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Conformality of atomic layer deposition analysed via experiments and modelling: case study of zinc oxide for catalytic applications

Title of the doctoral thesis	Conformality of atomic layer deposition analysed via experiments and modelling: case study of zinc oxide for catalytic applications
Content of the doctoral thesis	Atomic layer deposition (ALD) is a precise coating technique based on sequential self-terminating chemisorption reactions on solid supports using at least two different gaseous reactants. The unparalleled ALD conformality and sub-nanometer control over coating thickness make ALD useful across different industries, including semiconductor manufacturing, protective coatings, optoelectronics, energy storage, solar cells, and catalysis. However, studies have shown the necessity of optimizing processes to ensure ALD conformality, especially on high-aspect-ratio structures. This thesis work aims to demonstrate the potential of zinc acetylacetonate as an ALD reactant for adding ZnO on mesoporous particles, with a focus on catalyst preparation, and to explore the effects of various process parameters on ALD conformality, using experimental and diffusion–reaction modelling. An archetypical trimethylaluminum-water ALD process was used as a test vehicle on lateral high-aspect-ratio channels for conformality analysis. The reaction of zinc acetylacetonate on the oxide particles showed self-terminating behaviour, with approximately two zinc atoms deposited per square nanometer after one ALD cycle. The ZnO addition to the copper-on-zirconia catalyst promoted the hydrogenation of carbon dioxide into methanol the most compared to other copper-after-zinc or copper-only catalysts. Fingerprint ALD thickness profile characteristics were obtained in a free molecular flow regime when the channel filling with ALD film was less than 5%. This thesis bridges the gap between ALD conformality on high-surface-area supports and its use in catalyst preparation. The presented ZnO ALD process on porous particles using zinc acetylacetonate was a novel approach, expanding available precursors. The presented discussion and results highlight the cruciality of the optimization of the ALD process and thorough characterization to ensure ALD conformality on high-surface-area structures.
Field of the doctoral thesis	Chemical Engineering
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Opponent(s)	Professor Christophe Detavernier, Ghent University, Belgium
Custos	Professor Riikka L. Puurunen, Aalto University School of Chemical Engineering
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Keywords	ALD, conformality, ZnO ALD, high-aspect-ratio, coatings, diffusion–reaction modelling

Väitöskirja on julkisesti nähtävillä osoitteessa https://aaltodoc.aalto.fi/doc_public/eonly/riiputus/?lang=fi