Diffusion–reaction modeling for atomic layer deposition on spheres: comparison with experimental data

Niko Heikkinen, Jihong Yim, Jänis Järvilehto, Saeed Saedy, P. Brüner, T. Grehl, Eero Haimi, Jorge Velasco, Christine Gonsalves, J. Ruud van Ommen, Juha Lehtonen, Riikka L. Puurunen

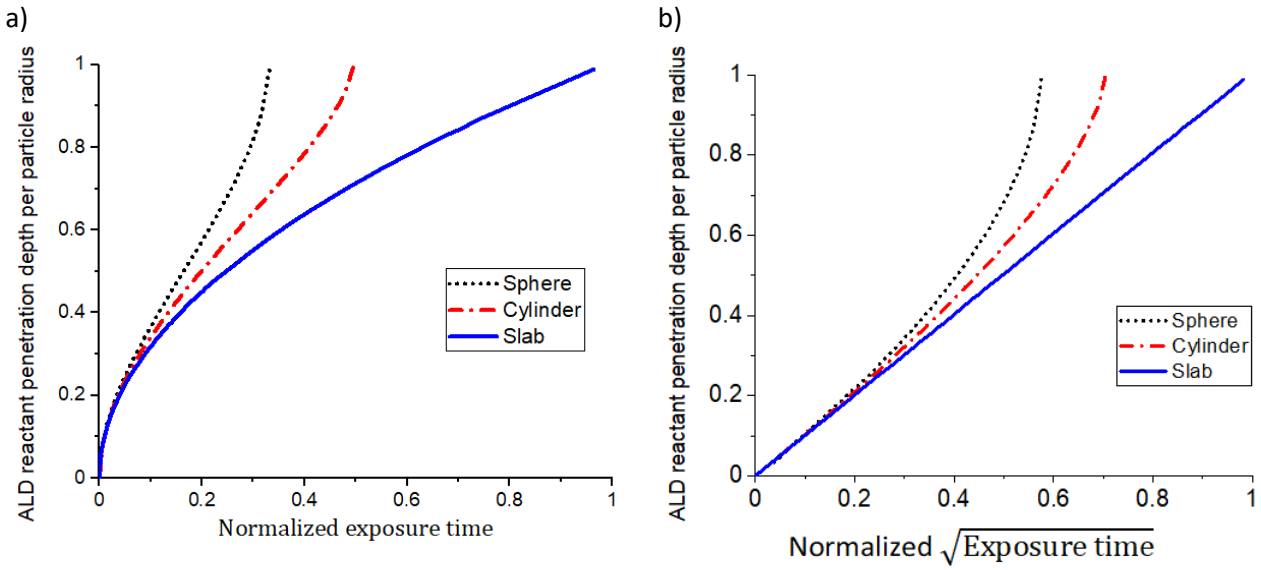

Figure 1, ALD reactant penetration depth into a porous particle. normalized by the particle radius, for three different geometries of slab (porous plate-type structure), cylinder and sphere: (a) as a function of normalized exposure time and (b) as a function of square root of the exposure time. Spherical and cylindrical particles require only ~0.3-0.5 of the exposure time with compared to slab-type particles.

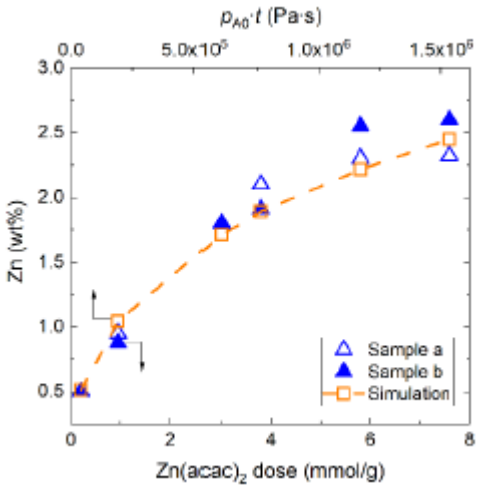

Figure 2. Average zinc loading (wt%) from ZnO/alumina with a particle size of 1.0 mm (Samples a and b) measured via ICP-OES and simulated using a diffusion–reaction model adapted for porous spheres. The Zn(acac)$_2$ dose (mmol/g) and the simulation exposure $p_{A0} \cdot t$ (Pa·s), having the corresponding ratios with respect to the experimental dose, were varied. Parameters used for simulations: R = 0.5 mm, ε = 0.2, τ = 4, d = 9.2 × 10^{-9} m, S = 158 m^2 g^{-1}, V_p = 5.4 × 10^{-7} m^3 g^{-1}, T = 473 K, MA = 263.61 g mol^{-1}, σ = 2 × 10^{18} m^{-2}, n_A = 1.84 × 10^{22} m^{-3}, p_{A0} = 120 Pa, and c = 0.01.