Supporting Information

Photothermal Transformation of Au-Ag Nanocages under Pulsed Laser Irradiation

Zachary D. Hood,[a,b,†] Kelsey P. Kubelick,[c,†] Kyle D. Gilroy,[c,†] Don Vanderlaan,[d] Xuan Yang,[c] Miaoxin Yang,[a] Miaofang Chi,[b] Stanislav Y. Emelianov,[c,d*] and Younan Xia[a,c,*]

[a] School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia 30332, USA

[b] Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

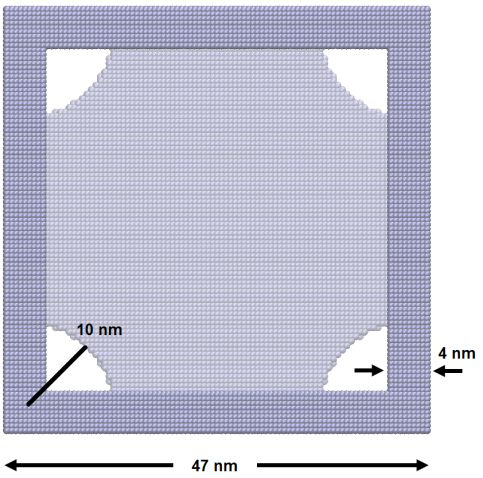
[c] Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology and Emory University, Atlanta, Georgia 30332, USA

[d] School of Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA

[†]These authors contributed equally to this publication

*Corresponding authors: Stanislav Emelianov (stas@gatech.edu) and Younan Xia (younan.xia@bme.gatech.edu)

Continuum Model for discrete dipole approximation (DDA) simulations. To create a continuum model that had a shape similar to that of the nanocage structure for the DDA calculations, we used molecular dynamics software (Large-scale Atomic/Molecular Massively Parallel Simulator, LAMMPS) to first generate a cubic continuum with a simple cubic (*sc*) lattice with 857375 dipoles. Then, a cubic region was deleted (minus 456533 dipoles) from the interior to leave behind a cubic hollow box with 400842 dipoles remaining. Finally, eight spherical voids were deleted from the corner sites, which correspond to 9066 dipoles from each corner site. The final structure contained 328314 dipoles, and a cross section of the final structure is shown in the drawing.



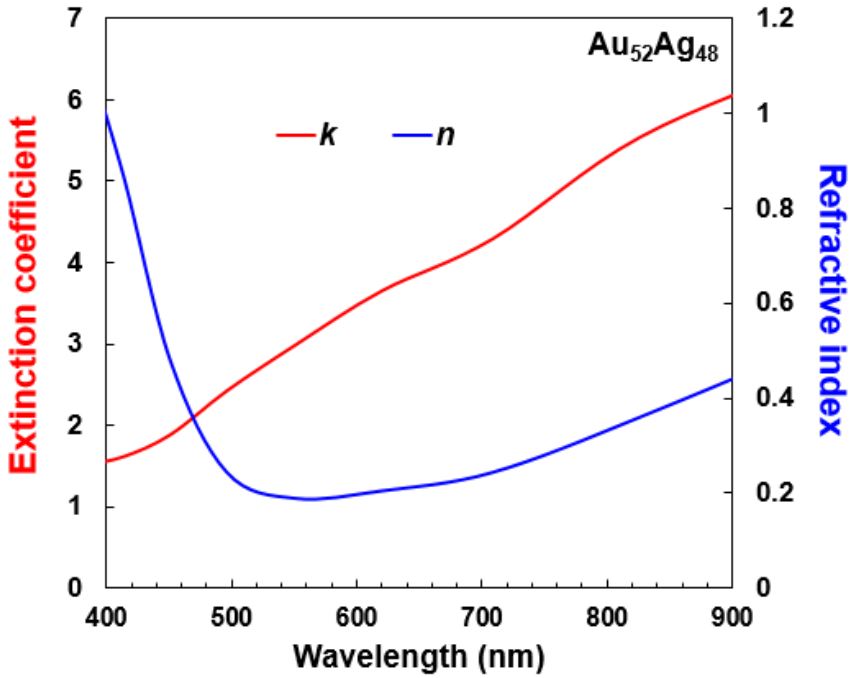


Figure S1. Plot of the dielectric constants for $Au_{52}Ag_{48}$ extracted from ref. 1, trending extinction coefficient and refractive index versus wavelength.

