Microstructure of vapor deposited coatings on curved substrates

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Thermal barrier coating systems consisting of a metallic bond coat and ceramic over layer are widely used to extend the life of gas turbine engine components. They are applied using either high-vacuum physical vapor deposition techniques in which vapor atoms rarely experience scattering collisions during propagation to a substrate, or by gas jet assisted (low-vacuum) vapor deposition techniques that utilize scattering from streamlines to enable non-line-of-sight deposition. Both approaches require substrate motion to coat a substrate of complex shape. Here, direct simulation Monte Carlo and kinetic Monte Carlo simulation methods are combined to simulate the deposition of a nickel coating over the concave and convex surfaces of a model airfoil, and the simulation results are compared with those from experimental depositions. The simulation method successfully predicted variations in coating thickness, columnar growth angle, and porosity during both stationary and substrate rotated deposition. It was then used to investigate a wide range of vapor deposition conditions spanning high-vacuum physical vapor deposition to low-vacuum gas jet assisted vapor deposition. The average coating thickness was found to increase initially with gas pressure reaching a maximum at a chamber pressure of 8–10 Pa, but the best coating thickness uniformity was achieved under high vacuum deposition conditions. However, high vacuum conditions increased the variation in the coatings pore volume fraction over the surface of the airfoil. The simulation approach was combined with an optimization algorithm and used to investigate novel deposition concepts to tailor the local coating thickness. © 2015 American Vacuum Society. [http://dx.doi.org/10.1116/1.4927162]

I. INTRODUCTION

Ongoing efforts to increase the efficiency of gas turbine engines are driving combustion gas temperatures well above the melting points of their metallic components.\(^1\) This has led to the adoption of thermal protection concepts that combine internal air-cooling of components with thermal barrier coating (TBC) systems to impede heat flow (and thermal damage) to the component surface. TBC systems typically consist of a metal alloy bond coat deposited on the surface of the metallic component to delay oxidation and hot corrosion, and an outer, low thermal conductivity ceramic layer.\(^1\)–\(^3\) Numerous methods have been proposed for the deposition of these coatings including liquid droplet processes such as air or vacuum plasma spray,\(^4\) and electron beam-physical vapor deposition (EB-PVD)\(^5\) concepts that create an atomically dispersed vapor plume, which is condensed on the substrate surface. More recently, hybrid techniques have been also proposed including plasma spray-PVD (PS-PVD),\(^6\)–\(^8\) which uses a high power plasma to evaporate liquid droplets in a high-pressure gas jet, and electron beam-directed vapor deposition (EB-DVD)\(^9\)\(^{,}\)\(^10\) in which an electron beam is used to evaporate a source material located in the throat of a helium gas jet forming nozzle.

Both the thermal protection provided by ceramic coatings and their durability in the engine environment are strongly influenced by the thickness and structure of the coating.\(^5\)\(^,\)\(^11\) In a ceramic layer deposited by PVD, the coating thickness, pore volume fraction (porosity), and inclination of the growth columns (and pores) govern the thermal resistance. Coatings applied by one of the PVD methods are usually used for components subjected to severe thermal cycling, since they have a columnar structure leading to a low in-plane modulus (a consequence of the many intercolumnar pores oriented perpendicular to the substrate surface) and increased delamination resistance.\(^12\)–\(^14\) Their expansion and contraction partially accommodates the substantial thermal strain during thermal cycling without creating stored (elastic) strain energy sufficient to drive delamination cracks. While thicker coatings could give increased thermal protection, the stored elastic strain energy in a coating is proportional to its thickness,\(^15\)–\(^17\) and therefore, thick coatings are subject to an increased risk of delamination. It is therefore important to balance the coating’s thickness to achieve the required temperature drop without overly increasing the risk of delamination.

The pore structures in TBCs deposited by EB-PVD (and its higher-pressure, EB-DVD counterpart) occur on several length-scales: large intercolumnar pores surround typically ~10 \(\mu\)m diameter growth columns, while smaller micron-scale pores, and isolated nanoscale pores exist within the columns.\(^10\)\(^,\)\(^18\) While the large intercolumnar pores reduce coating strain energy by accommodating mismatches in thermal expansion,\(^19\) the micron-scale pores provide a significant reduction in coating thermal conductivity in the heat-flux propagation direction.\(^10\)\(^,\)\(^20\) Nanoscale pores in many “as-deposited” coatings also reduce coating conductivity by increasing phonon scattering, but are quickly removed by sintering during operation of the engine.\(^21\)\(^,\)\(^22\)
A critical challenge posed by the use any of the PVD methods for TBC deposition is the requirement to deposit coatings onto complex shaped engine components such as turbine blades, vanes, and nozzles. Uniform deposition with the low-pressure EB-PVD method is not possible on substrates with nonplanar surfaces unless they are rotated during deposition.23 Sophisticated substrate translation and rotation schemes have been designed to improve the coating thickness uniformity on these components.24,25 The EB-DVD process utilizes a higher deposition chamber pressure (typically 1–45 Pa) and a gas jet to partially overcome this limitation by enabling the incident vapor to flow over the entire substrate surface; eliminating sharp coating thickness discontinuities in line-of-sight limited, low-pressure EB-PVD coatings. The EB-DVD method has been used to deposit coatings on several non-line-of-sight (NLS) substrates including fibers,26 polymer foam templates,27 and stationary airfoil shaped substrates.23 A similar capability has been reported for the gas flow sputtering method28–30 using a deposition chamber pressure of 47 Pa, and the PS-PVD method, which operates with chamber pressures in the 100–1000 Pa range.6–8

Vapor condensation onto a nonplanar substrate geometry affects both coating growth behavior during deposition and in-service performance of the ensuing coating. For example, the delamination resistance of a TBC appears to depend on the curvature of the substrate to which it is applied. Steinbrech et al.13 have shown that the lifetime of coatings applied to the outer surface of cylindrical tubes increased with the cylindrical substrate’s radius. Other investigations of the failure modes of coated airfoils removed from gas turbine engines have shown the failure mode to vary with location on the airfoil surface.11 This arises from a complex combination of factors including spatial variations of both the temperature and thermal stress experienced by the coating, the local substrate curvature, and the probability of impact by small or larger particles leading to erosion or foreign object damage.

The coating’s thickness and structure (such as its porosity or columnar growth angle) can affect its susceptibility to these degradation mechanisms. For instance, columnar coatings containing highly inclined growth columns are thought to be more susceptible to impact damage,31,32 while those that are highly porous can better resist thermocyclic failure modes, but may be more vulnerable to failure by the infiltration of liquid glasses (calcium magnesium aluminum silicates) that can accumulate on the hottest regions of the airfoil. Variation of the columnar growth angle has also been found to influence the through thickness thermal resistance, as well as the rate of intercolumnar sintering, and therefore stiffening of the top coat.33 If methods were developed to manipulate the local coating thickness and structure across the surface of the airfoil during the coating process, it might be possible to delay some failure modes, thereby significantly extending the lifetimes of thermal barrier coatings.

