Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Materials for

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

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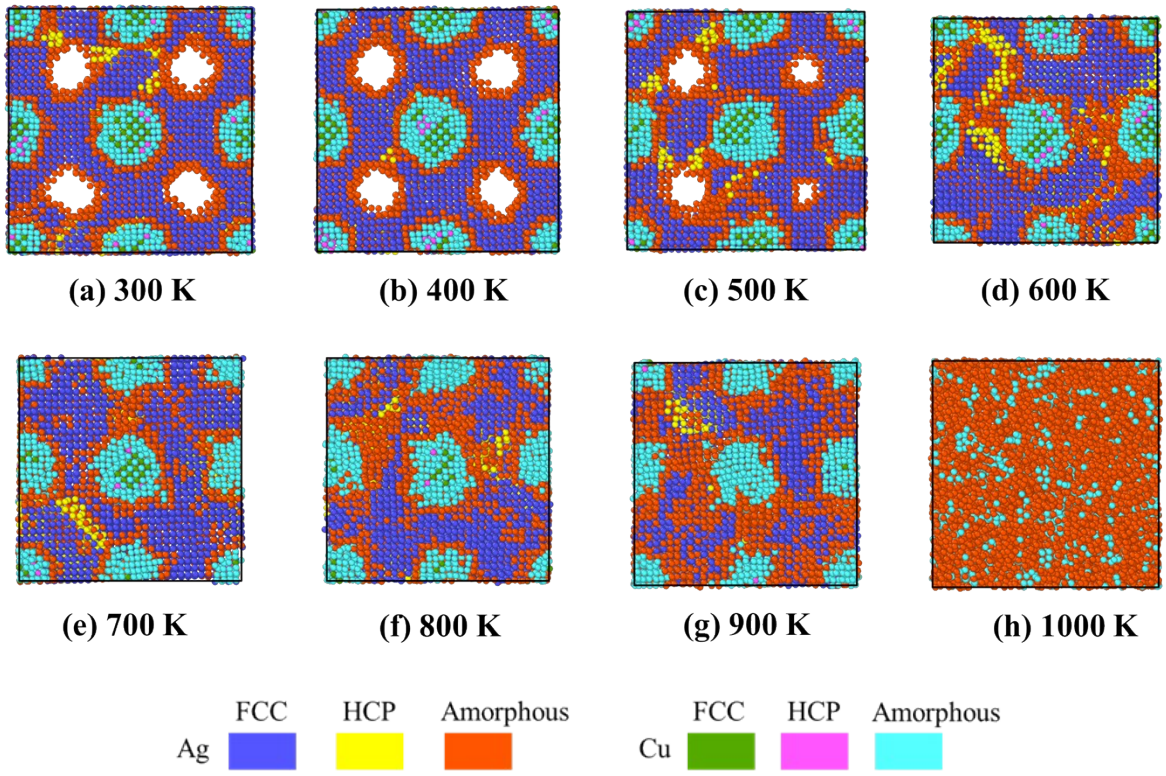

Figure S1: Final Morphology of sintered multiple-CS-NP model $Ag_5Cu_{2.5}$ at different temperatures (*T*'s). The pores are not eliminated under *T* of 500 K. As *T* increases from 600 K to 900 K, the porosity gradually decreases, thus a more densified structure is obtained, but still some pores are 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.

