Supplementary Information of

Intermetallic Reaction and Eutectic Transitions Tune the Reactivity in Core-Shell Mg/Ni Nanoparticles

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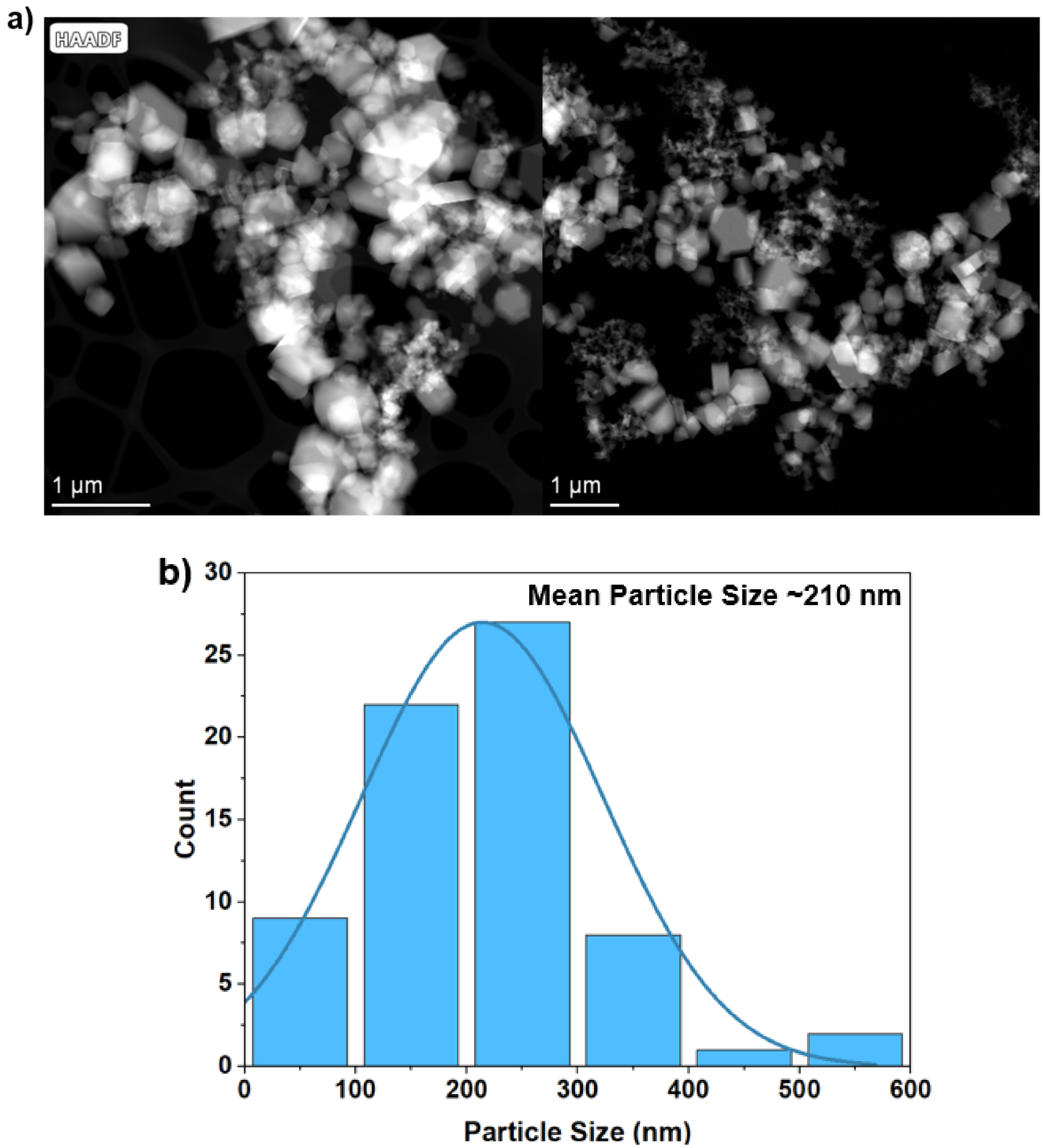

Figure S1. (a) TEM on the synthesized magnesium nanoparticles with various shapes b) corresponding size distribution

