

Supplementary information

Structure Evolution of NiAu Nanoparticles under Ambient Conditions Revealed Directly by Atom-resolved Imaging Combined with DFT Simulation

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Supplementary Figures

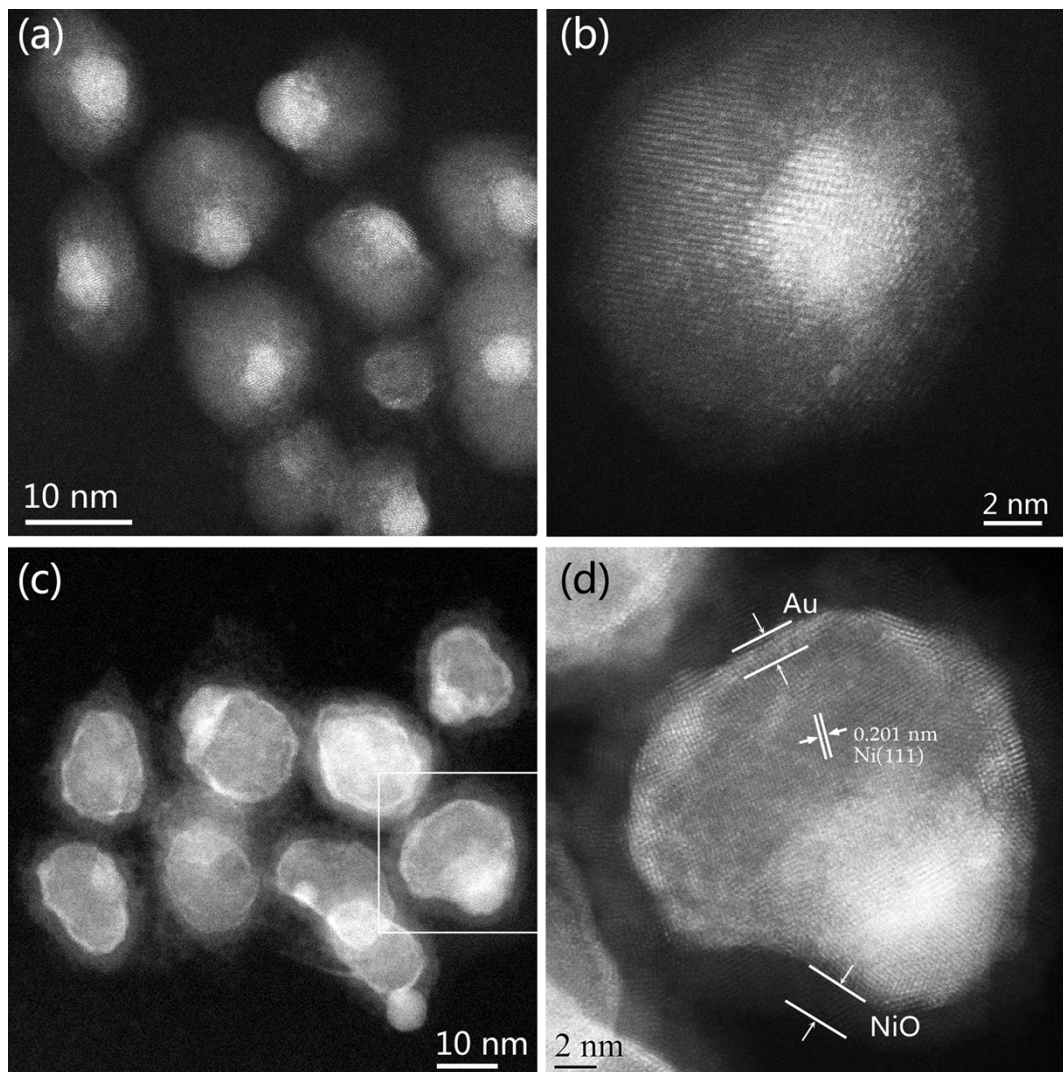


Figure S1 low and high magnified HAADF images of NiAu nanoparticles. (a~b) the original spindle-like NiAu particles, Au and Ni components are separated at two sides with some mono dispersed Au atoms embedded in the Ni matrix; (c~d) the reconstructed NiAu sandwich-like multilayer nanostructures after annealed in air at 350 °C for 8h. The lattice fringes of the three layers could be clearly distinguished.