A numerical simulation of coating deposition provides an efficient means of exploring the relationships between the local coating thickness, its structure, and the conditions used for its deposition. In principle, molecular dynamics provides a means for this, but the computational expense is prohibitive for coatings that are typically 100 μm thick and deposited at rates of a few microns per minute. The alternatives are more computationally efficient (but more approximate) atomistic kinetic Monte Carlo (kMC) techniques,35,36 continuum-based methods such as the level-set method,37 or finite element based methods.38,39 Of these, only the kMC technique can address structure at both the atomic and coating thickness scales. Advanced kMC methods have been developed with built in controllers to manipulate surface roughness and site occupancy,40 and even account for material elasticity.42,43 An overview of these methods has been recently published.44

Here, we use a combination of kMC modeling for simulating atomic assembly and a direct simulation Monte Carlo (DSMC) technique for vapor transport to investigate the deposition of a coating on a model airfoil-shaped substrate. Deposition onto both stationary and rotated substrates is investigated as the background pressure, gas jet velocity (via the changes to the pressure ratio across the nozzle used for its formation), and the homologous coating temperature are varied. Experimental coatings on both stationary and rotated airfoils are also deposited to assess the validity of the modeling approach. The dependence of the local coating thickness, columnar growth angle and porosity are reported as a function of the deposition conditions, and opportunities to control the spatial variation of these parameters are discussed.

II. METHODS

The airfoil substrate used for experimental and simulated depositions is shown in Fig. 1. The airfoil’s exterior surface shape was defined by three quadratic surfaces with varying radii and centers of curvature. To allow for the use of two-dimensional simulations, the airfoil’s cross-section remained constant through its thickness (it had no twist). Simulation airfoils were considered perfectly two-dimensional, while experimental airfoils had a width of 12.7 mm and were mounted to a thin backing plate during deposition. During stationary deposition, the substrate was aligned with the airfoil’s chord parallel to the gas jet flow direction, and oriented with the leading edge nearest to the vapor source, as shown in Fig. 1.

A schematic of the deposition geometry is shown in Fig. 2. The substrate was positioned in the vacuum chamber with the center of rotation located 21 cm above the center of the 12.5 mm wide vapor source. The evaporation rate of a model nickel source was set at 8.8 × 10^19 atoms m⁻² s⁻¹ for all simulations. A coaxial gas jet was formed around the vapor source by expansion of a 90 at. % He and 10 at. % O₂ gas mixture through a choked nozzle, Fig. 2. The velocity of the rarefied gas jet was governed by the ratio of the gas pressure up and downstream of the nozzle, the ratio of specific heats of the gas, and its initial temperature (taken to be 300 K here).18,20

A. Simulations

A two-step simulation method was used to encompass the range of length and time scales relevant to the deposition
process. First, the rarefied gas dynamics within a deposition chamber was simulated with a DSMC method described in detail elsewhere. The vapor species was taken to be nickel with scattering parameters calculated using the method of Venkattraman and Alexeenko. The local nickel atom flux incident on a surface, and its incidence angle distribution (IAD) obtained from these simulations were used as the input to a 2D on-lattice kMC method, which simulated atomic assembly and growth of the coating. The IAD is centered on the local surface normal \( \hat{n} \). The kMC method used here has been previously used to simulate the vapor deposition of porous coatings and microelectronic trench filling. The method simulates the deposition of individual vapor atoms on the substrate surface and links the deposition rate to single-atom diffusional jumps between lattice sites within, or on the surface of the existing coating. The energy barriers used to determine diffusion kinetics of nickel were precalculated using the embedded atom method and are tabulated in Hass. During both simulations, the Ni vapor was assumed to have a sticking coefficient of unity, and no re-evaporation of condensed vapor was allowed to occur.

The kMC method is well suited for simulation of the vapor deposition of a coating since it is sufficiently computational efficient to permit prediction of the thickness and microstructure of a coating grown at realistic deposition rates, angle of atom impacts, and substrate temperatures. The relationship between deposition rate and surface diffusion is determined by linking the sum of all single atom diffusional jump probabilities with the vapor atom arrival rate obtained from the DSMC simulation. The probability of a diffusional jump occurring is determined by the jump attempt frequency, the activation energy of the jump, and the temperature. For a jump over a barrier with activation energy \( E_i \), the successful probability is given by

\[
P_i = v_o e^{-E_i/kT},
\]

where \( v_o \) is the effective vibrational frequency of atoms in the solid (fixed at \( 5 \times 10^{12} \text{ s}^{-1} \) in this study), \( E_i \) is the activation barrier for the specific jump \( i \) in eV (tabulated in ), \( k \) is Boltzmann’s constant in eV/K, and \( T \) is the absolute temperature in Kelvin. The simulation advances by adding \((\Sigma P_i)^{-1}\) to the simulation time after each jump is performed. When the elapsed simulation time is greater than the time interval between vapor atom arrivals (the inverse of the deposition rate), an additional vapor atom is added to the simulation and the cycle repeats until the desired number of atoms have been deposited.

During simulation, each occupied lattice site can possess several activation energies (and thus jump probabilities)

![Fig. 1](image1.png)

![Fig. 2](image2.png)
corresponding to the different (atomic configuration dependent) diffusional pathways available to it. All possible pathways for a given lattice configuration are stored in memory, and a Monte Carlo algorithm is used to select a specific jump. The energy barrier values are stored in a binary tree to minimize computational effort when selecting a jump and updating the grid afterwards. A comprehensive discussion of the kMC procedure used here can be found in Yang.50

The convex and concave surfaces of the airfoil were divided into 40 independent kMC simulation regions to allow for microstructure simulation along the entire substrate surface. Each simulation region was separated from the next by a distance of 1.13 mm along the convex surface and 1.07 mm along the (shorter) concave surface. These kMC regions corresponded to the substrate surface elements used in the input DSMC simulations. Each kMC region was assigned a width of 4000 virtual lattice sites (≈1 μm wide). To reduce variability in columnar growth, an initial substrate roughness was used for the simulations.35 The effects of surface asperity size, shape, and spacing on simulated coating microstructure have been quantified in previous studies.47,51 The roughness used here consisted of flat-topped pyramidal asperities with a base width of 100 atoms, a height of 75 atoms, and a spacing of 256 lattice sites between asperity midpoints.

