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Technical paper

Simulation model for an EB-PVD coating structure using the level set method

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ABSTRACT

A comprehensive modeling approach to link machine dynamics, deposition, and substrate kinematics in an electron beam physical vapor deposition (EB-PVD) is presented in this paper. The machine dynamics in EB-PVD process are captured by finite element models, resulting in the prediction of evaporation rate and vapor distribution. The deposition process is modeled using the level set method, which is one of the computational techniques for tracking topographic evolution. The proposed simulation model is implemented in Matlab and is compared with experimental results published by other researchers. Results indicate that the proposed simulation model can be used to predict microstructure features such as zigzag and helical columnar shapes. The pitch of a zigzag microstructure can be predicted within 20% at the 0.3 to 6 μm level for Yttira-stabilized Zirconia (YSZ) coating.

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1. Introduction

Among the various deposition techniques, EB-PVD is versatile because it can simultaneously evaporate multiple materials of different types of compositions; it enables engineers to design tailored microstructures, such as functionally graded coatings and nano-laminated coatings; and new materials that could not be produced economically by conventional methods [2,3]. Coatings produced by the EB-PVD process usually have a good surface finish and a uniform microstructure. Singh and Wolfe [4] investigated the application of EB-PVD to the formation of net-shaped rhenium components with the shapes of ball, plate, and tube. EB-PVD can be a cost-effective solution for manufacturing surfaces with submicron and nano-sized microstructures with high hardness and strength as compared with chemical vapor deposition (CVD).

There has been an acute need for developing a scientific basis for coating processes, especially models and techniques for their real-time control [5]. The theory of evaporation was first established by Hertz in 1882 followed by Langmuir in 1913 and Knudsen in 1915 to model the evaporation rates from free solid surfaces and liquids [6]. One of the key results in the theory of evaporation is the cosine law of emission which models the directionality of evaporating molecules [6]. The cosine model and its variants have been used in several evaporation applications to model coating thickness of simple planar substrates [7,8]. Bernier et al. [9] proposed a modified Knudsen's cosine law of emission using experimentally measured thickness profiles of coatings deposited on stationary cylinders.

A computer program based on mathematical models explaining the physical phenomena such as evolution and deposition inside physical vapor deposition (PVD) chamber, can be used for process optimization in coating plants [10]. The main advantage of the software tool is that noticeable practical improvements can be achieved without any additional experimental tests. Pereira et al. [11] developed a computer program based on Knudsen's cosine law, which can calculate the coating thickness distribution around any component rotated about its axis. The kinetics of evaporation and vapor transport as well as deposition rate were simplified in reduced order models and a macroscopic balance was established between the intermediate process parameters, such as ingot temperature and deposition rate, and the input parameters [12]. The authors have developed a simulation tool to predict the coating thickness for simple geometric shapes such as the flat plate and the cylinder coated with titanium and tungsten, respectively [13,14]. The microscopic process of coating growth, however, cannot be accurately predicted using these models for the EB-PVD process.

For the atomic scale simulation, many studies have relied on the Monte Carlo (MC) technique which is a well known method that describes discrete atoms and their interactions in these microscopic processes without developing the mathematical models which are usually high dimensional and nonlinear and represents nanometer-scale phenomena on the surface of a substrate [15]. The deposition of thermal barrier coatings (TBCs) on a rotating planar substrate was modeled on an atomic scale by implementing the kinetic Monte Carlo (KMC) approach [16]. While such Monte Carlo (MC) techniques can directly account for the stochastic nature of an individual atom to describe nanometer-scale dynamics, MC models are not available in closed-form so that it is very difficult and computationally expensive to use them for system-level analysis. Thus, most researchers combine

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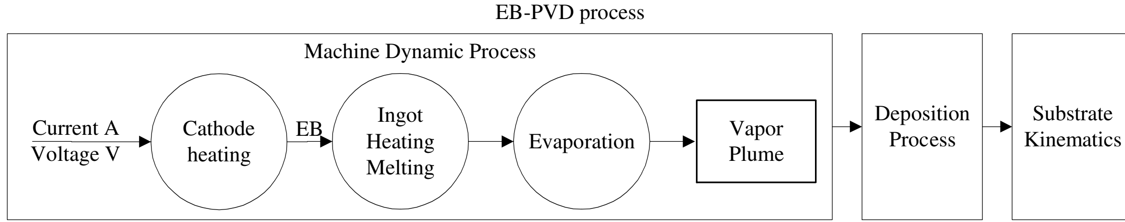

Fig. 1. Schematic diagram of the unified EB-PVD process model.

both machine level and microlevel simulations to link process parameters and thin film deposition parameters using the MC simulation approach [17,18].