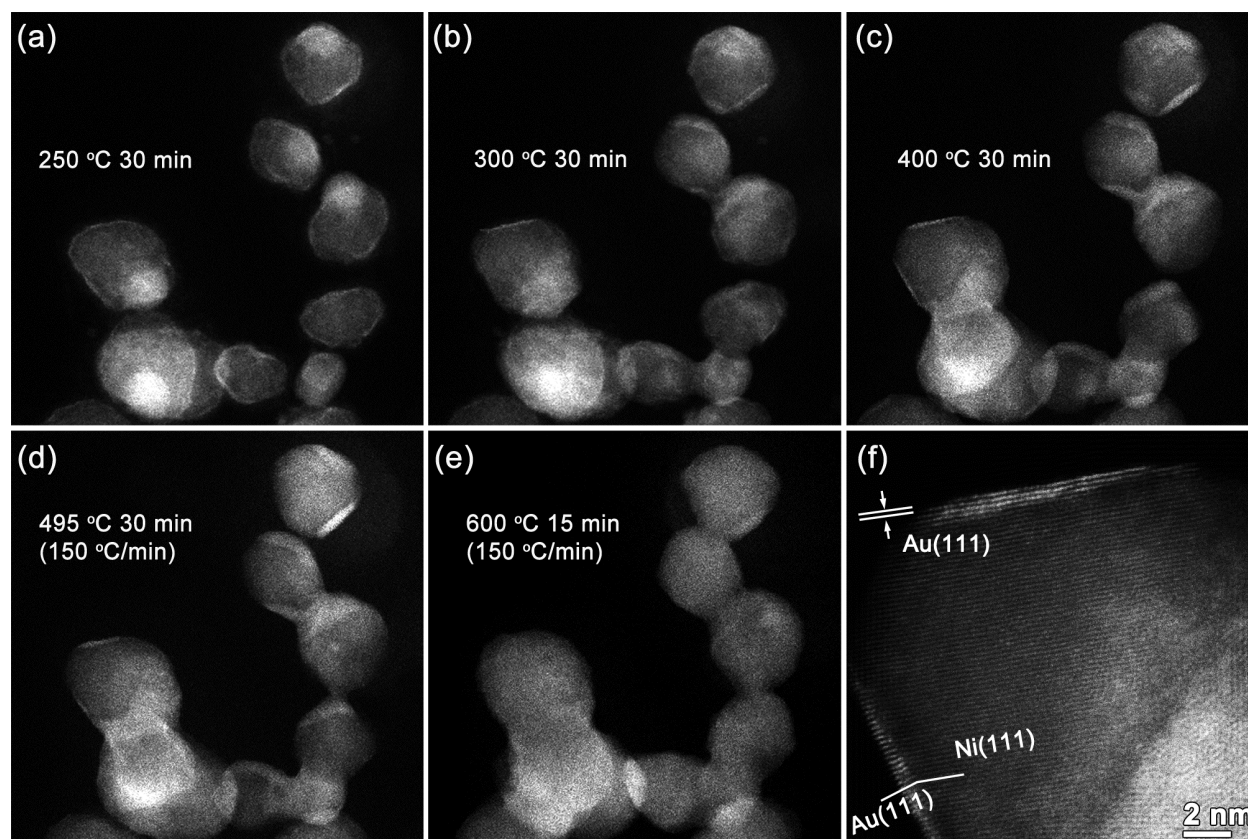


Figure S2 HAADF images of NiAu spindles after series of in-situ annealing in vacuum. (a) ~ (e) low magnified HAADF images of the same area after having been annealed at different temperatures ($^{\circ}\text{C}$) and durations (min); (f) high magnified HAADF image of the individual nanostructure after annealed at $400\text{ }^{\circ}\text{C}$ for 30 min. The NiAu nanospindles evolve along four distinct stages: i) the Ni matrix recrystallizes into polyhedron morphology (a~b); ii) Au component diffuses along Ni(111) facets via either epitaxial or compensating growth (c); iii) single crystallization of Ni matrix (d); iv) wrapping diffusion of Au component around Ni matrix forming Ni@Au structure (e).