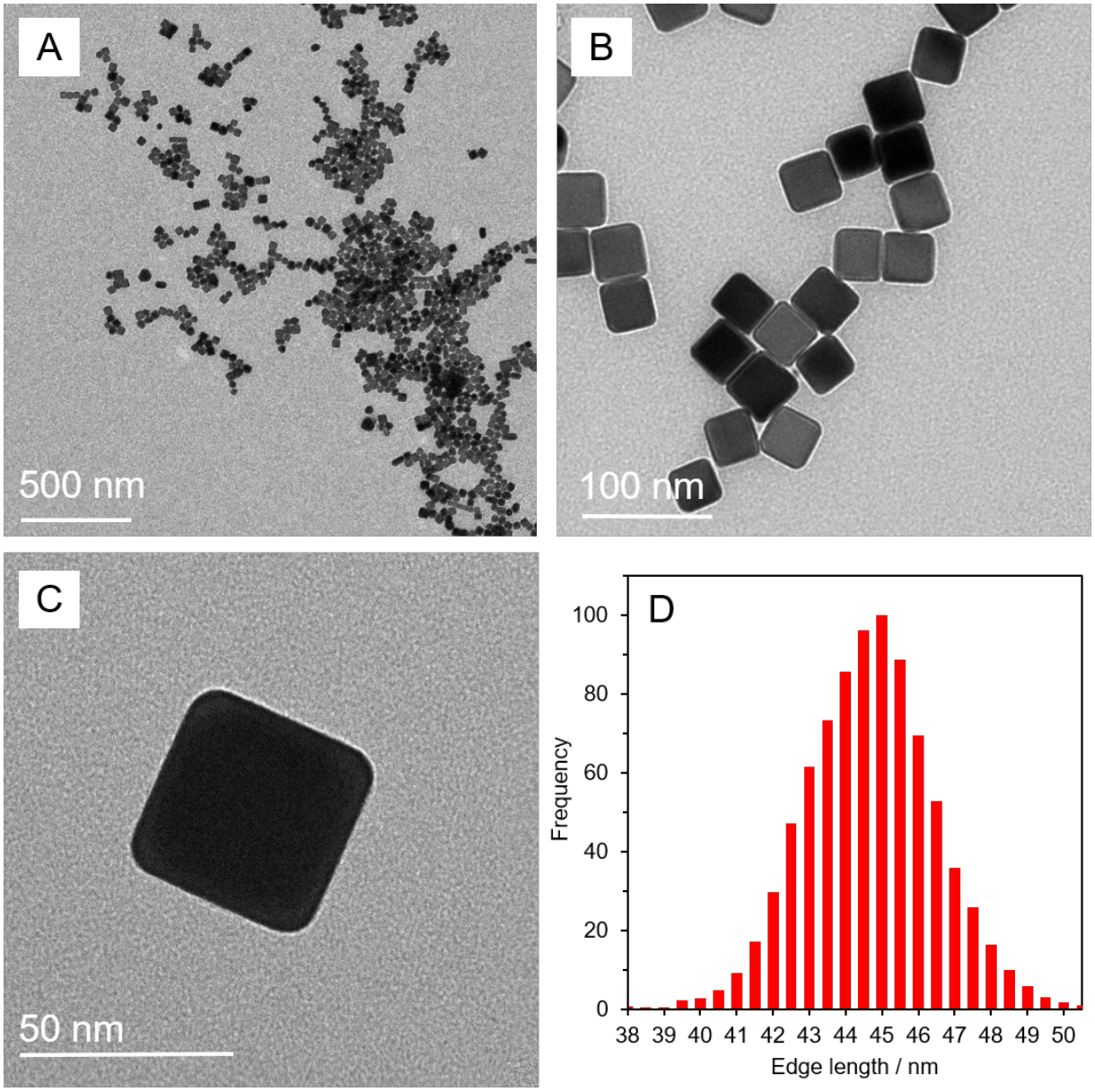


Figure S2. (A-C) TEM images of the as-prepared Ag nanocubes. (D) Histogram of the edge lengths of the Ag nanocubes.