The DSMC simulations yielded two variables that subsequently govern the thickness and structure variation across the substrate: the local deposition rate and IAD of the vapor atoms. The deposition rate influences the number of diffusional jumps possible between vapor atom arrivals and the final thickness of a coating deposited in a fixed time. The IAD specifies the likelihood that an incident vapor atom impacts a substrate at a specific incidence angle, θ, measured from the local surface normal [Fig. 3(a)]. Angles oriented toward the airfoil’s leading edge were taken as positive, while those oriented toward the trailing edge were negative. Atoms arriving with similar trajectories that impact opposite sides of the substrate (convex or concave) will have θ values of identical sign. Oblique atom arrivals are susceptible to shadowing by growth surface protuberances, leading to the eventual formation of pores under conditions of insufficient thermally activated surface diffusion.36,47

Simulations of deposition on rotated substrates were performed by sequentially combining data from a set of stationary DSMC simulations with substrate orientation specified by the angle α, as shown in Fig. 3(b). Eight stationary DSMC simulations, each separated by 45° of rotation, were used as input for each rotated kMC simulation. Substrate rotation was simulated by depositing a specified number of atoms (determined by the orientation-specific local deposition rate) from the IAD of each orientation. At DVD-like and higher chamber pressures, there was significant IAD overlap between neighboring orientations which ensured a smooth transition between orientations. The eight orientations were cycled through until the desired total number of atoms had been deposited.

![Fig. 3. (Color online) Definition of (a) the incidence angle, θ, of a vapor atom relative to the local surface normal, and (b) the orientation of the airfoil substrate, α relative to the jet flow axis. (c) An example of an incident vapor atom angle probability distribution (θm = 20°, θw = 87°) calculated by simulating jet flow near a tilted substrate (α = 45°) at a chamber pressure of 22 Pa and a pressure ratio of 5.45 (baseline DVD conditions). The distribution was recorded at a location 15 mm along the convex side of the airfoil.](image)

The kMC deposition rate was determined by assuming a maximum deposition rate of $D_{\text{max}} = 4.3 \, \mu \text{m/min}$ (Ref. 52) at the surface region with the highest deposition flux as calculated by DSMC. The deposition rate, $D$ at each surface
region along the remainder of the substrate was determined by normalizing the DSMC calculated fluxes by the maximum value

\[ D = D_{\text{max}}(f / f_{\text{max}}), \]

where \( f \) is the DSMC determined vapor flux at a surface region and \( f_{\text{max}} \) is the maximum vapor flux at each orientation. When rotated deposition was simulated, \( D \) was calculated at each orientation. The total number of atoms deposited in each simulation region, \( N \), was also scaled by the total DSMC flux

\[ N = N_{\text{max}}(f / f_{\text{max}}), \]

where \( N_{\text{max}} = 9,000,000 \). During rotated deposition, \( f \) and \( f_{\text{max}} \) were determined by summation of DSMC fluxes from all orientations.

An example of an IAD simulated at a distance 10 mm from the origin along the convex surface of a stationary airfoil is shown in Fig. 3(c). The distribution is defined from the local substrate normal, as shown in Fig. 3(a). The IAD is typically well defined by the peak’s maximum angle, \( \theta_m \), and the full width at half-maximum, \( \theta_w \). For a stationary deposition, the resulting coating microstructure is influenced by these two parameters. The columnar growth angle, \( \varphi \) (which is defined identically to \( \theta \)), is closely aligned (but smaller in magnitude) to \( \theta_w \). Coating porosity is influenced by both \( \theta_w \) and \( \theta_m \) as shadowing of the incident vapor increases with IAD width and incident angle. During substrate rotation, the local IAD constantly changed, and the coating structure depended on the sequence in which atoms were deposited, not simply a time-averaged IAD.

The simulations were performed first using baseline DVD conditions consisting of a chamber pressure of 22 Pa, a pressure ratio of 5.45, and a substrate homologous temperature \( T/T_m = 0.243 \) (where \( T_m \) is the absolute melting temperature of the deposited material, in this case nickel). The effects of varying these three baseline parameters were then systematically explored. When substrate rotation was modeled, the incident atom flux was scaled to simulate a rotation rate of 6 rpm. This was achieved by using the input variables from each orientation for a simulation time of 1.25 s and then advancing to the next orientation. Once simulations were completed, the columnar growth angles were measured by applying a Hough transformation\(^{53} \) to renderings of the simulation microstructure. The pore volume fraction was determined by measuring the fraction of occupied lattice sites in the inner 80% of the coating’s thickness. The outer boundary was excluded to avoid spurious porosity from column tip roughness.

**B. Deposition experiment**

To test the validity of the simulation approach, experimental depositions were performed using the EB-DVD method\(^{2,10} \). Nickel coatings were deposited onto grade 303 stainless steel substrates shaped by wire-cut electric discharge machining. The substrates surface was roughened before deposition by grit blasting. The RMS roughness of the resulting substrates was approximately 2 \( \mu \)m. Both rotated and stationary depositions were performed for approximately 70 min. Rotated substrate depositions were performed at 6 rpm. The coatings were deposited without substrate heating. However, heat radiated from the electron beam’s interaction with the vapor source resulted in a substrate temperature of 150 °C, which corresponds to a homologous temperature, \( T/T_m = 0.243 \); the same as that used during simulations. After deposition, the samples were cross-section, polished, and imaged in a scanning electron microscope (SEM) to determine their thickness and local columnar growth angle.

**III. SIMULATION AND EXPERIMENTAL RESULTS**

**A. Coatings from stationary deposition**

As indicated in Fig. 3(c), two key parameters of an IAD are the location of the distribution’s maximum (\( \theta_m \)) and the distribution’s full width at half maximum (\( \theta_w \)). The variation of both parameters for deposition using the baseline EB-DVD conditions is shown in Fig. 4. The variation in maximum angle along the concave and convex surfaces is shown in Figs. 4(a) and 4(b), respectively. The change in full width at half maximum along the concave and convex surfaces is shown in Figs. 4(c) and 4(d), respectively. The plots show that the IAD varied significantly between line-of-sight regions near the airfoil’s leading edge and the highly shadowed regions found closer to the trailing edge. In near line-of-sight regions (distance from leading edge < 20 mm), the IAD was narrow with \( \theta_m \) close to the incident angle of the carrier gas flow. Deposition in these regions was highly influenced by the carrier gas flow field.

In highly shadowed regions (substrate distance > 20 mm on both surfaces), the IAD was broad with a maximum angle close to the local surface normal. Vapor atoms deposited in this region had undergone multiple scattering collisions with the background gas and made impact with the substrate from a wide range of incident angles, including from directions that were opposite to the flow direction of the carrier gas. Deposition in these regions was weakly correlated with the local carrier gas flow properties. These NLS substrate regions had much lower deposition rates than the line-of-sight areas, with vapor atom arrivals the result of substantial gas phase diffusion transverse to the flow direction.

