Supporting Information for

A Quantitative Analysis of the Role Played by Poly(vinyl pyrrolidone) in Seed-mediated Growth of Ag Nanocrystals

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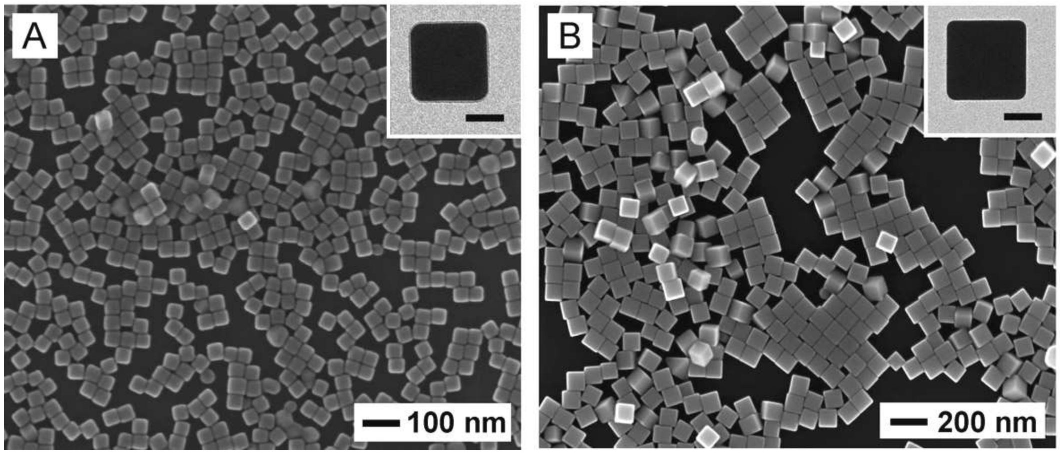

Figure S1. (A) SEM image of the cubic seeds of Ag with an average edge length of 40 ± 1 nm. The inset shows typical TEM image of the seed (scale bar: 20 nm). (B) SEM image of the cubic seeds of Ag with an average edge length of 100 ± 2 nm. The inset gives a typical TEM image of the seed (scale bar: 50 nm).

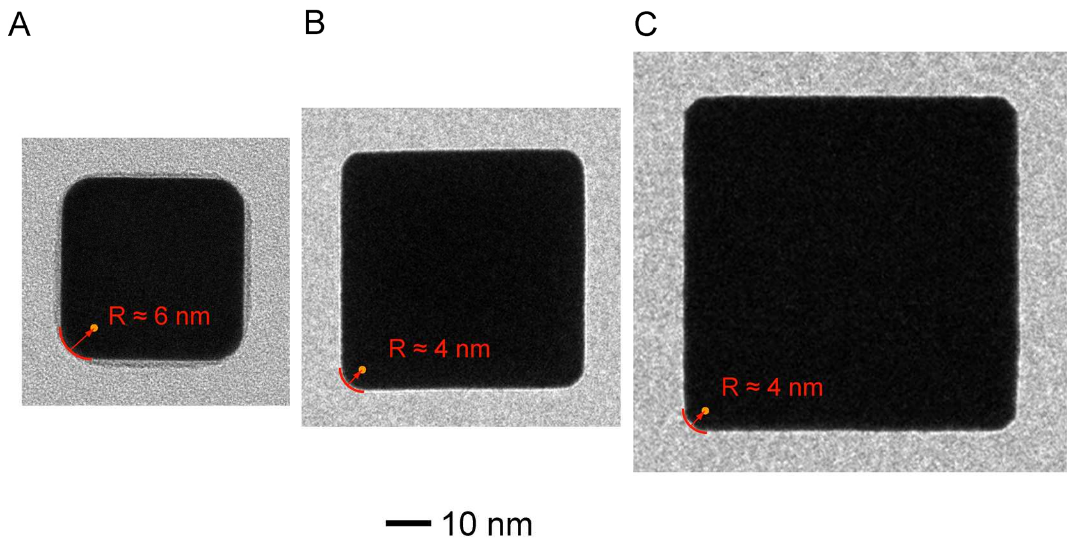

Figure S2. TEM images of a single (A) 40-nm Ag cubic seed, (B) 55-nm Ag cube as shown in Figure 2A, and (C) 75-nm Ag cube as shown in Figure 2C at a higher magnification. The red arc in each image indicates the corner site of a cube with a curvature of R in radius.