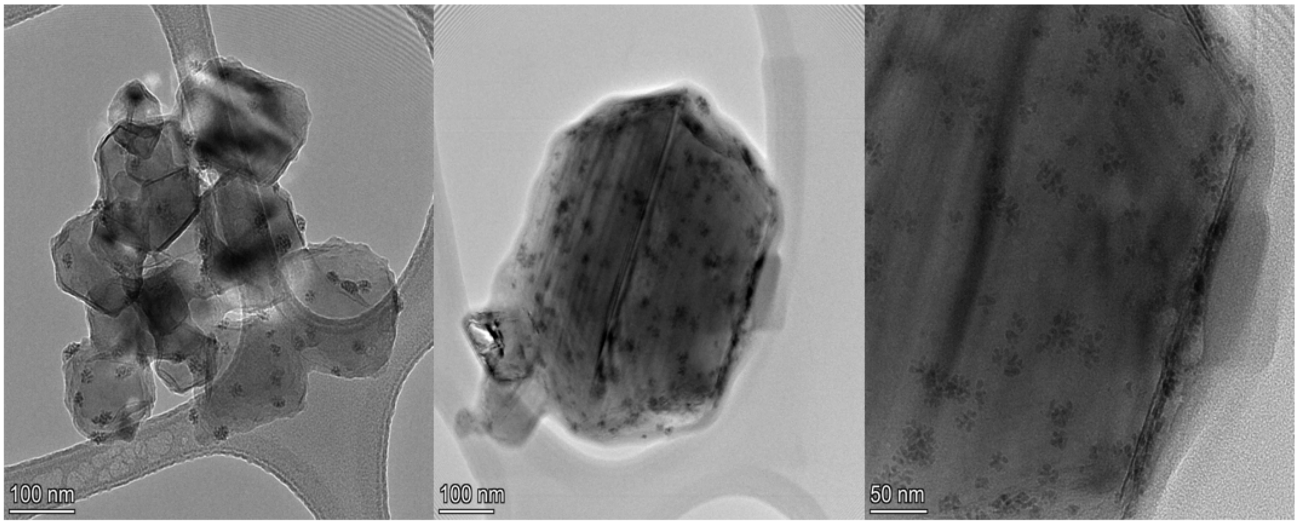

Figure S2. HRTEM on Ni-coated Mg nanoparticles

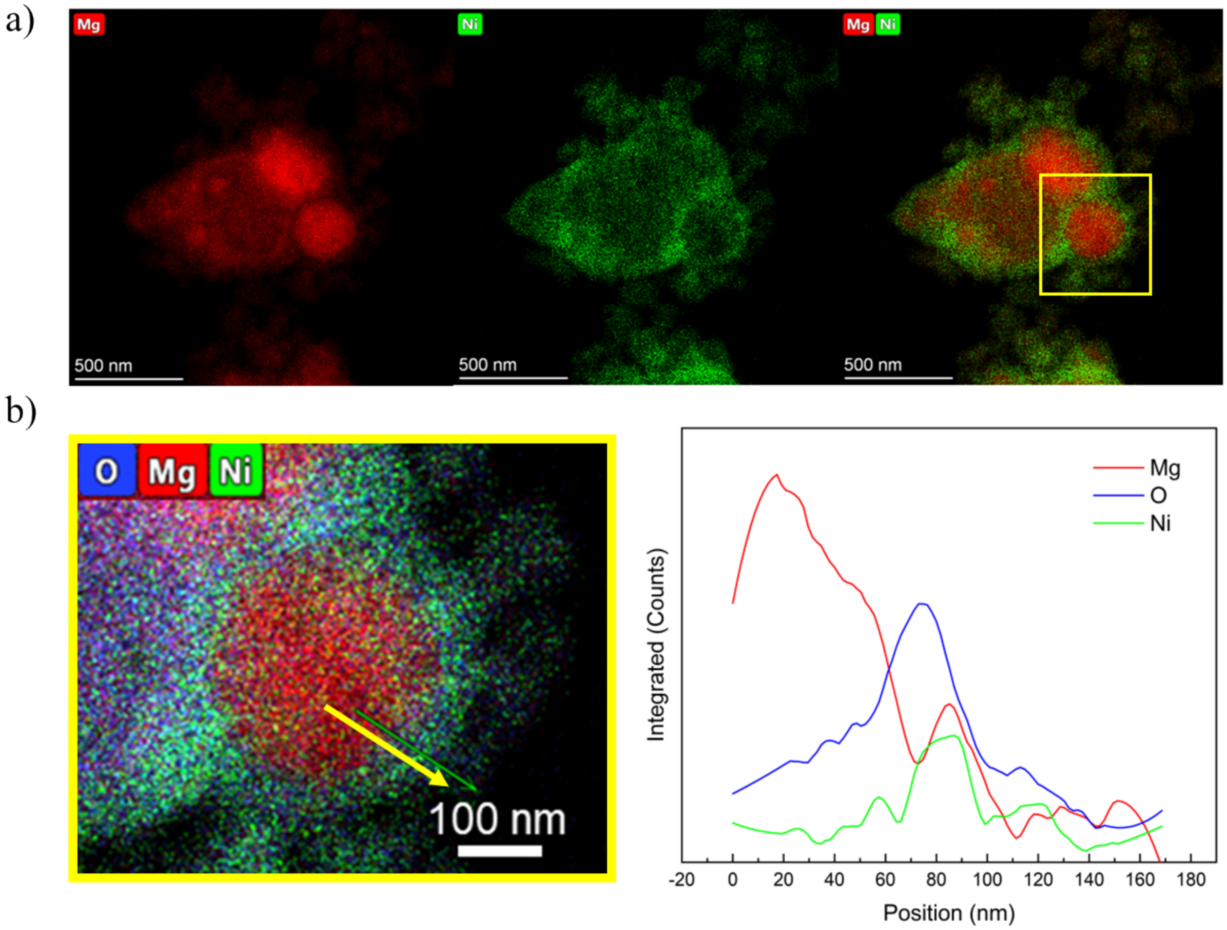

Figure S3: STEM EDS on the Ni coated Mg nanoparticles (Mg: Ni = 1 : 0.22) b) corresponding line scan profile

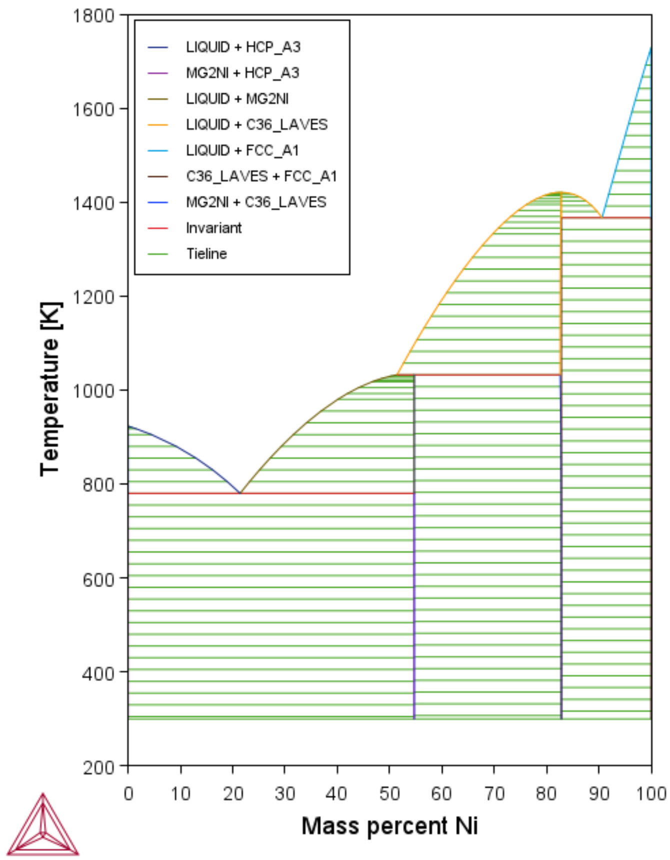

Figure S4. Phase diagram of Mg-Ni binary system calculated with Thermo-Calc software.