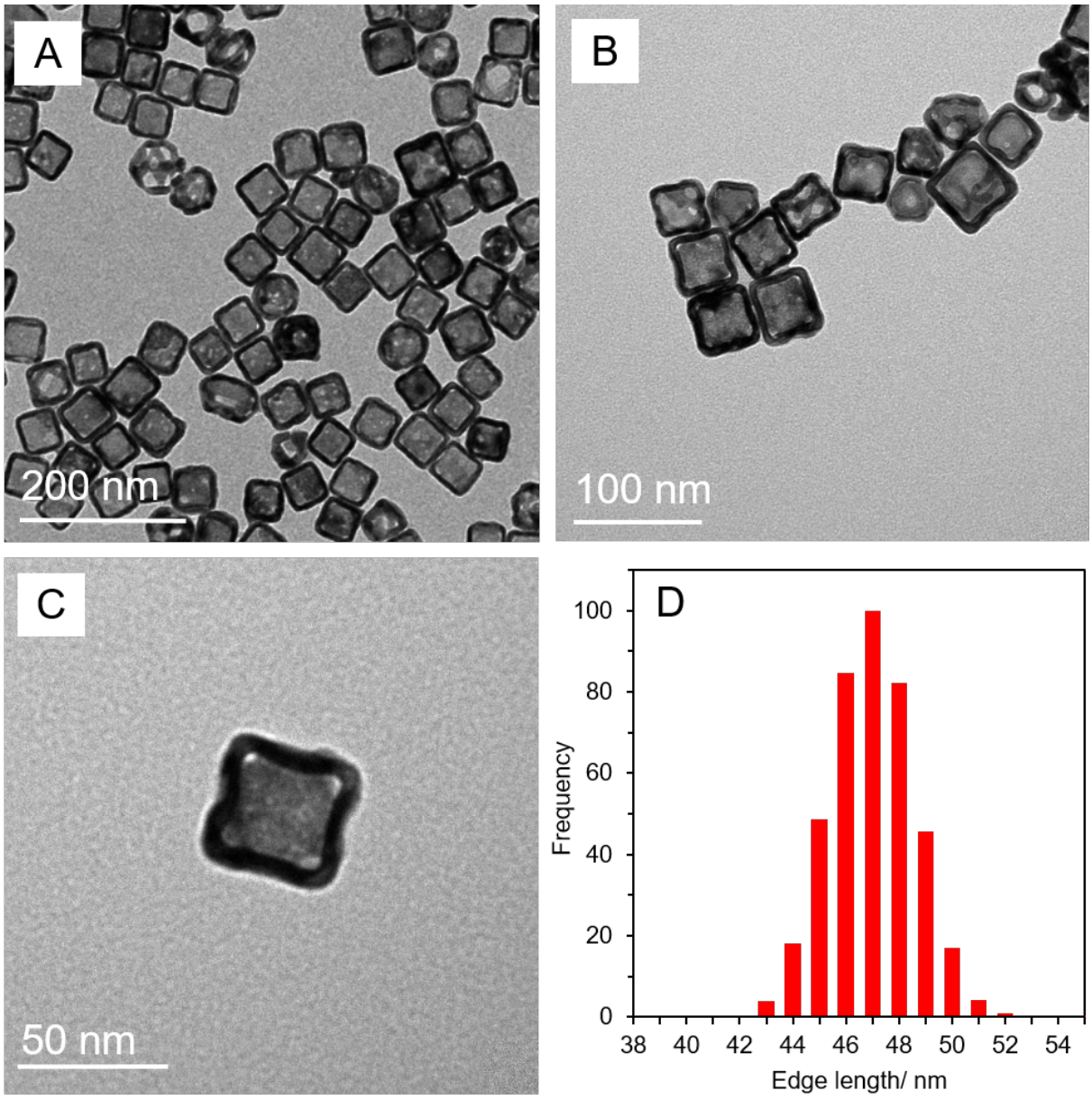


Figure S3. (A-C) TEM images of the as-prepared Au-Ag nanocages. (D) Histogram of the edge lengths of the nanocages.

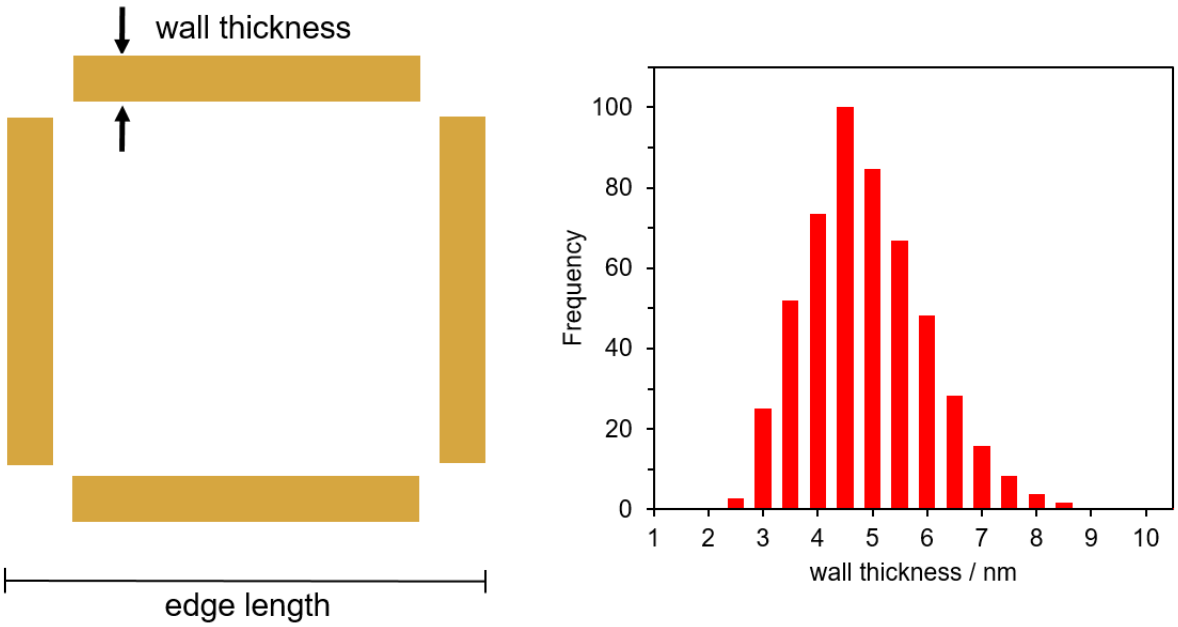


Figure S4. Definition of the wall thickness (left) and a histogram showing the thickness distribution for the nanocages (right). All particles were analyzed using ImageJ software.

