Supplementary Information

Synthesis and exceptional thermal stability of Mg-based bimetallic nanoparticles during hydrogenation.

Gopi Krishnan,[*a] *Raluca F. Negrea,*[b] *Corneliu Ghica,*[b] Gert H. ten Brink,[a] *Bart J. Kooi.*[a] and *George Palasantzas,*[a]

[a] Zernike Institute for Advanced Materials and the Materials Innovation Institute, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands.

[b] National Institute for Materials Physics, P.O. Box MG-7, Magurele, Ilfov, RO 77125, Romania

Corresponding Author

* Email: gopi.k.krish@gmail.com

A. Target configuration

Figure 1. Showing the different types of section target arrangement used for the production of nanoparticles.

B. Nanoparticle deposition source

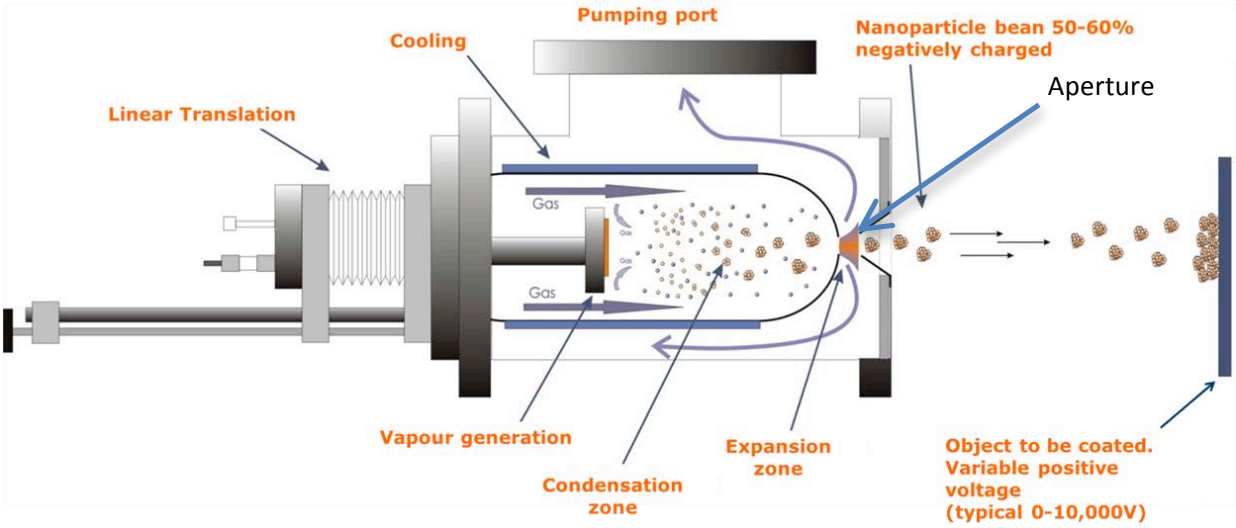

Figure 2. Schematic of the nanoparticle production set up (Mantis deposition Ltd).

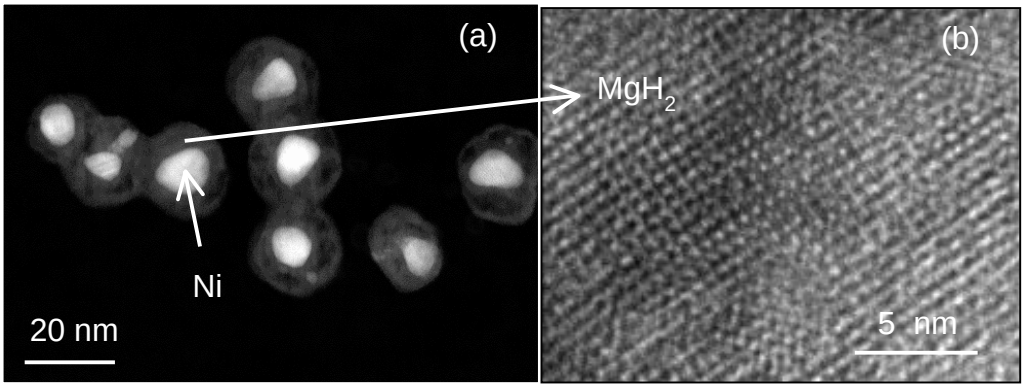

Figure 3 (a) HAADF-STEM image of the Mg-Ni nanoparticles after hydrogenation with a phase segregated Ni core and an MgH_2 shell. (b) HRTEM image of an NP showing that the orthogonal (110) and (110) planes of the MgH_2 phase are resolved. It confirms the presence of tetragonal α-MgH_2 structure. The arrow in which part of the NP shown in Figure 3 (a) the HRTEM image in 3 (b) was recorded.