The kMC simulations were initially performed for a stationary substrate oriented at \( \alpha = 0 \) deg, using the baseline deposition conditions. Figure 5 shows the thickness and structure of coatings that were deposited at six representative locations on the airfoil under these conditions. It is evident that the coating had a significant variation in both its thickness and structure along each surface. Reduced, but significant vapor deposition occurred on NLS regions as shown in an earlier study of the same problem\(^{23} \).

The simulated and experimental coating thickness, columnar growth angle, and pore volume fraction along the entire substrate surface are shown in Fig. 6 for the concave (left column) and convex (right column) surfaces of a
stationary airfoil. The variation in simulated and experimental thickness along the concave and convex surfaces of the airfoil is shown in Figs. 6(a) and 6(b). The thickest coating on each surface was formed at the leading edge, as vapor was quickly depleted (by deposition) from the carrier gas streamlines that traveled closest to the stationary substrate surfaces. The concave surface shows an increased thickness near the trailing edge, a consequence of this section of substrate curving back into less vapor depleted regions of the carrier gas jet stream.

The simulated and experimental columnar growth angles, $\phi$, are plotted versus position on the airfoil in Figs. 6(c) and 6(d) for both surfaces. Near the leading edge of both surfaces, the coating had a feathery appearance due to nucleation of secondary growth columns [Figs. 5(e) and 5(f)]. The primary intercolumnar pores at these leading edge locations were oriented toward the leading edge. However, the magnitude of this angle gradually decreased along the surface, and eventually approached the local surface normal. In NLS regions such as in Figs. 5(a)–5(d), the columnar growth angles were smaller as the highly scattered vapor atoms were deposited with a broad range of incident angles.

Measurement of the columnar growth angle in experimentally deposited coatings gave orientation results with significant scatter, a consequence of the substrate's long wavelength surface roughness, which caused local variation of the surface normal. The estimated standard deviation of the measured angle was 5°. Examination of Fig. 6 shows that the simulation predicted column angles agreed reasonably with experimental values (to within 10° on the concave surface) [Fig. 6(c)] and beyond a distance of ~15 mm from the leading edge [Fig. 6(d)]. However, the simulated growth angles were ~20° higher than the experimentally measured values on the convex surface near the airfoil's leading edge. Recent work has shown that for highly inclined incident angles, the instantaneous IAD experienced at the coating surface after formation of the feathery structure is significantly

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**Fig. 4.** (Color online) DSMC predicted parameters of the IAD along both surfaces of a stationary airfoil oriented at $\alpha = 0^\circ$. Results were calculated for baseline DVD conditions. The shaded regions were not in the line-of-sight of the vapor source.
different to that experienced at the substrate surface during initial deposition. Improved simulation accuracy might be obtained in future simulations by using an IAD defined by the angle with the instantaneous column surface as the coating develops. Fortunately, these large growth angles do not develop on rotated substrates, and as shown below, the simulations were then better behaved.

The columnar inclination angle, $\varphi$, formed on flat substrates by condensation of a collimated, monoangular flux with an incident angle, $\theta$, can often be well fitted by a Tangent rule\textsuperscript{55} given by

$$2 \tan \varphi = \tan (\theta).$$

Using the IAD peak angle, $\theta_m$ for $\theta$, the Tangent rule prediction has been plotted in Figs. 6(c) and 6(d), and correctly predicts that growth columns are tilted in the direction of the incident flux but with a columnar growth angle of smaller magnitude than the incidence angle. The Tangent rule growth column angle was found to agree reasonably with kMC simulations. It has been found that the predictive accuracy of the Tangent rule also decreases as the magnitude of the incidence angle increases beyond 70°.\textsuperscript{56–58} Several more complex empirical and semiempirical approaches have been attempted,\textsuperscript{54,59–61} but no universal empirical approach has been successfully proposed for high incident angle fluxes.

![Diagram of coating microstructures](image)

**Fig. 5.** (Color online) Simulated coating microstructures at six locations on a stationary airfoil substrate. Simulations were performed at baseline DVD conditions. The substrate’s homologous temperature, $T/T_m = 0.243$, and the highest deposition rate shown [at the (f) location] was $2.5 \times 10^{20}$ atoms m$^{-2}$s$^{-1}$. 

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The coating porosity was determined from the kMC simulations as function of location along the substrate surfaces [Figs. 6(e) and 6(f)]. The plots show the total pore fraction, the small length scale intracolumnar porosity, and larger intercolumnar porosity. Along both surfaces, porosity is greatest at the leading edge and gradually decreases along the surface before reaching near-constant values in NLS surface regions. The total porosity variation results from

FIG. 6. (Color online) Comparison between experimental and simulation results for a stationary airfoil (\(\phi = 0^\circ\)). (a) and (b) The simulated and experimental thickness profiles (normalized by the thickness at the origin of the concave surface). (c) and (d) The columnar growth angles along with those predicted by the Tangent rule. (e) and (f) The simulated total pore volume fraction together with the intracolumnar and intercolumnar components of the total porosity.
changes to the intercolumnar porosity, as the width of the intercolumnar pores decreased with distance along the substrate surfaces. To understand these observations, it is helpful to examine the jet flow and vapor atom concentrations near the airfoil.

The flow field behavior, as characterized by the carrier gas streamlines and contours of pressure for this stationary simulated deposition condition, is shown in Fig. 7(a). Figure 8(a) shows the corresponding vapor streamlines and concentration contours. The highest density of vapor particle streamlines terminated near the leading edge of convex side of the airfoil substrate, consistent with the thickness profile predicted by the simulation methodology. This region of highest deposition rate was within the line of sight of the vapor source and depleted the concentration of vapor in the gas jet flow that subsequently passed close to the airfoil surface. However, binary collisions between the vapor and gas jet atoms were able to scatter vapor atoms toward the substrate, resulting in significant (diffusive) coating of the NLS regions of the stationary airfoil.

![Diagram of gas jet streamlines and pressure contours](image)

**Fig. 7.** (Color online) Helium gas jet streamlines and pressure contours at the eight orientations used to simulate deposition onto a rotated substrate. Simulations were performed using baseline DVD conditions.
B. Rotated substrate deposition

The results above indicate that it is not possible to deposit a uniformly thick coating over all surfaces of a stationary airfoil substrate by EB-PVD. Even though gas jet assisted deposition processes result in some deposition onto NLS surfaces, the thickest coatings form on regions within sight of the vapor source. However, rotation of such a substrate during deposition allows all areas of the substrate to spend some time within the line of sight of the vapor source, and results in improved coating uniformity.