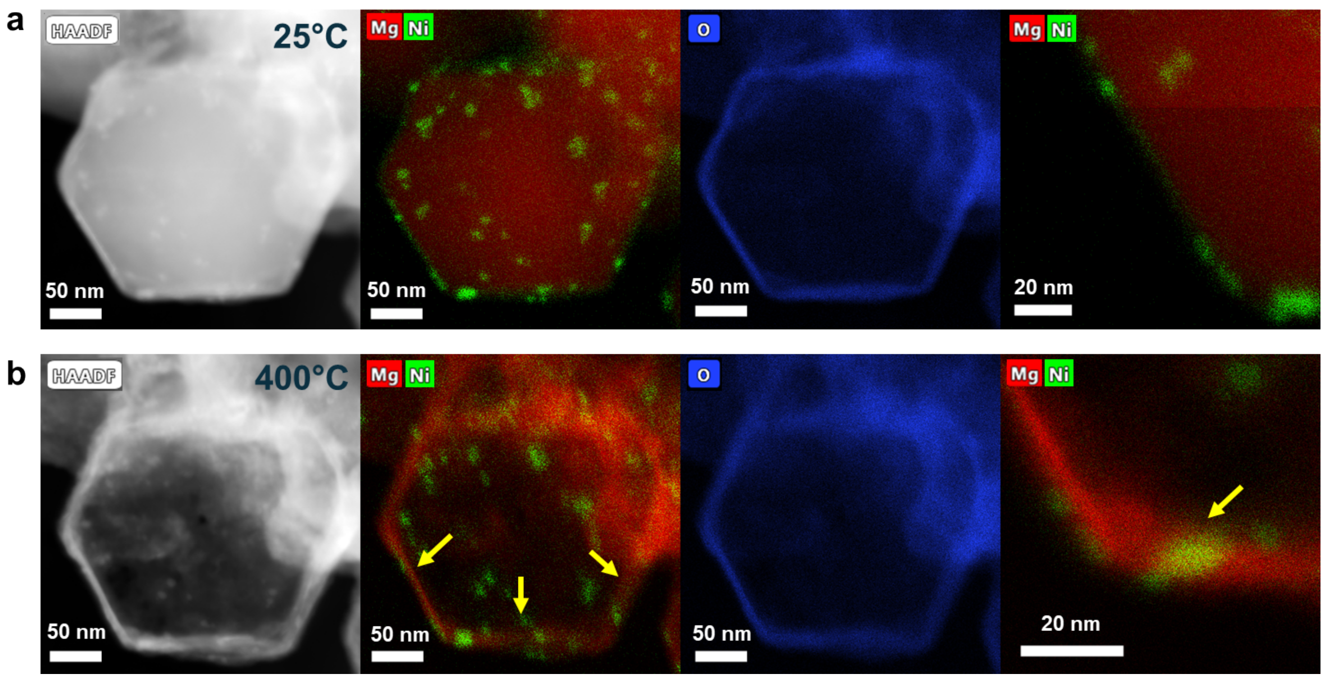

Figure S5. *In situ* heating STEM-EDS of Ni-coated Mg particles under vacuum. (a) Images at room temperature showing the initial Mg-Ni core–shell structure. (b) Images at elevated temperatures showing Mg diffusion into the Ni shell, providing evidence of alloy formation at the interface.

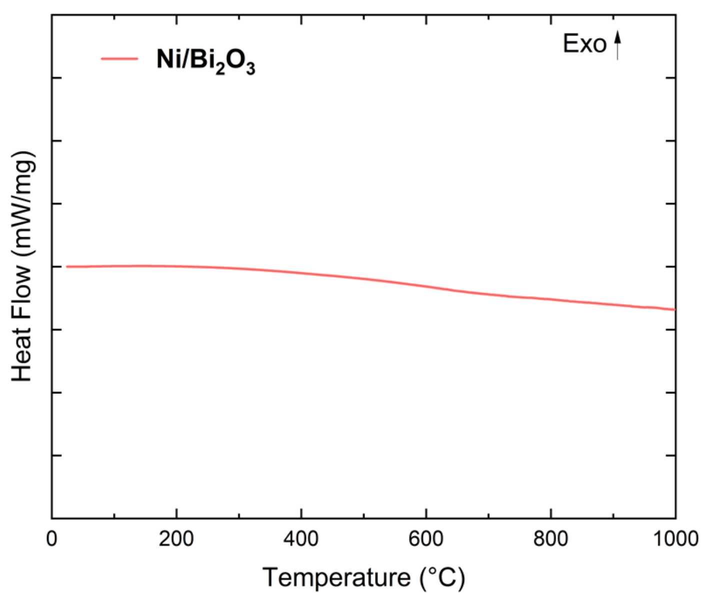

Figure S6. DSC curve of Ni/Bi_2O_3 in argon evironment at a heating rate of 10 K min^{-1}

Thermal calculation on temperature rise of particle from alloying reaction

$2Mg + Ni = Mg_2Ni$ $\Delta H = -59.61$ kJ/mol of Ni

Ratio of Mg and Ni = 1: 0.22 in the thick-coated sample

The enthalpy of formation for 0.22 mol Ni = 13.1 kJ

= 124.5 J/g

From DSC, the amount of heat released from calculating the area at a heating rate of 10 K/min = 52.56 J/g

% of Ni reacting with Mg = $\frac{52.56}{124.5} = 42.2\%$

The temperature increases of the particles,

$\Delta H = m_{Mg} \cdot c_{p,Mg} \cdot \Delta T + m_{Ni} \cdot c_{p,Ni} \cdot \Delta T + \Delta H_{fusion,Mg}$

$\Delta H_{fusion,Mg} = 8.7$ kJ/mol

$\Delta T = 107$ K

Therefore, the alloying reaction is sufficient to raise particle temperature by 107 K while overcoming the heat of fusion required for melting.

Diffusion Flux Calculations

The particle volume was estimated from the projected surface area obtained from TEM images and the particle thickness

$$V = A \times t$$

The particle mass was calculated from the volume and bulk density of magnesium ρ=1738 kg/m^3

$$m = \rho \times V$$

The number of moles of magnesium,

$$n = \frac{m}{M}$$

The instantaneous molar diffusion rate was determined from the finite difference of moles with respect to time at consecutive temperature measurements

$$Rate = \frac{\Delta n}{\Delta t}$$

The diffusion flux was calculated as follows whereas A_s is the effective particle surface area

$$J = \frac{Rate}{A_s}$$