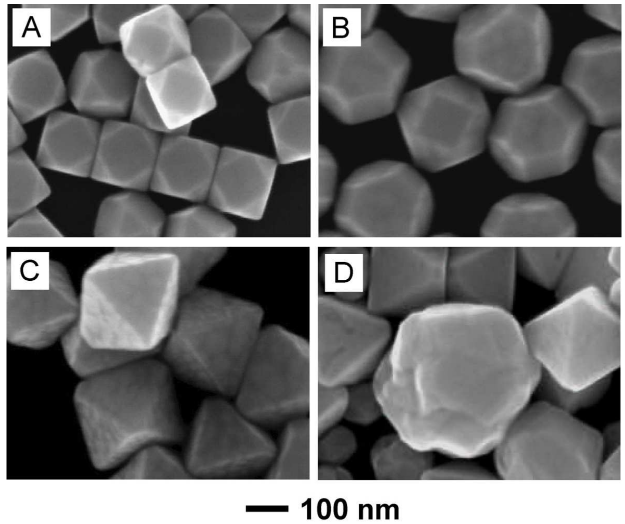

Figure S3. SEM images of Ag nanocrystals grown from the 40-nm cubic seeds with 1.0 mM PVP55 serving as the capping agent. The samples were obtained at different time points: (A) 25 min, (B) 45 min, (C) 75 min, and (D) 90 min.

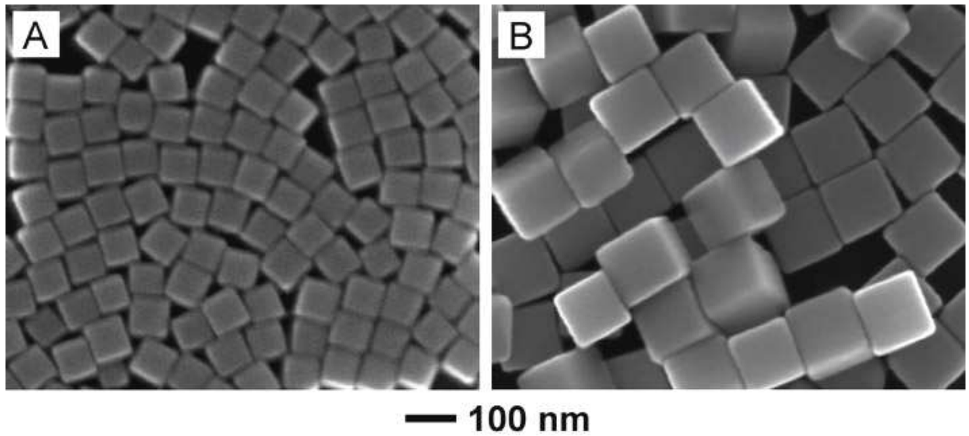

Figure S4. SEM images of Ag cubes grown from the 40-nm cubic seeds in the presence of 2.0 mM PVP55 as the capping agent. The samples were obtained after the growth had proceeded for (A) 5 min and (B) 20 min, respectively.

