THIN FILM DEPOSITION USING RAREFIED GAS JET

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Abstract: The rarefied gas jet of Aluminium is studied at Mach number *Ma = (U_j / \sqrt{kb T_j / m})* in the range *0.01 < Ma < 2*, and Knudsen number *Kn = (1/(\sqrt(2) \pi d^2 n_d H)* in the range *0.01 < Kn < 15*, using two-dimensional (2D) Direct Simulation Monte Carlo (DSMC) simulations [1, 2, 3, 4, 5, 6], to understand the flow phenomena and deposition mechanisms in a physical vapor deposition (PVD) process. Here, *H* is the characteristic dimension, *U_j* and *T_j* are the jet velocity and temperature, *n_d* is the number density of the jet, *m* and *d* are the molecular mass and diameter, and *kb* is the Boltzmann constant.

In 2D DSMC simulations we find that the jet velocities both before and after the substrate reduces as the Knudsen number is decreased (increasing the number density). As Knudsen number decreases, the gas jet became much more concentrated on the centerline, and the gas depleted region behind the substrate (flat plate) decreases due to the decrease in the streamwise velocity and hence increased residence time. The decreased Knudsen number (smaller mean free path) confined the gas jet to the centerline by reducing the rate of lateral diffusion. Increasing the jet Mach number also leads to a narrowing of the gas jet. This results from the higher jet velocity, and hence higher momentum of the gas jet along the streamwise direction, which reduces the transverse scattering effects of collisions. We examine the jet streamlines in the vicinity of the substrate by determining the average trajectories along the simulation cells.

The variation of the local fluxes along the streamwise direction away from the jet are studied. The qualitative nature of the local flux at high Mach number *(Ma = 2)* is similar to those in the incompressible limit *(Ma = 0.01)*. These include the initial fast decay, then slow variation, and finally rapid decay near the substrate. However, there are important differences. The amplitudes of the local flux increase as the Mach number increases. The flux decreases by an order of magnitude before reaching to the substrate. There is significant velocity and temperature slip ((Pradhan & Kumaran, *J. Fluid Mech*-2011); (Kumaran & Pradhan, *J. Fluid Mech*-2014)) at the solid surfaces of the substrate. In a compressible rarefied jet flow, we determine the local flux deposited on the substrate surface with the thermal accommodation coefficient equal to 1. The gas atom concentration in the jet slowly decreases due to the infrequent scattering, and deposition occurs due to the reduced diffusion distance. The gas flux profile at the front and rear surfaces of the substrate is determined, and show significant dependence upon the Knudsen number.

An important finding is that the capture width (cross-section of the gas jet deposited on the substrate) is symmetric around the centerline of the substrate, and decreases with increased Mach number due to an increase in the momentum of the gas molecules. DSMC simulation results reveals that at low Knudsen number *((Kn = 0.01);* shorter mean free paths), the atoms experience more collisions, which direct them toward the substrate. However, the atoms also move with lower momentum at low Mach number, which allows scattering collisions to rapidly direct the atoms to the substrate. At high Knudsen number *((Kn = 15);* longer mean free paths), the atoms travel greater distances without depositing onto the substrate. Changing the Mach number influences the flux profile by controlling the momentum of the incident gas atoms. At high Mach number *(Ma = 2)*, the gas atoms have large momentums, which increases the distance atoms traveled before depositing onto the substrate. A very small Mach number *(Ma = 0.01)* resulted in atoms depositing quickly near the centerline of the substrate.

Keywords: Thin film deposition, Rarefied gas jet, DSMC simulations.

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DSMC Simulation results:

