Final Report Summary - COCOON (Conformal coating of nanoporous materials)

CONTEXT - Nanoporous structures are used for application in catalysis, molecular separation, fuel cells, dye sensitized solar cells etc. Given the near molecular size of the porous network, it is challenging to modify the interior surface of the pores after the nanoporous material has been synthesized.

THE PROPOSAL - Atomic Layer Deposition (ALD) is envisioned for creating catalytically active sites and for controlling the pore size distribution in nanoporous materials. ALD is a self-limited growth method that is characterized by alternating exposure of the growing film to precursor vapors, resulting in the sequential deposition of (sub)monolayers.

KEY RESULTS - The following key achievements have been accomplished:

Development of novel in situ methodologies to study ALD in nanoporous materials - Synchrotron based x-ray fluorescence (XRF) and grazing incidence small angle x-ray scattering (GISAXS), and lab based ellipsometric porosimetry (EP) have been demonstrated to be excellent in situ methods for monitoring ALD processes in nanoporous materials. The element-specific XRF technique allows to identify and to quantify the amount of material that was deposited into the pores, while GISAXS and EP are powerful techniques for monitoring the reduction in porosity and average pore size during ALD.

Demonstration of pore size engineering by ALD - We have demonstrated controlled filling of nanopores using ALD. Thin mesoporous films with an average pore size between 4 – 12 nm were selected as model systems, and the in-situ XRF, EP and GISAXS techniques were used to monitor the density and porosity of the porous film during subsequent ALD cycles. ALD deposition inside the pores remained possible up to the exact point where the remaining entrance window to the pore had shrunk down to the size of the precursor molecules that were used for ALD deposition. At that point, the precursor molecules could no longer enter into the porous structure, and subsequent ALD cycles only resulted in coating of the external surface. This illustrates the potential of ALD for designing molecular filters.

Demonstration of the potential of ALD for creating catalytic sites in nanopores - We have managed to create catalytic sites in nanoporous thin films and powders, and have explored various possible applications of ALD-activated porous materials. In collaboration with catalysis groups, we have demonstrated that ALD deposited Al, Ti and V sites can be used for catalyzing hydrocracking and epoxidation reactions. ALD deposited TiO2 was demonstrated as a promising photocatalyst. In collaboration with a photonics group, we demonstrated that ALD based functionalization of a nanoporous thin film with acid sites can be used for building a novel type of NH3 gas sensor.

CONCLUSION - Due to its conformal nature, ALD proves an attractive technique for tailoring nanoporous materials, as both the pore size and the composition of the pore wall material can be tuned with atomic level precision.