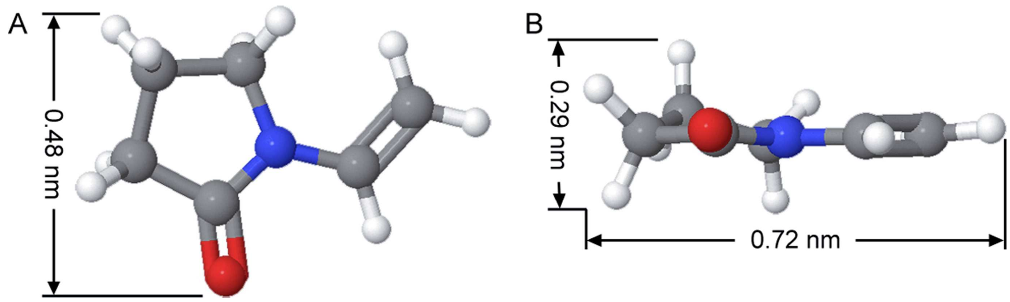

Figure S5. A schematic of the PVP monomer (*N*-vinypyrrolidone) viewed from two orthogonal directions. The red balls represent O atoms; the blue balls represent N atoms; the grey balls represent C atoms; and the white balls represent H atoms. When acting as a capping agent for Ag nanocrystals, the O atom will be used to bind to the Ag surface. From the length of C-C bond (0.154 nm), the dimensions of a PVP monomer were estimated and marked on the drawings. The area (0.29×0.72 nm = 0.21 nm^2) occupied by a PVP monomer can thus be calculated from the data in (B). The thickness of a monolayer of PVP repeating units is estimated to be 0.48 nm (see A). For a coverage density of 140 repeating units per nm^2, the number of PVP repeating units in each segment of PVP on the Ag surface is estimated to be around 29.

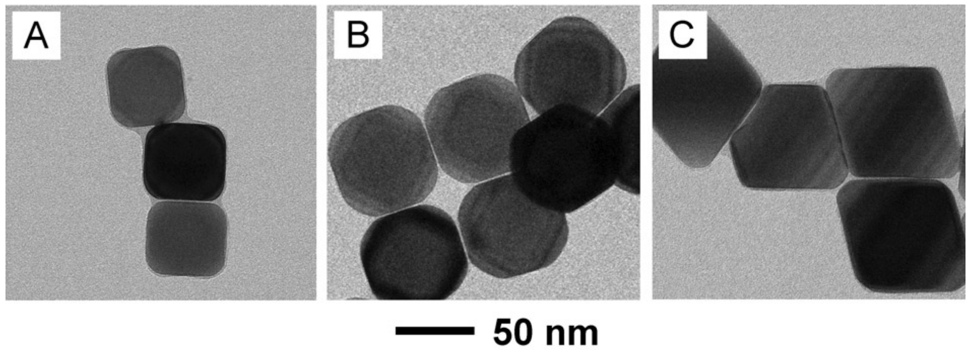

Figure S6. TEM images of the Ag polyhedrons shown in Figure 2, D-F.

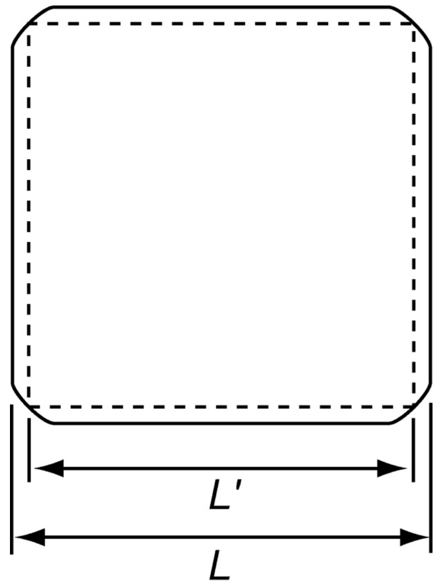

Figure S7. A schematic drawing of a Ag cubic seed viewed along the <100> directions. The corners of the seed are slightly truncated. The size (L) of a seed is defined as the distance between two opposite {100} facets. L' represents the size of a perfect cube encased by the cubic seed with its vertices located at the centers of facets formed by truncation. When the seed grows only along <100> directions, the size of the finally formed octahedron will be determined by L' rather than L.