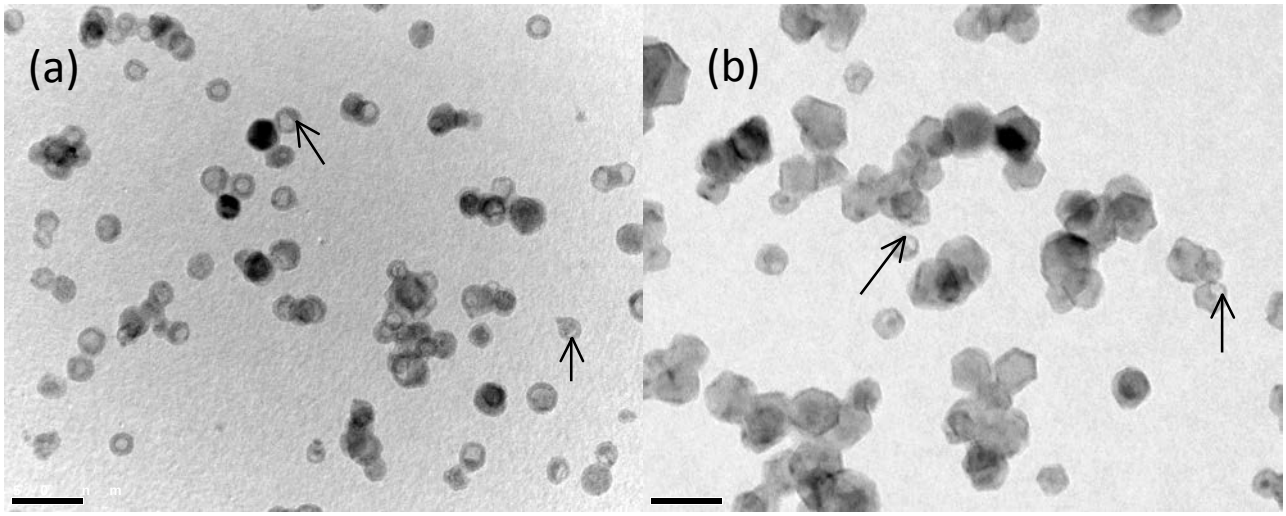

Figure 4 Bright-field TEM image of Mg based NPs. (a) Mg-Ni nanoparticles with 93±3 at % of Mg demonstrate void formation (hollowing) during production of the nanoparticles as also indicated by an arrow. (b) Void formation in the Mg-Ti nanoparticles with 88±3 at % of Mg during their production. Note that the void formation depends on the nanoparticle size.

