Title: Nanoparticle Sintering in Atomic Layer Deposition of Supported Catalysts: Kinetic Modeling of the Size Distribution

Authors: Fabio Grillo, Jacob A. Moulijn, Michiel T. Kreutzer, J. Ruud van Ommen

PII: S0920-5861(18)30071-3
DOI: https://doi.org/10.1016/j.cattod.2018.02.020
Reference: CATTOD 11245

To appear in: *Catalysis Today*

Received date: 28-12-2017
Revised date: 28-1-2018
Accepted date: 13-2-2018

Please cite this article as: Fabio Grillo, Jacob A.Moulijn, Michiel T.Kreutzer, J.Ruud van Ommen, Nanoparticle Sintering in Atomic Layer Deposition of Supported Catalysts: Kinetic Modeling of the Size Distribution, Catalysis Today https://doi.org/10.1016/j.cattod.2018.02.020

Nanoparticle Sintering in Atomic Layer Deposition of Supported Catalysts: Kinetic Modeling of the Size Distribution

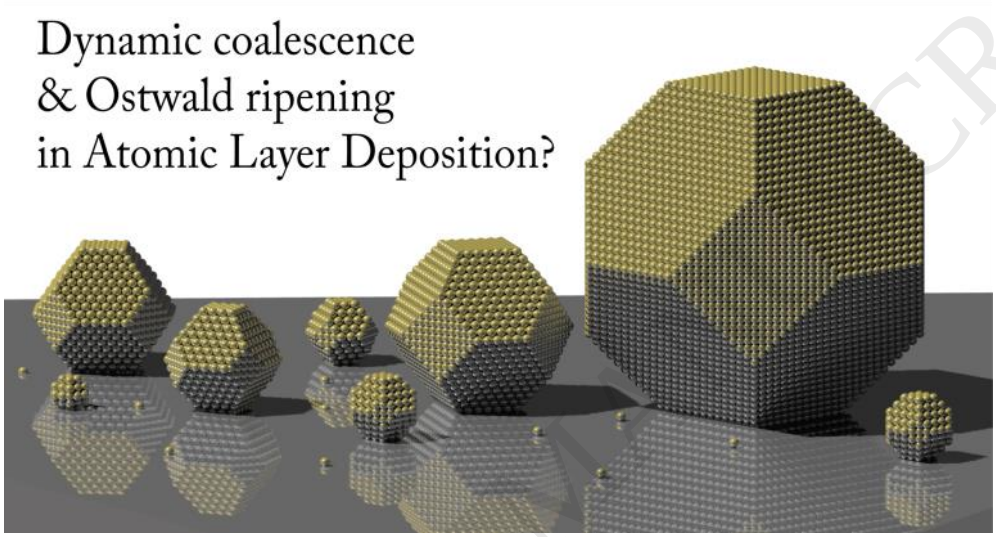
Fabio Grillo[a], Jacob A. Moulijn[b]*, Michiel T. Kreutzer[a], J. Ruud van Ommen[a]

[a]*Chemical Engineering Department, Delft University of Technology, 2629 HZ Delft, The Netherlands*

[b]*Delft IMP B.V., 2629 JD Delft, The Netherlands*

corresponding author: j.a.moulijn@tudelft.nl

Graphical abstract



Abstract

In industrial catalysis, the sintering of supported nanoparticles (NPs) is often associated with the loss of catalyst activity and thus with periodic plant downtime and economic burdens. Yet, sintering mechanisms are at play also during the synthesis of the catalyst itself. They can, in fact, determine the size distribution of the NPs, and thus the activity and the stability of the catalyst. Here, we examine the role of nanoparticle sintering in a technique borrowed from the semiconductor industry that promises to reconcile atomic-scale precision with scalability: atomic layer deposition. By modeling the cyclic influx of single atoms in concomitance with NP sintering via either dynamic coalescence or Ostwald ripening, we establish the "signature" of different growth regimes: the size distribution. In contrast, we show that integral quantities such as the mean diameter, the number of NPs per unit area, and the material loading are poor indicators of the underlying growth mechanism. In particular, a constant number of NPs cannot be interpreted as a sign of no sintering. Finally, we argue that NP sintering, if properly understood, can open up new avenues for the control over the size distribution of NPs, and thus over their catalytic activity and stability.

Key words: dynamic coalescence, Ostwald ripening, nanoparticle growth, size distribution, modeling, mechanisms