The behavior of the gas jet near the substrate varies significantly during substrate rotation. This variation is shown by the carrier gas streamlines and pressure contour plots in Fig. 7 for the baseline DVD simulation conditions. The figure shows that flow remains laminar for all orientations. At orientations where the airfoil’s chord was roughly parallel to the flow direction (\( \alpha = 0^\circ \) and \( 180^\circ \)) [Figs. 7(a) and 7(e)], the streamlines flow past the substrate with modest perturbation. However, isolated regions of stagnation that resulted in an elevated pressure (\( \sim 1.3 \) times the background) above the

Fig. 8. (Color online) Nickel vapor atom streamlines and concentration contour plots at the eight orientations used to simulate deposition on a rotated substrate. Simulations were preformed using baseline DVD conditions.
The variation of gas flow near the airfoil shown in Fig. 7 greatly affected the vapor atom streamlines near the substrate. The average vapor atom trajectories and contour plots of the vapor atom concentration are shown in Fig. 8 for each simulated orientation. The results were also calculated at baseline simulation conditions. When the substrate was oriented in-line with the jet axis (z = 0° and 180°) [Figs. 8(a) and 8(e)], both the convex and concave surfaces received a significant vapor flux. Surface regions closest to the vapor source (the leading edge at z = 0° and trailing edge at z = 180°) received the highest vapor fluxes. Airfoil regions downstream from the leading or trailing edge received a reduced flux because of earlier depletion from the gas jet streamlines by condensation onto the leading or trailing edges.23 When the substrate was oriented perpendicular to the jet axis (z = 90° and 270°) [Figs. 8(c) and 8(g)], the surface facing the vapor source received a much higher vapor flux compared to that on the shadowed surface. At other intermediate substrate orientations [Figs. 8(b), 8(d), 8(f), and 8(h)], significant parts of one surface were in the line-of-sight of the vapor source while others were shadowed, resulting in a strong spatial variation in the local flux incident upon the surface.

The orientation of the substrate also affected the IAD at all locations on the substrate. For example, Fig. 9 shows the IAD at the midpoint of the concave surface for each angle of rotation. When the midpoint of the concave surface was in the line-of-sight of the gas jet origin [Figs. 9(f)–9(h)], the distribution maximum angle was closely correlated with the angle between the local surface normal and the gas jet axis. However, when this midpoint location was in a NLS position, the IAD received a much more isotropic flux [Figs. 9(b) and 9(e)], though in some cases with a still substantial shift in 0m from zero [Fig. 9(a)].

The KMC simulated coatings at six locations on the substrate (the same locations used for stationary deposition in Fig. 5) using baseline deposition conditions are shown in Fig. 10. The variations with location of the coating thickness, the columnar growth angle and the porosity were much reduced compared to the stationary case. As with coatings created by stationary deposition, each protuberance on the substrate acted as a nucleation site for columnar growth. On the concave surface, the growth columns typically extended through the entire coating thickness, and the number density of column tips on the coating’s exterior surface was similar to the density of nucleation sites. Along the convex surface, the coating microstructure was comprised of wedge-shaped columns that increase in width as they grew out from the substrate surface. Many columns intersected with each other during this competitive growth process, and as a result, the coating surface was composed of fewer, wider column tips, each covering several nucleation sites.

SEM micrographs of a nickel coating deposited on a rotated airfoil substrate using a chamber pressure of 22 Pa, a pressure ratio of 5.45, and a substrate temperature T/TM = 0.243 (the same as the simulations above) are shown in Fig. 11 for similar locations to those shown in Fig. 10. The experimental coatings exhibited generally similar trends in coating thickness, and columnar growth angle as the simulations. The experimental coatings also had similar variations of surface morphology to those found on the simulated coatings. Along the concave surface, the growth columns were narrower and neighboring columns typically grew parallel to each other with vertical sides. Along the convex surface, columns were often wider and more fanlike, with neighboring columns often intersecting each other during growth.

Rotation of the substrate greatly improved the uniformity of coating thickness along the concave [Fig. 12(a)] and the convex [Fig. 12(b)] surfaces compared to stationary deposition [Figs. 6(a) and 6(b)]. The experimental coating thickness is also plotted on Figs. 12(a) and 12(b) and was in reasonable agreement with that simulated. Once again, the thickness profiles on both sides were normalized by the thickness at the convex surface’s origin at the leading edge as shown in Fig. 3. The coatings located near the leading and trailing edges were thicker than at the center of the substrate surfaces. It is also evident that the coating on the concave side of the airfoil was thinner than that on the convex surface.

The growth column angle variation with location along the concave and convex substrate surfaces can be seen in Figs. 12(c) and 12(d). Comparison with Figs. 6(c) and 6(d) for the stationary case shows that substrate rotation greatly reduced the average growth angle and angle variation along both surfaces. For much of the substrate, the rotated coating’s growth columns were almost normal to the local substrate surface. The most significant deviations (of 5°–15°) from normal were confined to locations near the leading and trailing edges of the substrate. Agreement between simulated and experimental growth angles was also much improved.

C. Porosity

The intracolumnar pores in the experimentally grown coatings were ~10–100 nm in length while those between the growth columns had widths (intercolumnar gaps) of ~1 μm and a length comparable (in some cases equal) to the coating thickness. The volume fraction of intracolumnar pores was typically independent of the initial roughness of the substrate, whereas the intercolumnar pore volume fraction was very sensitive to the surface topology of the substrate, especially during early stages of deposition when the gap width depended sensitively upon the surface asperity spacing.
The total porosity (and its two constituent types) of a coating simulated using the baseline DVD conditions is shown as a function of location along the concave and convex surfaces of a rotated airfoil in Figs. 12(e) and 12(f). Examination of the figure shows that the total and two components of the pore volume fraction (for a rotated deposition using the baseline conditions) were approximately independent of position along the airfoil surface. However, while the intracolumnar porosity was approximately the same on both the concave and convex surfaces (with a pore fraction of \( \alpha = 0.25 \)) , the intercolumnar component of porosity on the convex surface was almost twice that of the concave surface coating. By comparing Figs. 10(c) and 10(d), it can be seen that this difference resulted from the formation of wider intercolumnar pores on the convex surface of the rotated airfoil. This occurred because of the increased fraction of oblique atom trajectories that impact the convex surface. On the concave surface, the airfoil’s leading edge and trailing end shadowed many of the atoms traveling along these highly inclined trajectories.

Porosity evolution during vapor deposition resulted from flux shadowing in combination with insufficient surface diffusion to replace the local adatom deficit. The surface roughness, and therefore pore fraction of a coating, is consequently temperature and deposition rate dependent since the rate of (thermally activated) surface diffusion is sensitive to

FIG. 9. (Color online) Nickel vapor particle incidence angle distributions used to simulate rotated deposition at the center of the concave side of the airfoil. Simulations were performed using baseline DVD conditions.
the substrate’s temperature during the deposition process. The porosity increased with deposition rate, due to the reduced interval of time available for surface diffusion between atom arrivals. However, coating porosity was less sensitive to deposition rate than to temperature since it has a linear effect on the degree of surface diffusion, while the temperature dependence is exponential [Eq. (1)]. Simulations were performed at homologous temperatures, $T/T_M$ from 0.2
to 0.515 to investigate the effects of temperature on the two components of the total porosity. The simulations were again performed using baseline DVD parameters for a rotated airfoil.

