

ALD Applications

Room 116-118 - Session AA3-WeA

Functional Film Application

Moderator: Han-Bo-Ram Lee, Incheon National University

4:00pm **AA3-WeA-11 Catalyst Synthesis and Modification via Atomic Layer Deposition: From Supported Metal Catalysts to Complex Systems, Mar Piernavieja Hermida, R Naumann d'Alnoncourt, K Knemeyer, Technische Universität Berlin, Germany; V Stempel, BASF SE, Process Research and Chemical Engineering; A Trunschke, R Schlögl, Fritz Haber Institute of the Max Planck Society, Germany; M Driess, Technische Universität Berlin, Germany; F Rosowski, BASF SE, Germany**

Even though microelectronics has been one of the major adopters of atomic layer deposition (ALD) during the past 20 years, many other applications such as synthesis of battery materials, fuel cells or catalysis have been of increasing interest. A recent review from Junling Lu, Jeffrey W. Elam and Peter C. Stair summarizes the literature reports in the field of catalysis [1]. The vast majority of the cited contributions involve supported metal nanoparticle catalysts. Although in a lesser magnitude, metal oxides have been used as well due to their unique properties.

Our main focus lies on catalysts used for selective oxidation reactions, typically consisting of mixed metal oxides or phosphates. We aim to modify properties of bulk catalysts by changing the catalysts surface via ALD or using ALD for bottom up synthesis of complex systems as mixed metal phosphates or oxides on suitable supports. Thus, our main application of ALD is deposition in a submonolayer regime or deposition of very thin films (< 1 nm) rather than deposition of metal nanoparticles. A small number of ALD cycles can lead to homogeneous coverage of a catalyst surface with adatoms, leading to a higher catalytic performance.

For example, a combination of a thermal magnetic suspension balance and a fixed bed reactor [2] was used to deposit phosphorous on the surface of vanadia, changing its catalytic performance from total oxidation towards maleic anhydride formation [3]. The set-up was also used to deposit different compounds (promoters or poisons) on the surface of vanadyl pyrophosphate to influence its catalytic activity and selectivity. Our next step will be the deposition of vanadium containing layers, e.g. $(VO)_2P_2O_7$ or $VOPO_4$, on a suitable support.

[1] J. Lu, J. W. Elam, P. C. Stair, *Surf. Sci. Rep.* 2016, 71, 410

[2] V. E. Stempel, R. Naumann d'Alnoncourt, M. Driess, F. Rosowski, *Rev. Sci. Instrum.* 2017, 88, 074102

[3] V. E. Stempel, D. Löffler, J. Kröhnert, K. Skorupska, B. Johnson, R. Naumann d'Alnoncourt, M. Driess, F. Rosowski, *J. Vac. Sci. Technol. A Vacuum, Surfaces, Film.* 2016, 34, 01A135

4:15pm **AA3-WeA-12 Atomically Controllable Ru@Pt Core Shell Nanoparticles Towards PROX's Reactions Modulated by Pt Shell Thickness, Yun Lang, K Cao, J Zhang, B Shan, R Chen, Huazhong University of Science and Technology, China**

Preferential oxidation of CO under excess H_2 (PROX) is an effective way to remove CO from steam reforming of hydrocarbons for application in proton exchange membrane fuel cell.^[1] For PROX, the bimetallic core shell nanoparticles can tremendously improve total activity and selectivity of PROX reactions^[2]. However due to the lack of precise control over the core shell structures, the studies of relationship between PROX reactions with nanoparticles' structural parameters remain very limited. Herein, we demonstrate synthesis of Ru@Pt core shell nanoparticles using area-selective ALD techniques based on precursors' partial pressure and deposition temperature adjustment. A near linearly growth rate of Pt on Ru surface monitored with in-situ quartz crystal microbalance indicates well-controlled shell thickness by varying ALD cycles. The catalytic activity and selectivity of Ru@Pt core shell structure are enhanced compared with single component Ru, Pt or alloyed structure, which results from electron transfer from Ru to Pt. The catalytic performance is sensitive with shell thickness that influences the extent of electron modification and lattice mismatch. A monolayer of Pt shell shows optimal catalytic performance and minimal Pt loading. Density functional theory simulations have also been carried out to verify the results.

[1] H. Xu, Q. Fu, X. Guo, X. Bao, *ChemCatChem.* 2012, 4, 1645

[2] A. U. Nilekar, S. Alayoglu, B. Eichhorn, et al, *J. Am. Chem. Soc.* 2010, 132, 7418

Author Index

Bold page numbers indicate presenter

— C —

Cao, K: AA3-WeA-12, **1**

Chen, R: AA3-WeA-12, **1**

— D —

Driess, M: AA3-WeA-11, **1**

— K —

Knemeyer, K: AA3-WeA-11, **1**

— L —

Lang, Y: AA3-WeA-12, **1**

— N —

Naumann d'Alnoncourt, R: AA3-WeA-11, **1**

— P —

Piernavieja Hermida, M: AA3-WeA-11, **1**

— R —

Rosowski, F: AA3-WeA-11, **1**

— S —

Schlögl, R: AA3-WeA-11, **1**

Shan, B: AA3-WeA-12, **1**

Stempel, V: AA3-WeA-11, **1**

— T —

Trunschke, A: AA3-WeA-11, **1**

— Z —

Zhang, J: AA3-WeA-12, **1**