

Feature-scale conformality of atomic layer deposition from continuum to free molecular flow: how Knudsen number influences thickness profile characteristics

Jorge A. Velasco,¹ Christine Gonsalves,¹ Gizem Ersavas Isitman,² Jihong Yim,¹ Emma Verkama,¹ Daulet Izbassarov,² Ville Vuorinen,² Riikka L. Puurunen¹

¹ Aalto University, School of Chemical Engineering, Department of Chemical and Metallurgical Engineering,

² Aalto University, School of Engineering, Department of Mechanical Engineering

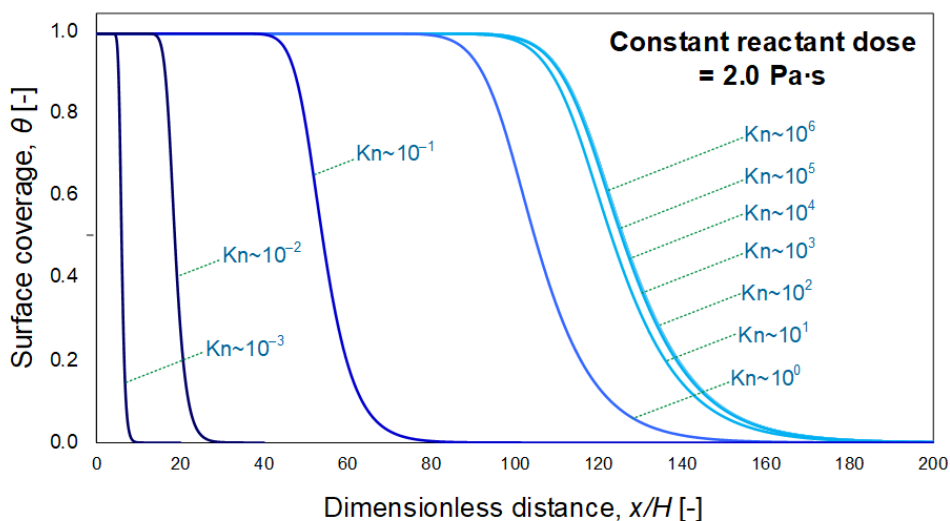


Figure 1: Surface coverage (θ) vs. dimensionless distance (x/H), simulated with the 1-dimensional diffusion-reaction model [1,2] for a constant dose (dose = $p_A t$) at different flow regimes (Knudsen numbers). Different Knudsen numbers were obtained by varying the channel height H (10^{-7} to 10^{-5} m) and initial partial pressure of Reactant A p_{A0} (10^{-3} to 10^5 Pa). To have the dose constant, the ALD pulse time t_1 was varied between 2×10^3 and 2×10^{-4} s. Parameters that were kept constant: $T = 250$ °C, $p_i = 4 \times p_{A0}$, $d_A = 5.91 \times 10^{-10}$ m, $d_l = 3.74 \times 10^{-10}$ m, $M_A = 0.075$ kg/mol, $M_l = 0.028$ kg/mol, $P_d = 10^{-5}$, $c = 10^{-2}$, $q = 4 \times 10^{18}$ m⁻², $N = 1$.

References

[1] M. Ylilammi, O. Ylivaara, and R.L. Puurunen, J. Appl. Phys., 123, 205301, (2018).

<https://doi.org/10.1063/1.5028178>

[2] J. Yim and E. Verkama et al., Phys. Chem. Chem. Phys., in press (2022),

<https://doi.org/10.1039/D1CP04758B>