The pore volume fractions midway along the convex airfoil surface are shown in Fig. 13(a) (the trend at the midpoint of the concave surface was nearly identical and therefore not shown). Increasing the substrates temperature resulted in a rapid densification of the growth columns, Fig. 13(b). The intracolumnar pore fraction decreased from \(0.27\) at \(T/T_M = 0.206\) to approximately \(0.12\) at \(T/T_M = 0.515\), consistent with increased surface diffusion during the deposition process. However, the intercolumnar porosity at first increased with increasing temperature before reaching a maximum at \(T/T_M = 0.36\) and then decreasing at higher temperatures. This was a result of a gradual increase in the width of the intercolumnar pores until \(T/T_M = 0.36\), Fig. 13(c). Further increases in temperature resulted in more surface diffusion, the sintering of some growth columns and a reduction in the width of intercolumnar pores along the substrate surface, Fig. 14(d). The microstructure variation with increasing temperature was consistent with a transition from zone I to zone II of the Movchan, Demchishin, and Thornton Structure Zone Model.62,63

IV. PRESSURE AND JET FLOW EFFECTS

The results above show that the local thickness, growth column inclination, and pore volume fraction within a...
coating deposited on a rotated, airfoil shaped substrate are controlled by many parameters. The deposition temperature, vapor atom IAD (determined by vapor phase scattering, which in turn depends upon the pressure, flow field, and scattering coefficients of colliding species), and deposition rate all significantly influence the structure, and therefore thermophysical and mechanical properties of the coatings. In order to investigate the effects of process conditions,
Simulations were performed at a broad range of conditions including a low chamber pressure of 0.015 Pa and a pressure ratio of unity (typical of a high-vacuum EB-PVD coating process). Additional simulations at chamber pressures of 1, 16, and 45 Pa (using a pressure ratio of 5) typically accessible by an EB-DVD process were performed. Simulations using the much higher chamber pressure (of 100 Pa with a pressure ratio of 5) typical of a PS-PVD process were also performed. A substrate temperature, $T/T_M = 0.243$, an evaporation rate of $8.8 \times 10^{20}$ atoms m$^{-2}$s$^{-1}$, and a rotation rate of 6 rpm were used for all simulations. The effect of the chamber pressure upon the incident vapor flux (closely related to local coating thickness), growth column orientation, and pore volume fraction were all investigated.

Simulated microstructures calculated for high-vacuum EB-PVD conditions are shown in Fig. 14 at identical locations to those in similar figures above. They show that the coating thickness uniformity was significantly better than for the high-pressure EB-DVD conditions. However, increased variation of coating porosity was evident around the substrate. The porosity was highest in regions that received a significant amount of flux from oblique incident angles [Figs. 14(b) and 14(d)–14(f)]. In these regions, the intercolumnar gaps were wide, and competitive growth between neighboring columns was found. In the regions near the trailing edge on the concave surface [Figs. 14(a) and 14(c)], the microstructures were much denser with narrow intercolumnar pores. In these regions, oblique incident atom trajectories were shadowed by the airfoil’s edges, and most atoms were deposited from trajectories oriented near the surface normal.

A. Coating thickness variations

The ratio of the number of vapor atoms deposited in each (~1 mm wide) simulation region to the total number of evaporated atoms (the deposition efficiency) is a key factor contributing to the local thickness of a coating. This local deposition efficiency is plotted as a function of the position on the two surfaces of a rotated airfoil in Figs. 15(a) and 15(b), and used as a surrogate for normalized coating thickness. Deposition under the lowest pressure (high vacuum EB-PVD) conditions resulted in coatings of an almost constant thickness along each surface. Comparison of Figs. 15(a) and 15(b) for this case also shows that the local deposition efficiency on the convex and concave sides was also...
identical, and varied little with position. However, the vapor flux incident on each 1 mm wide region was slightly less than $10^{-3}$ of the emitted vapor. When integrated over the 40, 1 mm-wide regions, this resulted in a deposition efficiency of 0.034 for the concave surface and 0.039 for the convex side. This deposition efficiency of $\sim 4\%$ of the evaporated flux was due to lateral expansion of the vapor plume during propagation from the source, and would decrease further with increasing source to airfoil (standoff) distance. Increasing the chamber pressure to 1 Pa began to laterally confine the vapor plume, and increased the fraction of flux deposited on both surfaces, but with that deposited on the convex surface rising more rapidly. As the pressure was further increased, the deposition efficiency at first increased on both sides of the airfoil, but then reached a maximum before falling with further pressure increases. This drop in local efficiency was most dramatic on the concave surface, where the flux eventually decreased below that of the lowest pressure depositions. This phenomenon contributed to the development of a substantial difference in coating thicknesses on the two surfaces. Increasing the chamber pressure also increased the variation in deposited flux with location along each surface; the maxima in incident flux occurred at the ends of the airfoil, and increased relative to the minima at midpoint locations.

The effects of the chamber pressure and pressure ratio on the fraction of vapor that was deposited at the midpoints of the concave and convex surfaces can be seen in Figs. 16(a) and 16(b). An increase in pressure to 10 Pa was accompanied by a substantial increase in the fraction of the evaporated flux deposited at the midpoints.
flux that condensed on the substrate. This increase in local deposition efficiency reached a maximum at a chamber pressure of \( \sim 5 \) Pa, and was relatively insensitive to the pressure ratio. Figure 16(c) shows the variation of the ratio of the concave to convex surface midpoint coating thicknesses for the same conditions. The asymmetry in coating thickness between concave and convex surfaces was small while the chamber pressure remained below about 1 Pa. Above this
pressure, the thickness ratio dropped rapidly as the pressure was increased. Beyond a chamber pressure of 10 Pa, the deposition efficiency began to decrease, and both the deposition efficiency and concave/convex thickness ratio quickly decreased.

The trend in local deposition efficiency at the surface midpoints was quite similar to that for the overall deposition efficiency determined by integration of the local efficiency distribution over the entire substrate surface. Table I shows the ratio of the number of deposited atoms to the number evaporated along the concave, convex, leading edge, and entire substrate surface at several chamber pressures all at a pressure ratio of 5. Deposition efficiency along all of the surfaces increased with chamber pressure until it reached a maximum at 10 Pa of about 18.3% (compared with 7.6% at a pressure of 0.01 Pa). The total deposition efficiencies at 0.01 and 100 Pa were quite similar. While the 0.01 Pa efficiency of 0.01 Pa was low due gas phase spreading, at high pressures, the low efficiency resulted from short diffusion distances of the vapor transverse to the vapor streamlines. This slow transverse diffusion resulted in many vapor atoms flowing past the substrate without impacting and condensing upon its surface.

Coatings deposited at a chamber pressure typical of EB-DVD conditions possessed thickness variations over the airfoil surface quite different to those deposited under high-vacuum EB-PVD conditions (Figs. 15 and 16). The differences were a result of two effects of the carrier gas jet: Deposition from gas streamlines close to a substrate edge and the creation of a wall jet for substrate orientations perpendicular to the gas jet. The influence of both effects increased with chamber pressure. Deposition from gas flow around a substrate edge was most significant when the airfoil was oriented with the leading edge nearest the vapor source, but slightly inclined, as in Fig. 8(f). Under high-vacuum (0.015 Pa) conditions, no vapor was deposited onto the shadowed surface region (in this case, the convex surface). Although there is a significant concentration of vapor just above this surface region, no scattering collisions occurred to knock atoms from their straight-line trajectories, and onto the substrate surface. However, these collisions were present during DVD-like deposition, and significant amounts of vapor were deposited from the gas jet flow around the airfoil’s edges. This contributed to thicker coatings near the airfoil edges under DVD conditions. The frequency of these collisions increased with chamber pressure, resulting in a higher deposition rate onto the shadowed surface.

Deposition onto the substrate ends was also enhanced when the substrate was oriented transverse to the gas jet (\(\varphi = 0^\circ\) and 90°). At higher chamber pressures, the gas jet...
sensed the substrate and flowed around it. This created a wall jet\(^{14}\) that transported incident vapor parallel to the substrate surface, decreasing the amount that reached the substrate’s midpoint, and increasing the amount able to impact near the substrates ends. As the chamber pressure increased, multiple scattering collisions in the boundary flow made it increasingly less likely for vapor to reach the substrate surface, and the overall deposition efficiency decreased. The low-pressure used in PVD deposition, resulted in the incident vapor plume being uninfluenced by the substrate’s orientation, resulting in a uniform deposition rate along the entire line-of-sight region of surface. The PVD profiles have slight rises near the center of each surface, as these regions remain in the line-of-sight of the vapor source for a longer duration during rotated substrate deposition.

**B. Growth column orientation**

The variation in columnar growth angle, \(\phi\), along the convex and concave surfaces is shown in Figs. 15(c) and 15(d). Deposition at the lowest chamber pressure (0.015 Pa) resulted in a substantial (\(\sim 20^\circ\)) variation of the growth column orientation angle along the concave and convex surfaces. Figure 15(d) shows that on the concave surface, columns grown near the leading edge at the high-vacuum pressure of 0.015 Pa were oriented away from the leading edge and gradually transitioned to perpendicular growth with increase in distance from the leading edge. On the convex surface near the leading edge, the high-vacuum EB-PVD growth column orientation angle was about 7\(^\circ\) away from the leading edge. Fig. 15(d), similar to that reported for EB-PVD coatings by Darolia.\(^{11}\) At the trailing end of the convex surface coating, the growth column angle was \(\sim 12^\circ\), with the columns sloped toward the leading edge. Under the lowest pressure deposition condition, the column angle on the convex surface changed progressively between these two limits so that near the midpoint of the coating, the columns were oriented normal to the local substrate surface.

The use of a gas jet with chamber pressures up to 100 Pa led to significant changes to the angle of the growth columns. (It is noted that multibody collisions at high pressures are likely to have resulted in nanoparticle formation. This effect has not been addressed in the simulations.) On the convex surface, coatings grown at higher pressures [Fig. 15(d)] formed columns that were oriented very nearly perpendicular to the surface except for regions within \(\sim 5 \text{ mm}\) of the convex origin and \(\sim 10 \text{ mm}\) of the trailing end. Between \(\sim 5\) and 35 mm from the convex origin, the columns were only slightly tilted (by about 5\(^\circ\)) toward the leading edge. Near the trailing edge, the growth angle was more severely tilted toward the leading edge, reaching maximum angle of 10\(^\circ\)–20\(^\circ\). On the concave surface [Fig. 15(c)], the use of a higher chamber pressure resulted in column growth in the opposite orientation from those grown at high vacuum between the leading edge and surface midpoint (i.e., they oriented toward the leading edge). From the midpoint to trailing edge, the coatings grew at an angle within 5\(^\circ\) of the local surface. Columns grown at 1 Pa show a different pattern to those deposited at other conditions. These columns tended to point toward the nearest substrate edge. Unlike the high vacuum (0.015 Pa) case, vapor experiences scattering collisions at this pressure. However, their frequency is insufficient to cause significant diffusion transverse to, or against the direction of the gas jet. Atoms therefore arrive at the surface from trajectories closely aligned to the local gas jet flow.

The columnar growth angle was significantly affected by the introduction of a gas jet into the deposition process. For high-vacuum EB-PVD conditions, growth angles were aligned to the least-shadowed directions, while the introduction of a carrier gas causes the columns to tilt toward the directions with the most incident gas flow. This is most apparent near the leading edge along the concave surface [Fig. 15(c)]. Under high-vacuum EB-PVD-like conditions, this surface area is shadowed by the leading edge at many orientations. Thus, the majority of vapor arrives from the trailing edge direction, and the columns were tilted toward it. With introduction of a carrier gas, a significant amount of vapor flows around the leading edge and deposits on the nearby substrate surface. Vapor arriving from the trailing edge’s direction must first flow along the concave surface, and is likely to deposit before reaching the leading edge. This resulted in columns that were oriented toward the leading edge.

**C. Porosity**

The coating porosity is shown for both airfoil surfaces in Figs. 15(e) and 15(f). Deposition at the lowest pressure led to a pore volume fraction of \(\sim 0.4\) at the leading edge of both the convex and concave surfaces. This then progressively decreased toward the trailing edge of the coatings. This decrease occurred more rapidly with distance along the concave surface, and fell to a lower value (\(\sim 0.2\)) than on the convex side. Coatings deposited at chamber pressures of 16 Pa and above had a nearly uniform pore volume fraction of \(\sim 0.27\) on both sides of the airfoil. The porosity varied little with position along either airfoil surface. The porosity near the leading edge of the concave side initially decreased rapidly with pressure, but for pressures above 1 Pa, was independent of pressure. However, beyond a distance of the \(\sim 25 \text{ mm}\) from the leading edge, the porosity of the high-vacuum EB-PVD condition coating decreased below that of the high-pressure coatings. On the convex surface, increasing the pressure above 0.015 Pa resulted in a decrease in porosity. Above 1 Pa, the porosity continued to decrease with increasing pressure, but at a much slower rate. In this higher-pressure regime, the porosity was substantially less than that of a high-vacuum EB-PVD coating.