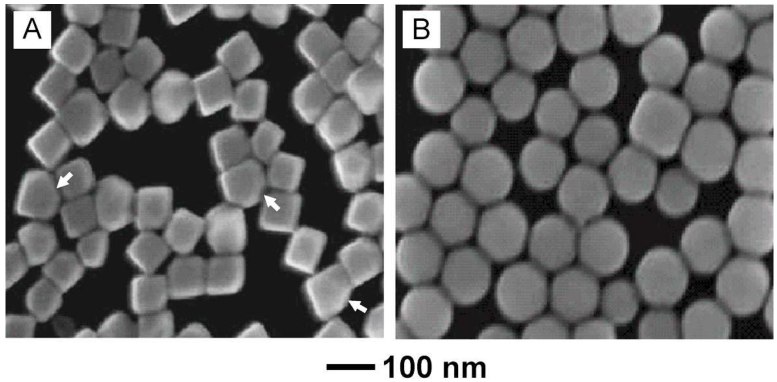

Figure S8. SEM images of Ag nanocrystals grown from the 40-nm cubic seeds in the absence of additional PVP. The samples were obtained after the growth had proceeded for (A) 5 min and (B) 10 min, respectively. White arrows in (A) indicate the Ag cubes with heterogeneous truncation at the corner sites (*i.e.*, some of the corners have not been truncated while the rest have been).

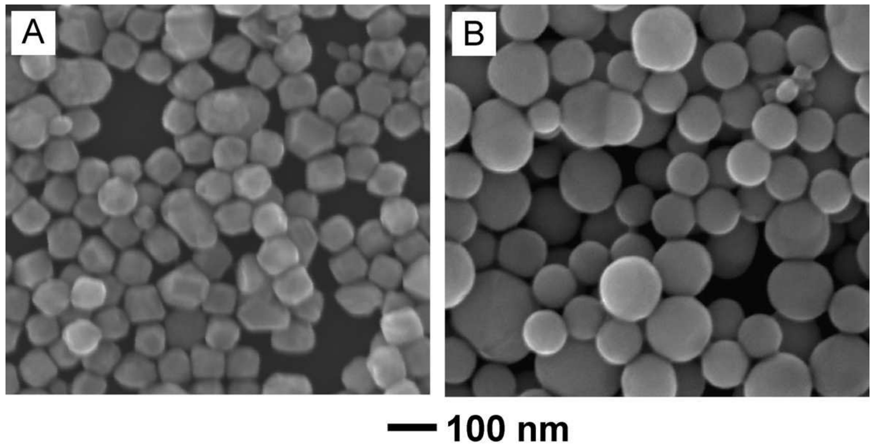

Figure S9. SEM images of Ag nanocrystals grown from the 40-nm cubic seeds in the presence of 0.1 mM 1-mehyl-2-pyrrolidinone as the capping agent. The samples were obtained after the growth had proceeded for (A) 5 min and (B) 10 min, respectively.

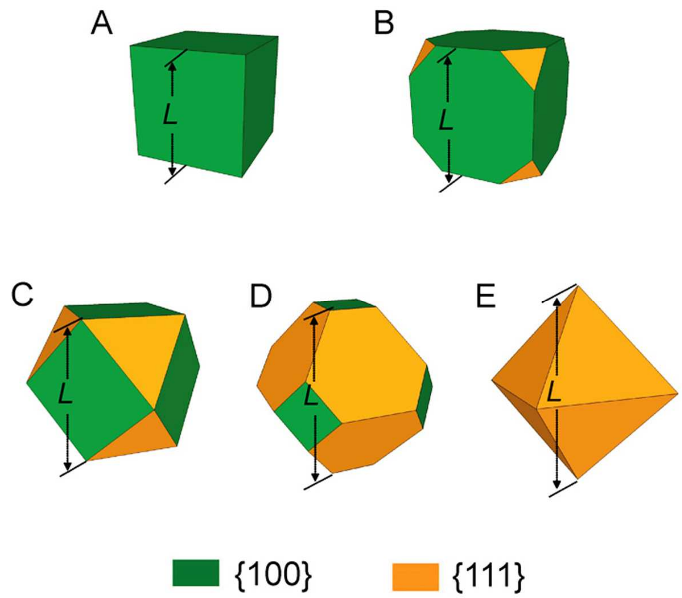

Figure S10. Definition of the size (L) for different types of Ag polyhedrons: A) cube; B) truncated cube; C) cuboctahedron; D) truncated octahedron; E) octahedron. Here L is defined as the distance between two opposite {100} facets.

