Electronic Supplementary Information (ESI)

# Efficient Shape Transformation of Palladium Nanocrystals by Biphasic Oxidative Etching and Regrowth

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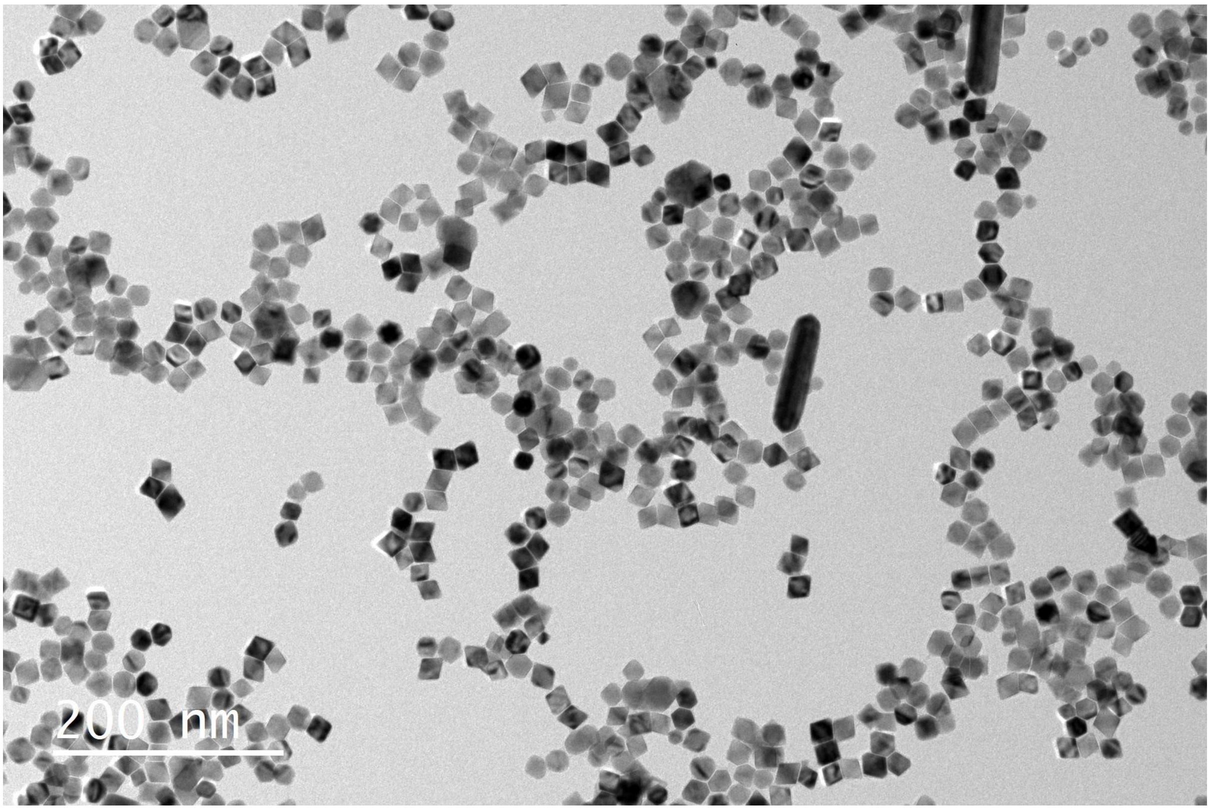


**Fig. S1.** A low-magnification TEM image of the Pd octahedrons (average edge length, 21.3 nm) obtained from a typical synthesis.

