Island-type growth of Au-Pt heterodimers: Direct visualization of misfit dislocations and strain-relief mechanisms

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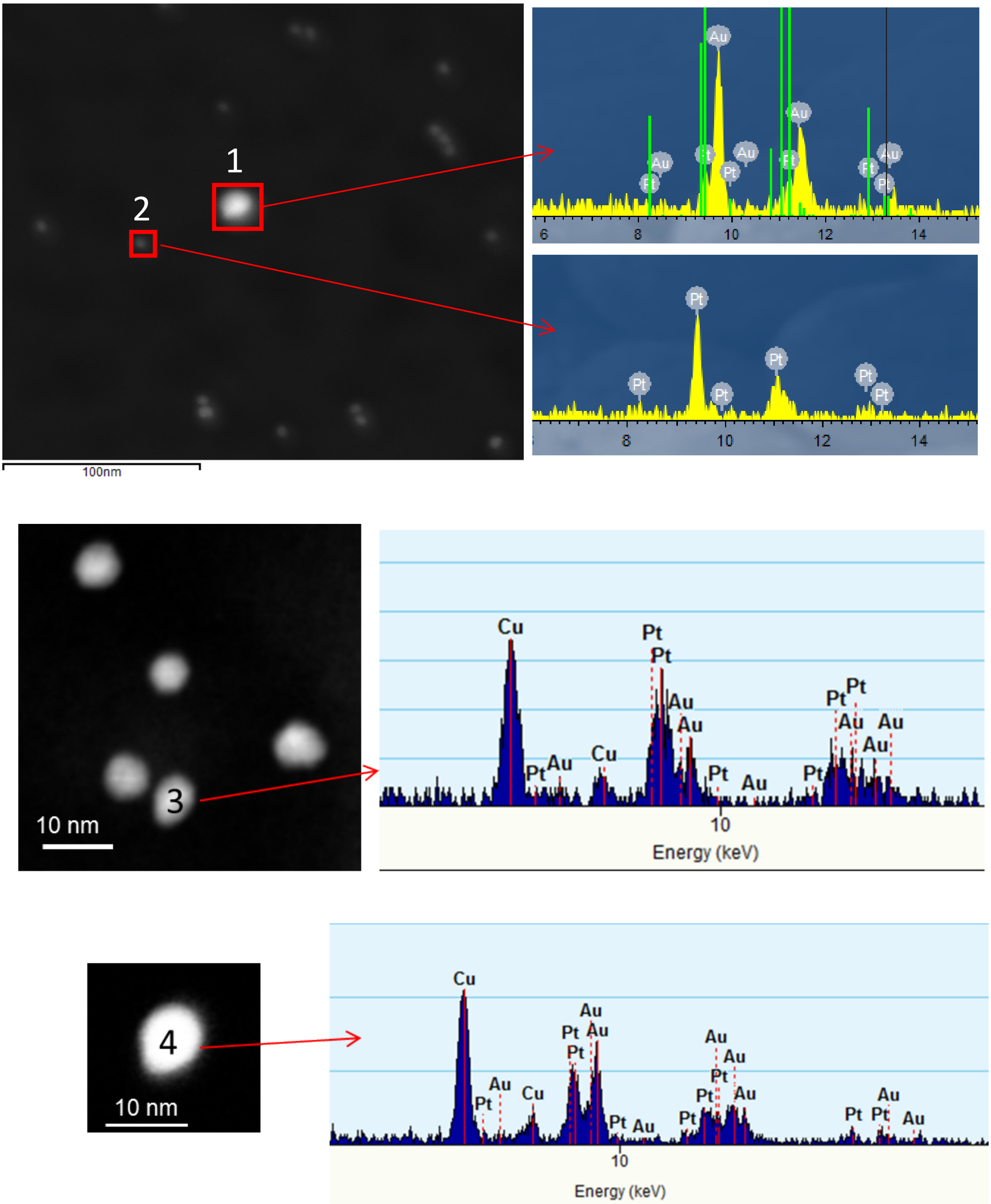
Electronic Supplementary information

Figure S1. STEM-HAADF/EDX analyses of particles found in the reaction medium after reaction for two hours: Cubeoctahedrally-derived 1) Big Au particle, 2) Pt particle, 3) particle containing both Au and Pt, 4) octahedrally-derived particle containing both Au and Pt.