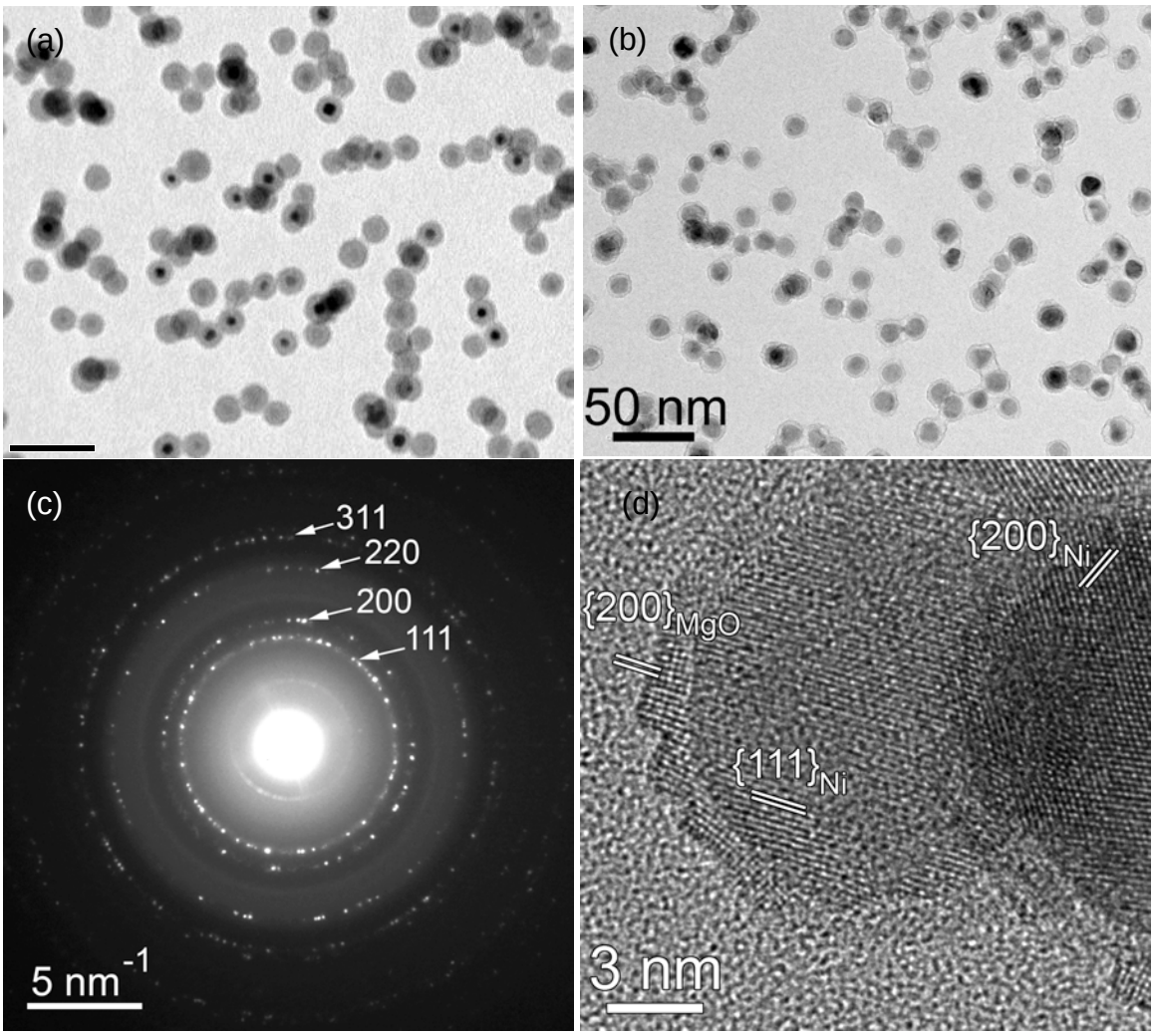

Figure 5. (a) Bright field TEM image of Mg-Ni NPs with multi shell structure before hydrogenation. (b) Bright field TEM image of the same Mg-Ni nanoparticles after hydrogenation at 150 ^{O} C and 5 bar H_2, resulting in a Ni/MgO core-shell structure with an average core size of 10 nm and a shell of ca. 1-3 nm thickness,. (c) Corresponding SAED pattern showing cubic Ni as main crystalline phase, no Mg phase. (d) HRTEM image of Mg-Ni NPs revealing a crystalline Ni core surrounded by a crystalline MgO shell.