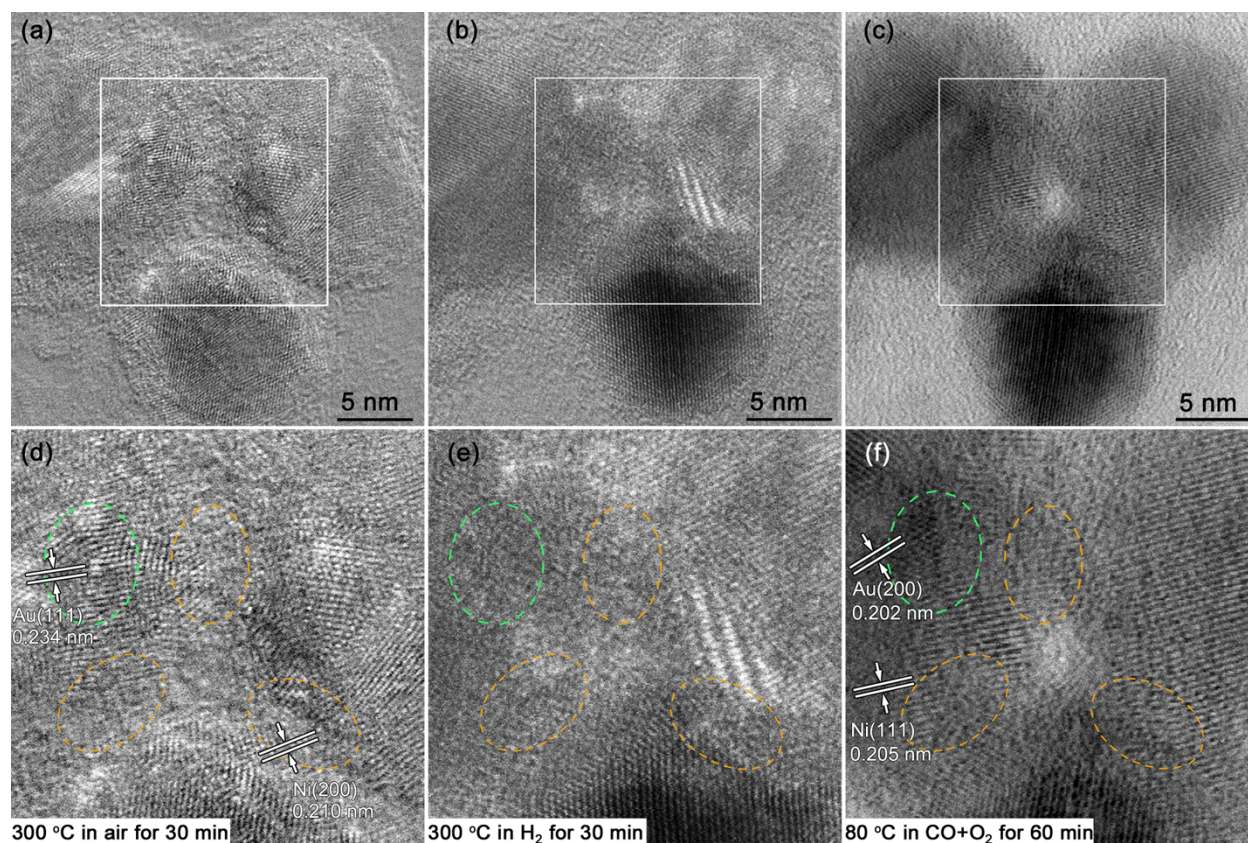


Figure S3 The BF-STEM images of NiAu reconstruction in atmospheres series simultaneously acquired with Fig. 3. (d~f) the corresponding high magnified images from the marked regions of image (a~c), respectively. Obvious structure evolution of hydrogen-reduction induced amorphization (d to e) and catalytic-reaction induced recrystallization (e to f) can be observed in the regions where the NiO layer locates as marked out by yellow circles. Meanwhile, the migration trend of Au component including the dispersion during reduction and the surface segregation in catalytic reaction is demonstrated in the green circled area. All the images are used in their original form without any processing for signal promotion.

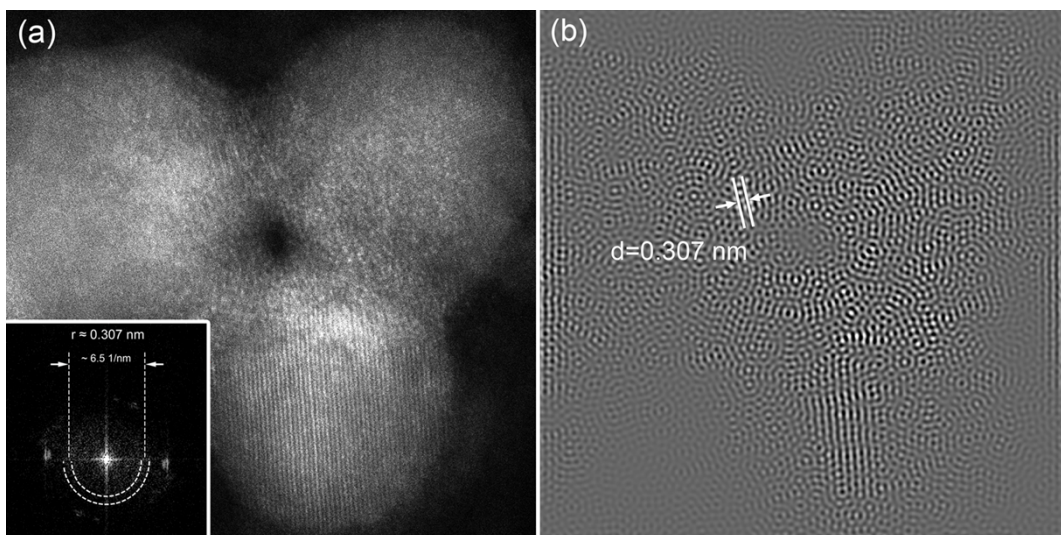


Figure S4 The NiAu nanoparticles after hydrogen reduction at 300 °C for 30 min. (a) the HADDF image demonstrating amorphous condition of the surface, the FFT pattern reveals that the diffraction ring of $\sim 6.5 \text{ nm}$ in diameter mainly contributes to the amorphous contrast; (b) the digital dark-field image from the diffraction region marked by circle dashed lines, which illustrates the mean size of NiAu clusters to be 0.307 nm, identical with the value of Au_3Ni FCC configuration.