



Structure-activity investigation of Ni-Ga model catalysts for CO₂ hydrogenation to Methanol

Spiga, Cristiano; Almind, Mads Radmer; Silva, Hugo José Lopes; Wagner, Jakob Birkedal; Chorkendorff, Ib; Damsgaard, Christian Danvad

Publication date:
2016

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):
Spiga, C., Almind, M. R., Silva, H. J. L., Wagner, J. B., Chorkendorff, I., & Damsgaard, C. D. (2016). *Structure-activity investigation of Ni-Ga model catalysts for CO₂ hydrogenation to Methanol*. Abstract from Material Science and Engineering 2016, Darmstadt, Germany.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Structure-activity investigation of Ni-Ga model catalysts for CO₂ hydrogenation to Methanol

Cristiano Spiga^{1,2*}, Mads R. Almind^{1,2}, Hugo J.L. Silva², Jakob B. Wagner¹, Ib Chorkendorff², and Christian D. Damsgaard^{1,2}

¹Center for Electron Nanoscopy, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

²Center for Individual Nanoparticle Functionality, Department of Physics, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

*: presenting author, email:crispi@cen.dtu.dk

Metal nanoparticles (NPs) dispersed on a high surface area support are widely used as catalysts for heterogeneous catalysis. The atomic structure of the active NPs is highly linked to the performances of the catalyst. An Environmental Transmission Electron Microscope (ETEM) equipped with a differential pumping system to confine a controlled gas flow around the specimen, offers a unique tool to investigate individual NPs at the atomic level in a gaseous environment [1]. Nevertheless, the morphology of the high surface area support tends to complicate the interpretation of TEM micrographs on the atomic level and blurs the spectroscopic information due to limited depth of field and multiple scattering events. One way to circumvent this is to synthesize NPs on a low surface area support representing the “real” high surface area supported catalyst.

δ -Ni₅Ga₃ catalysts prepared by incipient wetness impregnation on a high surface area SiO₂ support (Figure 1A), have shown promising for CO₂ hydrogenation to methanol with comparable turn-over frequencies to the preferred commercial Cu/Zn/Al₂O₃ catalyst system[2-3].

This study presents ETEM investigation of Ni-Ga NPs dispersed on ~200 nm SiO₂ spheres. The catalyst shows similar size distribution and activity pr. surface area as the low-surface area supported catalyst.

The SiO₂ spheres supported model catalyst features numerous NPs that can be illuminated directly with the electron beam (Figure 1B). This enables atomic resolved structural (HRTEM) (Figure 1C) and spectroscopic information (EELS) of the individual NPs.

The catalyst formation process and pre-dominant deactivation mechanism at the atomic level are investigated in the ETEM by following the morphology (surface structure, facets, NP size, crystal structure, material composition) during catalyst synthesis and CO₂ hydrogenation to methanol. The investigation is supported by complementary techniques such as *in-situ* X-Ray Diffraction (XRD) and catalytic activity measurements (fixed-bed reactor) using a Gas Chromatograph (GC) and a Mass Spectrometer (MS).

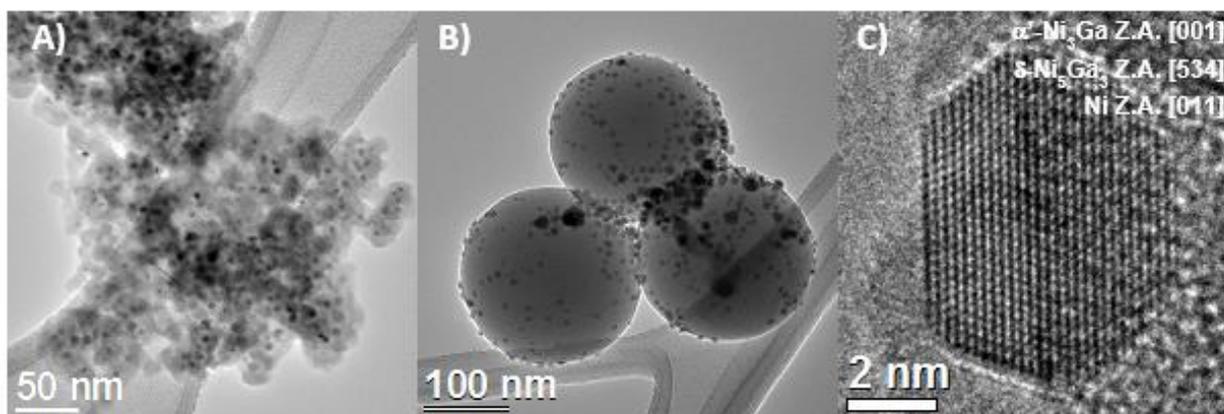


Figure 1. TEM micrographs of NiGa NPs supported on A) High surface area SiO₂ support B) Ni-Ga NPs on ~200 nm SiO₂ spheres, and C) HRTEM micrograph of Ni-Ga NPs on top of SiO₂ spheres ($P(H_2)=110$ Pa, $T=700$ °C).

References

- 1) Hansen, T.W., et al., Materials Science and Technology 11(2010), p. 1338.
- 2) Studt, F., et al., Nature Chemistry 6(2014), p. 320.
- 3) Sharafutdinov, I., et al., Journal of Catalysis, 320(2014), p. 77.