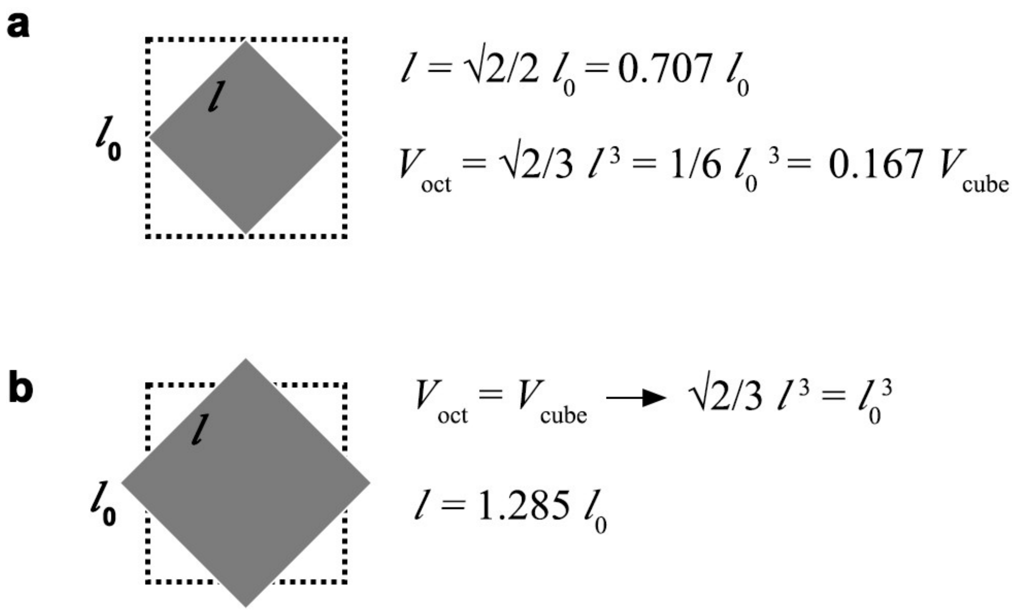


**Fig. S2.** Geometric calculations of the nanocubes and the octahedrons after the shape transformation. (a) A nanocube is etched into an octahedron without further regrowth. In this case, the relationship between the edge length of the octahedron ($l$) and that of the cube ($l_0$) should be $l = 0.707\ l_0$. The volume of the octahedron is 1/6 the volume of the cube. (b) A nanocube is transformed into an octahedron with 100% atomic efficiency, i.e., without the loss of volume. In this case, the edge length of the octahedron should be 1.285 times that of the original cube.

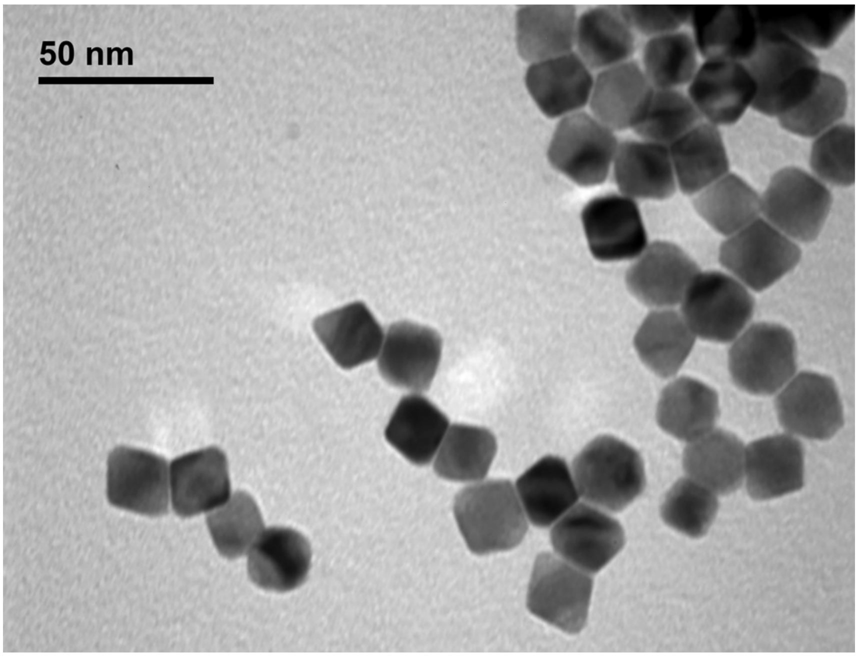


**Fig. S3.** TEM image of the Pd octahedrons obtained from a typical synthesis in an $N_2$ atmosphere. This result suggests that the shape transformation of the Pd nanocrystals does not rely on the $O_2/Cl^-$ pair.

