Supplementary Materials for

“Sintering of Multiple Cu-Ag Core-Shell Nanoparticles and Properties of Nanoparticle-Sintered Structures”

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Figure S1: Final Morphology of sintered multiple-CS-NP model Ag$_5$Cu$_{2.5}$ at different temperatures ($T$'s). The pores are not eliminated under $T$ of 500 K. As $T$ increases from 600 K to 900 K, the porosity gradually decreases, thus a more densified structure is obtained, but still some pores are left inside within the sintered structures. At 1000 K, the whole system melts, the core-shell structure is collapsed and a Cu-Ag alloy is obtained. Color scheme is explained as: Blue: Ag FCC; Yellow: Ag HCP; Red: Ag amorphous; Green: Cu FCC; Magenta: Cu HCP; Cyan: Cu amorphous.
Figure S2: Mean square displacement ($\langle d^2 \rangle$) during the sintering of multiple-CS-NP structures with (a) Ag$_8$Cu$_4$ and (b) Ag$_{11}$Cu$_{5.5}$, respectively. Cross-sectional images of multiple-CS-NP structures with (c) Ag$_8$Cu$_4$ and (d) Ag$_{11}$Cu$_{5.5}$ at critical $T$'s. Slow solid diffusion can be observed at 900 K in (a) while no solid diffusion can be observed after the liquid diffusion of surface premelted atoms at surface premelting temperature ($T_{sm}$) 1100 K. However, continuous diffusion is observed at both 1100 K and 1160 K in multiple-CS-NP Ag$_{11}$Cu$_{5.5}$ due to the continuous pore narrowing. Pores are eliminated at $T_{sm}$ (1100 K) in multiple-CS-NP structures with Ag$_8$Cu$_4$; thus, no solid diffusion can be observed in (a). However, for Ag$_{11}$Cu$_{5.5}$, pores survive even at $T_{sm}$ (1160 K), causing continuous solid diffusion following by initial liquid diffusion. The Ag shell atoms are colored with green, while the Cu core atoms are colored with blue.
Figure S3: Final sintered structure of multiple Ag$_5$Cu$_9$ NPs (pure Ag NPs) at 600 K. Pores are not eliminated at this $T$, while the pores do not survive in multiple CS NPs at 600 K, which proves that the interfacial atoms have higher mobility in CS NP and contribute to a higher densification.
Figure S4: Mean square displacement ($\langle d^2 \rangle$) of the (a) surface and (b) shell atoms during the sintering of multiple Ag$_5$Cu$_{2.5}$ NPs. The self-diffusivity (in the unit of Å$^2$/ps) obtained by linear fitting is also shown after each $T$. The dots in each curve represent the starting and ending points, during which the $\langle d^2 \rangle$ is used to calculate the self-diffusivity and activation energy.
Figure S5: Stress-strain plots for structures sintered by multiple NPs (a) Ag$_5$Cu$_0$, (b) Ag$_5$Cu$_{2.5}$, (c) Ag$_8$Cu$_4$, and (d) Ag$_{11}$Cu$_{5.5}$ at different $T$'s. Note that all tensile simulations are performed at 300 K, i.e., the final sintered structures are quenched to 300 K before executing the tensile simulations.
Figure S6: Potential energy ($E_p$) evolution during the quenching process of the sintered structures of multiple NPs (a) Ag$_5$Cu$_0$, (b) Ag$_5$Cu$_{2.5}$, (c) Ag$_8$Cu$_4$, and (d) Ag$_{11}$Cu$_{5.5}$. No steep decrease of $E_p$ is observed in these curves, indicating the formation of metallic glass after the quenching process.
Figure S7: Plots of \((-\Delta \frac{V}{V_0} - \Delta \rho)\) of structures sintered by multiple NPs (a) Ag₅Cu₀, (b) Ag₅Cu₂.₅, (c) Ag₈Cu₄, and (d) Ag₁₁Cu₅.₅ at different T's. Isothermal compressibility is the slope of the linear fitting lines.
Figure S8: Plots of $(\Delta V/V_0 - \Delta T)$ of structures sintered by multiple NPs (a) Ag$_5$Cu$_0$, (b) Ag$_5$Cu$_{2.5}$, (c) Ag$_8$Cu$_4$, and (d) Ag$_{11}$Cu$_{5.5}$ at different $T$'s. Coefficient of thermal expansion is the slope of the linear fitting lines.