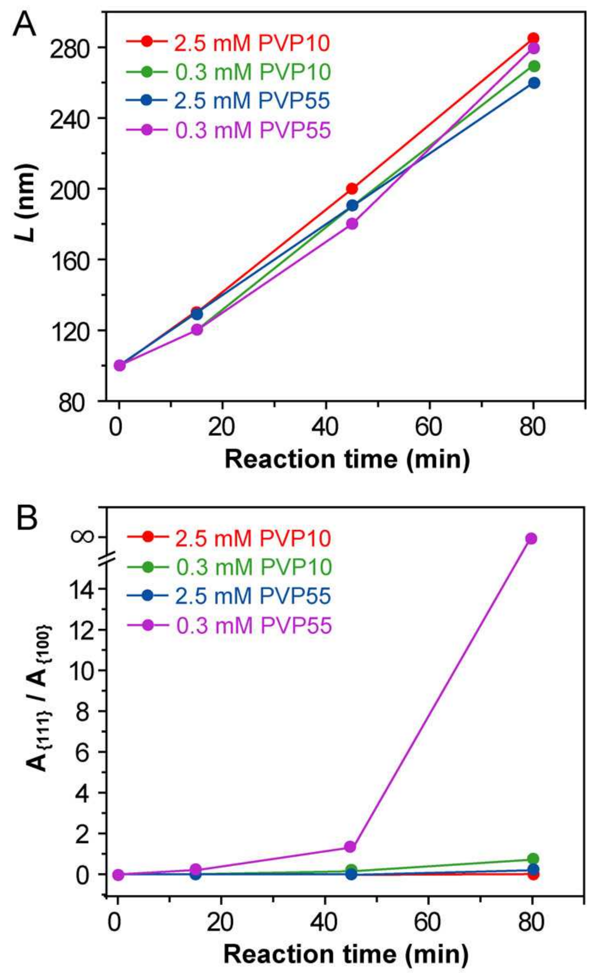

Figure S11. Plots of (A) size (L) and (B) the ratio between the areas of {111} and {100} facets for the Ag polyhedrons shown in Figures 5 and 6 as a function of reaction time.

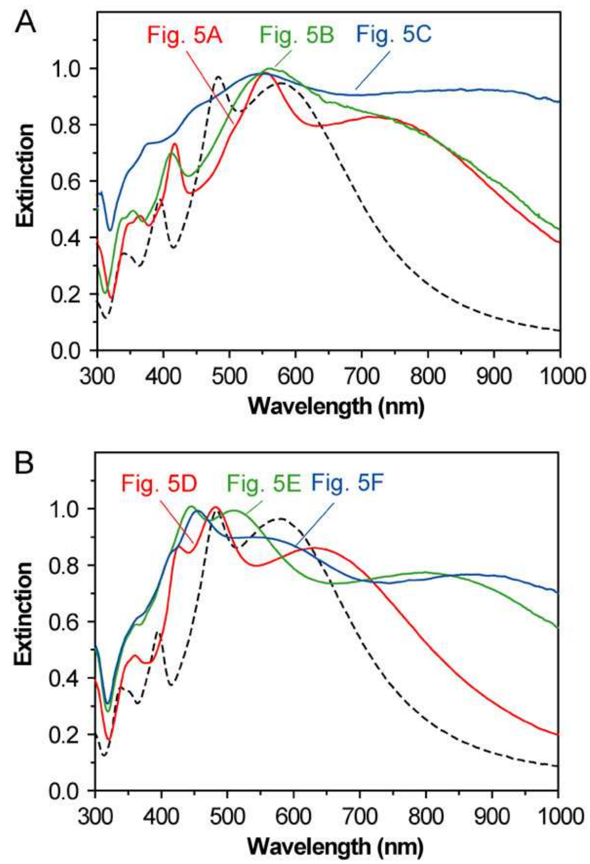

Figure S12. Normalized UV-vis spectra of samples shown in Figure 5 (as indicated in the plots). Dashed lines represent UV-vis spectra of the 100-nm cubic seeds of Ag.