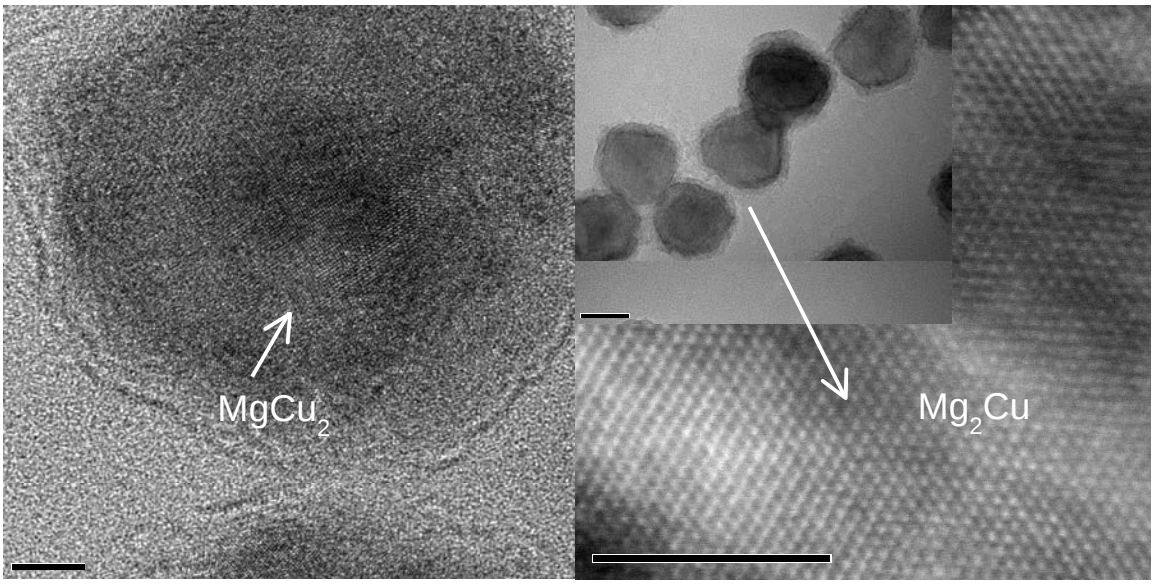

Figure 6. (a) HRTEM image of Mg-Cu NP formed at 0.250 A with a multi-phase structure. The center (core) of the NP is an $MgCu_2$ phase identified by lattice plane of (222) (b) HRSTEM image of (another) Mg-Cu NP where the Mg_2Cu phase is present in the region of the NP core. The inset shows a bright- field TEM image of Mg-Cu NPs with an arrow indicating the specific particle viewed in HRSTEM.

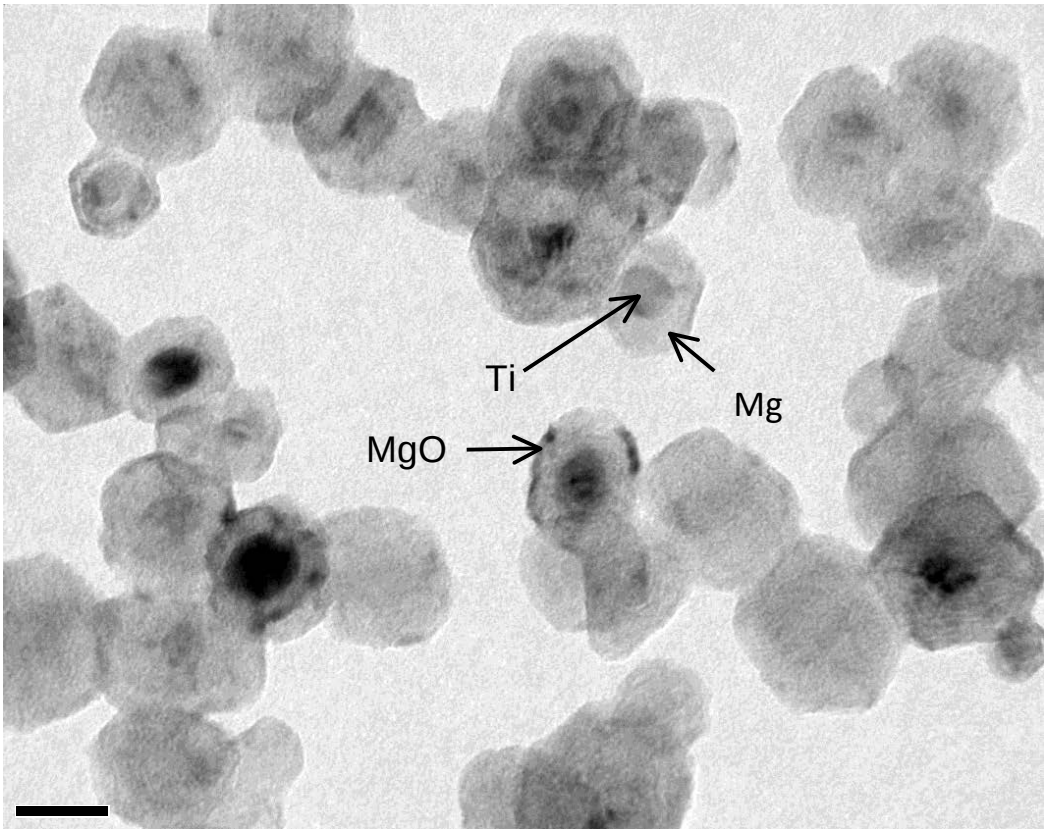

Figure 7. Bright-field TEM image of Mg-Ti nanoparticles produced at 0.250 A discharge current. Here, Ti act as nuclei of the Mg growth, and forms a core-shell structure as indicated in the image by an arrow. The contrast in the outer shell of the Mg-Ti NP arises from the crystalline MgO shell. It is important to note that an amorphous MgO shell is formed in the case of Mg-Ni and Mg-Cu NPs. No subsurface shell of Ti is observed here (also in contrast to Mg-Ni and Mg-Cu NPs, where such subsurface shells of Ni and Cu are present, respectively).