**V. LOCAL COATING OPTIMIZATION**

The simulations above have revealed that the thickness of a coating and its microstructure vary with position on an airfoil surface in a manner that is sensitive to the deposition conditions. Usually, these deposition conditions are fixed during the application of the coating. However, modifying the evaporation rate (by modulating the electron beam power), the dwell time at each airfoil orientation (with a
variable rotation rate), or the standoff distance (by eccentric substrate rotation), could enable the deposition of coatings whose thickness and microstructure were locally controlled. This might provide a means to form coatings that provided protection against the most life limiting threat to each specific region of the substrate’s surface. Rapidly varied parameters of the jet flow (pressure ratio or gas composition) could also be used for a similar purpose.

To investigate such an optimization, the dwell time at specific angles of airfoil rotation were varied with the objective of eliminating the difference in coating thickness between the concave and convex surfaces of an airfoil substrate. The simulated incident vapor fluxes at the eight stationary orientations used to simulate a rotation were each assigned a variable weight coefficient. The total flux incident on each surface region, \( j \), was then given by

\[
j = \sum_{m=1}^{8} a_m f_m,
\]

where \( f_m \) is the incident flux at each orientation and \( a_m \) is the orientation coefficient to be determined. The minimize function in the Scipy Python suite was then used to determine the \( a_m \) resulting in the minimum total flux difference between the two airfoil surfaces expressed by

\[
\Delta J = \sum_{n=1}^{40} |j_{1,n} - j_{2,n}|,
\]

where \( j_{1,n} \) and \( j_{2,n} \) are the total flux at each of the \( n \) substrate regions along the concave and convex surfaces (\( n = 1 \rightarrow 40 \) surface regions). The summation began at the convex and concave surface origins (near the leading edge) and proceeded along each surface toward the trailing edge (increasing \( n \)). The coefficients were constrained so that each deposition had a maximum/minimum rotation rate ratio of 8 (the maximum allowable dwell coefficient was eight times larger than the minimum).

The resulting coatings obtained using the optimized rotation coefficients exhibited less than a 10% difference in flux (and thickness for a nonvarying porosity) between the midpoint on their concave and convex surfaces, and combinations of coefficients could be found at all chamber pressures that maintained this level of resulting uniformity. The optimized coefficients are presented in Table II for depositions at 0.01, 2.625, 16, 45, and 100 Pa using a pressure ratio of 5 (except at 0.01 Pa where the ratio was 1). At the two lowest pressures, the coefficients varied only slightly from the coefficient for constant rotation (of 0.125). However, as the chamber pressure was increased, less uniform rotation patterns were required to achieve uniformity.

The total amount of flux incident on a substrate at each orientation can also be manipulated by adjusting the evaporation rate of the material source. In the current optimization design, this is mathematically equivalent to varying the rotation rate. In either case, a coefficient is used to adjust the deposition rate along the entire substrate surface.

\[
j_{1T}(x) = 1 - 0.027x.
\]

Along the convex surface, it was defined as

\[
j_{2T}(x) = \begin{cases} 
1 - 0.041x, & x \leq 27, \\
0.1, & x > 27,
\end{cases}
\]
where $x$ was the distance from each surface origin in millimeters. The difference between the target and simulated flux profiles was then minimized using

$$
\Delta J = |j_{\text{Leading}} - 1| + \sum_{n=1}^{40} |(j_{1,n} - j_{1T}(\Delta n)) + (j_{2,n} - j_{2T}(\Delta n))|,
$$

where $\Delta x$ is the distance between simulation surface regions (1.13 and 1.07 mm for the convex and concave surfaces, respectively) and $j_{\text{Leading}}$ is $j$ at the single leading edge surface region. During optimization the rotation rate was bounded between 0.5 and 10 times the constant rotation rate value, while the normalized evaporation rate was allowed to vary by no more than a factor of 5 (from 0.2 to 1.0), consistent with experimental observations.$^{18}$ The optimization

![Flux profile schematic](image_url)

![0.015 Pa target and optimized flux profiles](image_url)

![22 Pa target and optimized flux profiles](image_url)

![0.015 Pa optimized rotation pattern and evaporation rate](image_url)

![22 Pa optimized rotation pattern and evaporation rate](image_url)

Fig. 17. (Color online) Optimization-generated thickness profiles at two deposition conditions. [(b) and (c)] The objective and optimization procedure generated flux profiles incident upon the convex and concave surfaces. [(d) and (e)] The dwell fraction and evaporation rate sequences that came closest to achieving the objective profiles. A chamber pressure of 0.015 Pa and pressure ratio of 1.0 was used in (b) and (e) while a chamber pressure of 22 Pa and pressure ratio of 5.45 was used for (c) and (e). The ability to match the desired flux profile decreased with increasing chamber pressure.
was performed at a chamber pressure of 0.015 (high-vacuum EB-PVD conditions).

The resulting optimized flux profiles are shown in Fig. 17(b) along with their respective target flux profiles. The optimized profiles achieved the flux objectives fairly well, especially near the leading edge. However, both surfaces exceeded the thickness objective as the trailing edge was approached. The rotation pattern and evaporation rate variation used to obtain the optimized coating are shown in Fig. 17(d). Wider bars indicate a larger dwell fraction, while taller bars indicate a higher evaporation rate. The plot shows that the majority of deposition flux was concentrated at 45° and 225° orientations. Significant additional deposition occurred at the 0° orientation. Both the evaporation rate and the dwell fraction were minimized for all other orientations. Finally, it is noted that the ability of the optimization process to meet this thickness objective gradually decreased with increasing chamber pressure. This is shown in Figs. 17(c) and 17(e) for chamber pressures of 22 Pa and pressure ratio of 5.45. The resulting flux profiles poorly matched the objective profiles due to a rapid decrease in flux from the leading edge and an increased flux near the trailing edge on both surfaces. The use of more simulated substrate orientations (beyond the eight used here) might improve the optimization at high pressures by providing additional variable coefficients.

VI. CONCLUSION

DSMC simulations to analyze vapor phase transport in a rarefied, gas jet assisted deposition process have been combined with a kMC method to enable prediction of the thickness and structure of a porous coating applied to an airfoil. Coatings applied to substrates that were not rotated during deposition were found to have nonuniform thickness and contained acute growth column inclination angles. Rotation of the substrate was found to result in uniform thickness coatings grown under EB-PVD like conditions, but the coating microstructure varied substantially with location. Introducing a gas jet and raising the pressure during deposition led to the growth of coatings whose growth columns were almost all oriented perpendicular to the airfoil surface. However, under constant rate rotation, the thickness of the coating on the concave surface was only a half that on the convex surface. The simulation method has shown that by modulating the rate of evaporation, it is possible to deposit coatings with both uniform thickness and the majority of the growth columns oriented normal to the local airfoil surface. Dynamic modulation of deposition also offers opportunities to “tune” the local coating thickness and structure to potentially better resist the damage mechanisms associated with specific locations on the airfoil surface.

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