Level set approaches are being increasingly used for their robustness to topological changes, which describe the evolution of a surface by solving a Hamilton–Jacobi equation in a computational grid in a computationally efficient manner [19]. Adalsteinsson and Sethian [20,21] applied the level set method to develop a unified model of surface advancement including the effects of deposition, etching, and lithography. Their level set formulation was solved by numerical techniques developed for the solution of hyperbolic conservation law. Hsiau et al. (1997) showed that the boundary movement method, including the level set method, is practical in 2D, and competitive for larger scale or 3D application. O'Sullivan et al. [22] used the level set method to model the topographic evolution of high aspect ratio trench using physical vapor deposition and validated the numerical simulation by comparing with experimental data for Ti/TiN barrier layers. Since the 3D flux could be obtained from molecular dynamics computations, their approach represents a hybrid atomistic/continuum model. The level set method can be made more accurate by decreasing the grid size, offering prospects of virtual experimentation [23]. Hansen et al. [24] also linked the film growth rate obtained from molecular dynamics in angstrom-scale to the morphology of growing film using the level set method. The level set equation has been coupled to a physics-based model to compute the etch rate. It has also been shown that the level set formulation is amenable for integration with continuum codes commonly used in reactor modeling in etching processes to predict profile evolution during silicon etching [25].

In this paper, the level set approach is extended into the EB-PVD process to develop computational models which are efficient compared to MC techniques. First, an FEM-based unified EB-PVD machine dynamic model from our prior work [13] is summarized in Section 2. Section 3 illustrates the level set method and the derivation of an evolution speed function in the EB-PVD process. Section 4 summarizes the simulation results for YSZ deposition on the flat work-piece with rotation, which are compared with published experimental results to validate the developed simulator. Finally, Section 5 concludes with directions for future research.

2. Unified model of EB-PVD process

The unified model of EB-PVD process developed by the authors [13] uses a finite element model to combine various dynamic aspects of an EB-PVD machine as well as deposition process and substrate kinematics. As shown in Fig. 1, the key processes in EB-PVD can be simplified into three sub processes: machine dynamic, deposition, and substrate kinematics.

In the machine dynamic process, 'Cathode heating' shown in Fig. 1 results in the emission beam current I_e from input current A and voltage V of an EB gun. Next, the emission beam current is absorbed by finite elements of an ingot computed in a sequential order based on the given beam scanning pattern. The absorbed beam power $p_A(t)$ on the ingot is assumed to have the Gaussian rotationally symmetrical power density distribution [26]. 'Ingot Heating/Melting' shown in Fig. 1 solves an energy balance equation in each element of the ingot using the given absorbed beam power, resulting in a temperature profile T_{ij} of (i, j) element for $i, j = 1, \ldots, n_{mesh}$, where n_{mesh} is the number of elements along the diameter of the ingot mesh. From the temperature profile, vapor pressure P_{ij} of (i, j) element can be computed using the Clausius–Clapeyron formula as follows [27]:

$$\log_{10} P_{ij} = -\frac{A}{T_{ij}} + B + C \log_{10} T_{ij} + DT_{ij}. \tag{1}$$

Assuming that the evaporation rate is constant over the surface of an individual element of the mesh, the evaporated mass per unit time, a_{vij}, of (i, j) element is obtained from T_{ij} and P_{ij} as follows:

$$a_{vij} = F_p \cdot a_{v1ij} \tag{2}$$

where F_p is the area of an element in the ingot mesh in mm^2 and a_{v1ij} is the amount evaporated per unit time per unit area in $g \cdot cm^{-2} s^{-1}$, which is given by

$$a_{v1ij} = \alpha \cdot 4.4 \cdot 10^{-4} \cdot P_{ij} \cdot \left(\frac{M_D}{T_{ij}}\right)^{1/2} \tag{3}$$

where α is the evaporation coefficient which becomes 1 for idealized evaporation and M_D the molecular weight of the evaporant [28]. Based on the assumption that each element acts as a vapor source, 'Evaporation' shown in Fig. 1 determines the final distribution of the vapor plume by superimposing an individual vapor plume from an element on the others. The shape of an individual vapor plume depends on the beam collimation parameter n_{ij} that can be estimated using T_{ij}, P_{ij}, and a_{vij} in Eq. (2) as follows:

$$n_{ij} = K_n \left[f\left(a_{vij}\right)\right]^{1/4} \tag{4}$$

where

$$f\left(a_{vij}\right) = \frac{10^{10}}{\rho \cdot F_p} \cdot K_a \left(1 - \frac{P'_{ij}}{\sqrt{T'_{ij}}} \Big/ \frac{P_{ij}}{\sqrt{T_{ij}}}\right) \cdot a_{vij} \tag{5}$$

where ρ means the material density, K_a is a coefficient calculated from the ratio of surface area between a vapor plume and an ingot, and T'_{ij} and P'_{ij} refer to the temperature and pressure of environment for an (i, j) element, respectively, that are calculated using the isentropic expansion equation as follows [12]:

$$T'_{ij} = T_{ij} \left(\frac{P'_{ij}}{P_{ij}}\right)^{\frac{\gamma_{ij}-1}{\gamma_{ij}}} \tag{6}$$

where γ_{ij} is the heat capacity ration of the (i, j) element.

In the deposition process shown in Fig. 1, a substrate is represented by finite elements where coating thickness will be computed using the deposition process model derived from the geometry of the vapor flux with an assumption of isothermal cell

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