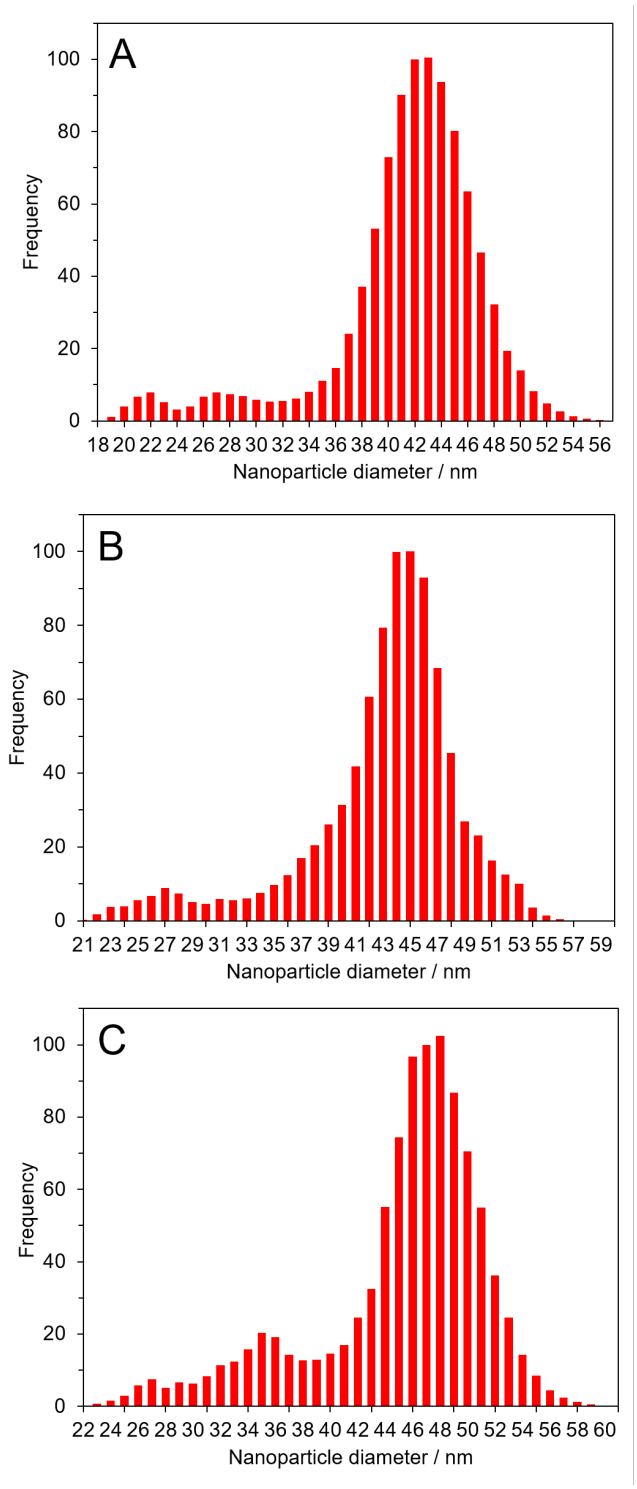


Figure S5. Histograms showing the diameters of the pseudo-spherical, solid nanoparticles obtained after 300 pulses at (A) 8, (B) 12, and (C) 20 mJ cm^{-2}.

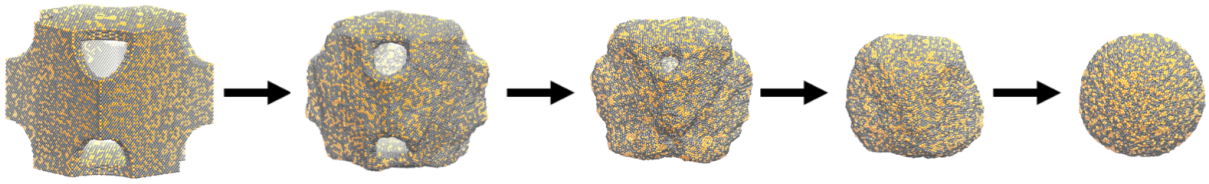


Figure S6. Schematic illustration of the proposed transformation process. The evolving structures in this schematic were generated using molecular dynamics software (LAMMPS, ref. 2). The depictions are not meant to represent the actual data and merely serve as a proposed pathway for structural evolution.

References

1. Peña-Rodríguez, O.; Caro, M.; Rivera, A.; Olivares, J.; Perlado, J. M.; Caro, A. *Opt. Mater. Express* **2014**, *4*, 403.
2. Humphrey, W., Dalke, A., Schulten, K., VMD - Visual Molecular Dynamics, *J. Molec. Graphics*, **1996**, *14*, 33.