placed outside the circle-of-orbit; in (b), the source is placed inside the circle-of-orbit.

In a more conventional design, shown in (a), the substrates are mounted on a 6-planet fixture that undergoes a double rotation; the center of an 8-inch magnetron cathode is placed outside the circle-of-orbit of the planets. The deposition rate of 20 nm/min can be reached with 4000 watts of power applied to the cathode. The thickness uniformity is 0.4% across the entire substrates; the vapor capture is 25.6%, which is typical of a planetary rotation process.

In an alternative and innovative design, shown in (b), pioneered by Vacuum Process Technology (Plymouth, MA), the 6 substrates are mounted on the same fixture [6]. The center of the cathode (of the same kind) is placed inside the circle-of-orbit. The same deposition rate of 20 nm/min can be obtained with 2350 watts of power to the cathode. The thickness uniformity is 0.3%; the vapor capture is 43.9%. The numedical modeling results are consistent with experiments. The second process, with an *M* value of 2.91, is far more efficient than the first process which has an *M* value of 0.99. While both processes satisfy the production needs, the second process does so by consuming 40% less power and 42% less source material than the first process.

CONCLUSIONS

In PVD, the mathematically convoluted relationship between a geometry and its outcome poses significant challenges for engineers to achieve a set of objectives which may include efficient use of raw materials and energy, in addition to qualifying the fabricated materials. We have shown that numerical modeling is capable of providing the crucial information needed to enable an engineering approach that is quantitative, accurate and prognostic.

A figure-of-merit, *M*, is introduced to gauge the efficiency of a PVD process. This metric can be employed in optimization of existing coating apparatus as well as in designs of new production plants from conception. A high *M* value indicates a PVD process that is efficient in consumption of raw material and energy (low cost as a result) and, therefore, consistent with the goal of sustainable manufacturing.

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FOR FURTHER INFORMATION

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