Hall-Williamson method. In this method the integral breadth of the diffraction peak is determined. The integral breadth is given by the integral intensity divided by the maximum intensity. Thus, the observed peak broadening (B_0) may be represented as (ref. 28 in the main text):

$$B_0 = B_i + B_r \qquad (1)$$

Where B_0 is the observed peak broadening in radians, B_i is the instrumental broadening in radians and B_r is the broadening due to the small particle size and lattice strain. Eq.2 holds very well if the diffraction peaks exhibit purely Cauchy profile. For cases where the diffraction peaks are partly Cauchy or partly Gaussian in profile, further modifications can be also introduced (ref. 29 in the main text). Now, according to the Scherrer equation, the broadening due to the small particle size may be expressed as:

$$B_c = \frac{K\lambda}{t} + \cos\theta \qquad (2)$$

Where B_c is the broadening due only to the small crystallite size, K is a constant whose value depends on particle shape but which is usually taken as unity, t is the crystallite size in nm, θ is the Bragg angle and λ is the wavelength of the incident X ray-beam in nm. Similarly, the broadening due to the lattice strain may be expressed as (ref. 28 in the main text):

$$B_s = \varepsilon\tan\theta \qquad (3)$$

Where B_s is the peak broadening due to the lattice strain, ε is the strain distribution within the material and θ is the Bragg angle. Based on equations (3) and (4) the total peak broadening B_r can be expressed as (ref. 28 in the main text):

$$B_r = \frac{K\lambda}{t} + \varepsilon\tan\theta \qquad (4)$$

Which can be written as:

$$B_r\cos\theta = \frac{K\lambda}{t} + \varepsilon\sin\theta \qquad (5)$$

The plot of $B_r\frac{\cos\theta}{\lambda}$ vs $\frac{\sin\theta}{\lambda}$ is a straight line with a slope equal to ε and the particle size, t, can be estimated from the intercept.

Figure S2. a) HAADF-STEM image of an octahedral Pt seed sample where a particle used for EDX mapping is marked through the green inset; b) Pt map; c) Mn map; d) Pt and Mn maps are represented by red and yellow colours respectively; e) EDX spectra.

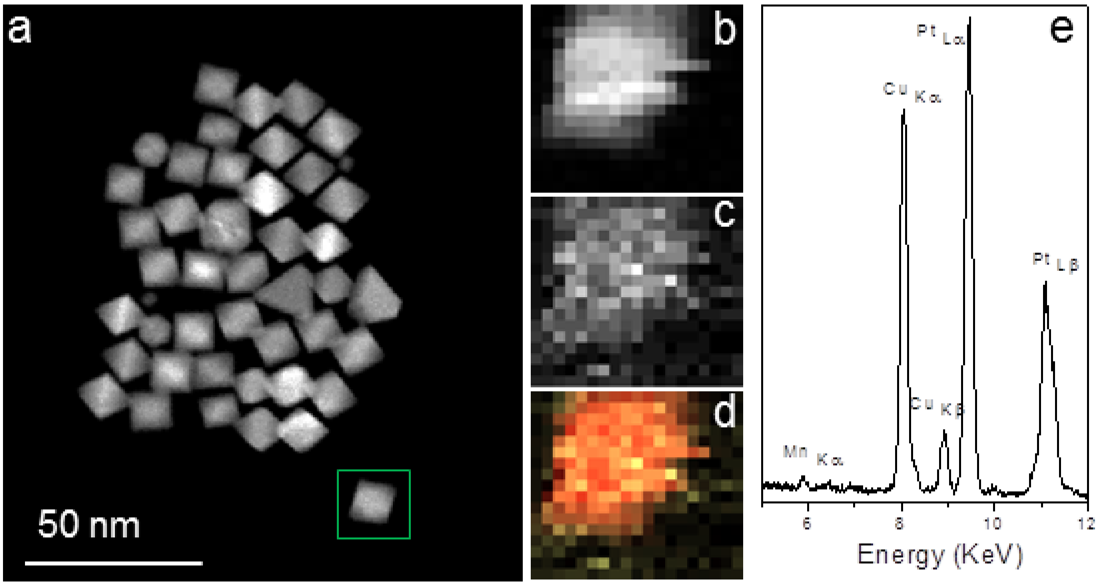


Figure S3. a) HAADF-STEM image of a cubeoctahedral Pt seed sample where a particle used for EDX mapping is marked through the green inset; b) Pt map; c) Co map; d) Pt and Co maps are represented through red and yellow colours respectively. e) EDX spectra.