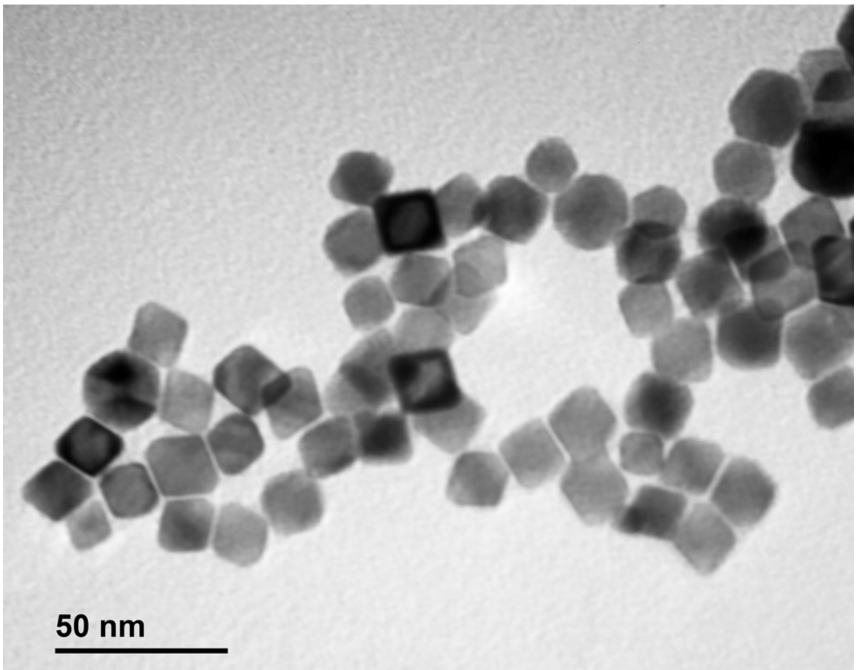


**Fig. S4.** TEM image of the Pd octahedrons obtained from a synthesis in ethylene glycol (EG). This result suggests that TEG in the typical synthesis can be replaced by other polyols, EG for example, without satisficing the overall quality of the Pd octahedrons obtained from this synthesis.

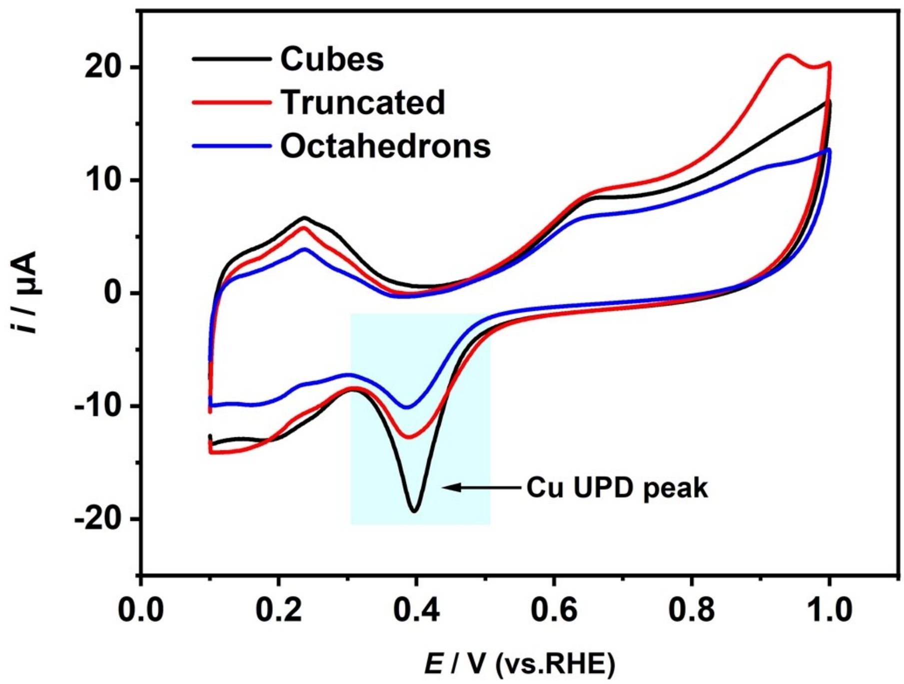


**Fig. S5.** Underpotential deposition of $Cu^{2+}$ on Pd nanocrystals of different shapes for determining the ECSA of the nanocrystals.

**Table S1.** Electrochemical properties of the Pd nanocrystals of different shapes.

| Sample | Peak current density in FAOR (mA cm$^{-2}$) | Current density at 0.3 V in FAOR (mA cm$^{-2}$) | Potential of HCOOH oxidation peak (V) | Potential of CO oxidation peak (V) | Potential of PdO reduction peak (V) |
|---|---|---|---|---|---|
| Pd nanocubes | 5.72 | 2.09 | 0.544 | 1.002 | 0.788 |
| Truncated Pd nanocrystals | 7.47 | 4.25 | 0.453 | 1.029 | 0.768 |
| Pd octahedrons | 8.07 | 5.14 | 0.409 | 1.031 | 0.768 |