

Simulated Conformality of ALD Growth Inside Lateral HAR Channels: Comparison Between a Diffusion–Reaction Model and a Ballistic Transport–Reaction Model

Jänis Järvillehto,¹ Jorge A. Velasco,¹ Jihong Yim,¹ Christine Gonsalves¹ and Riikka L. Puurunen¹

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

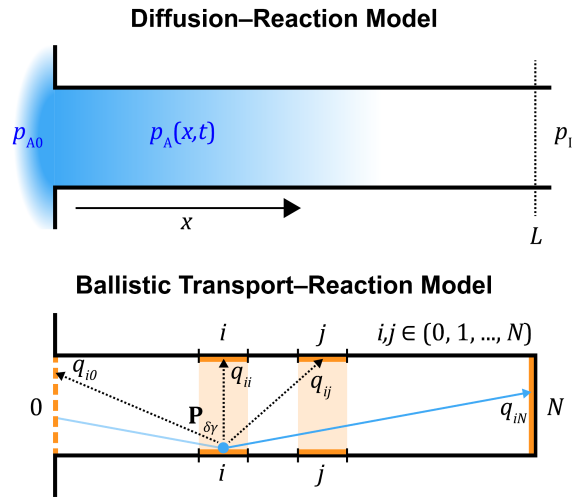


Figure 1. Simplified schematic depicting how the models treat particle transport inside the lateral high-aspect-ratio channel. The diffusion–reaction model [1,2] (upper) uses the diffusion equation to determine the partial pressure of the reactant, while the ballistic transport–reaction model [3,4] (lower) calculates reactant fluxes between discretization sites using a probability matrix based on the channel geometry.

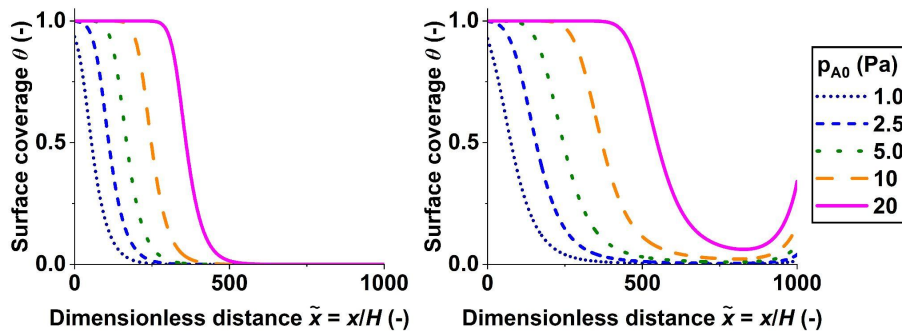


Figure 2. Saturation profiles showing the evolution of the surface coverage with penetration into the channel in the diffusion–reaction model [1,2] (left) and the ballistic transport–reaction model [3,4] (right). The initial partial pressure of the reactant was varied as indicated in the legend, while the other simulation parameters were as follows: $T = 573.15$ K, $p_1 = 0$ Pa, $M_A = 0.1$ kg/mol, $M_l = 0.028$ kg/mol, $M_{\text{film}} = 0.05$ kg/mol, $H = 0.5$ μm , $W = 0.01$ m, $L = 500$ μm , $t_{\text{end}} = 1$ s, $c = 0.001$, $P_d = 0.0001$, $q = 4$ nm^{-2} , $s_0 = 0.25$ nm^2 , $\rho = 3500$ kg/m^3 , $b_A = 1$, $b_{\text{film}} = 1$, $d_A = 0.6$ nm, $d_l = 0.4$ nm, $\Phi_p = 2$ and $\Phi_s = 4$.

References

- [1] M. Ylilammi et al., J. Appl. Phys. 123 (2018) 205301.
- [2] J. Yim and E. Verkama et al., Phys. Chem. Chem. Phys. 24 (2022) 8645–8660.
- [3] A. Yanguas-Gil and J.W. Elam, Theor. Chem. Acc. 133 (2014) 1465.
- [4] A. Yanguas-Gil and J.W. Elam, (2013) <https://github.com/alddsim/machball>, accessed Feb 13 2023.