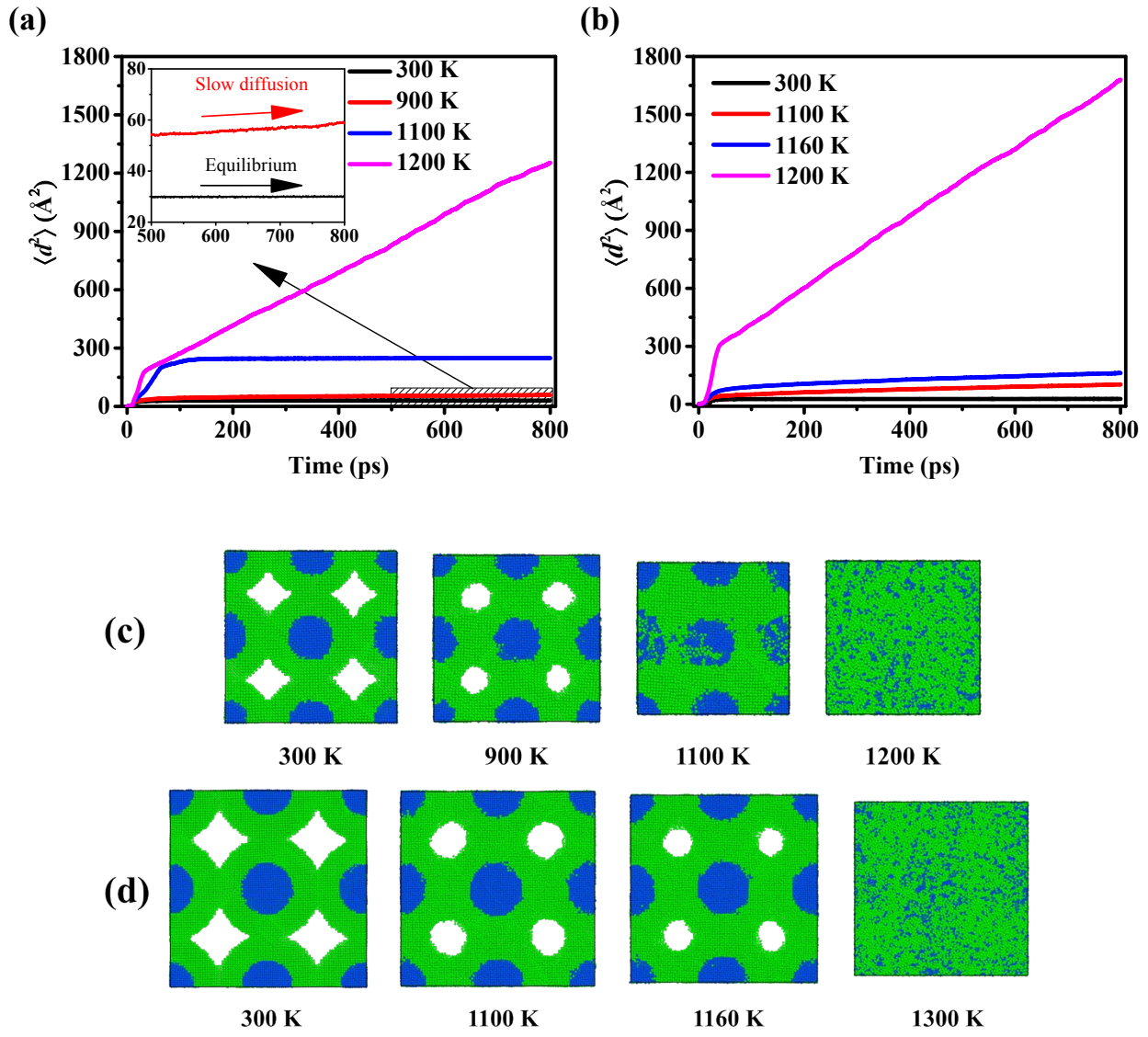

Figure S2: Mean square displacement ($\langle d^2 \rangle$) during the sintering of multiple-CS-NP structures with **(a)** Ag_8Cu_4 and **(b)** $Ag_{11}Cu_{5.5}$, respectively. Cross-sectional images of multiple-CS-NP structures with **(c)** Ag_8Cu_4 and **(d)** $Ag_{11}Cu_{5.5}$ at critical T's. Slow 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_8Cu_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.

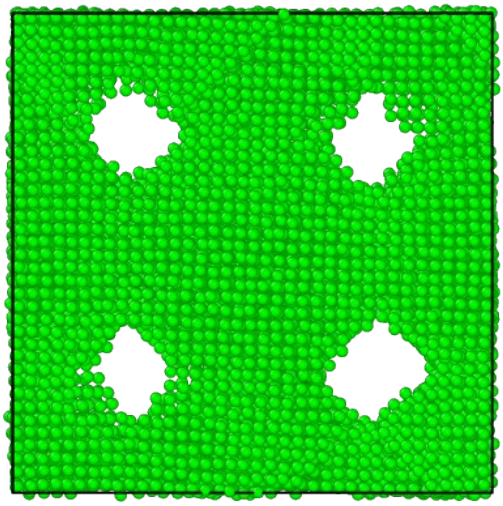

Figure S3: Final sintered structure of multiple Ag_5Cu_0 NPs (pure Ag NPs) at 600 K. Pores are not eliminated at this *T*, while the pores do not survive in multiple CS NPs at 600 K, which proves that the interfacial atoms have higher mobility in CS NP and contribute to a higher densification.

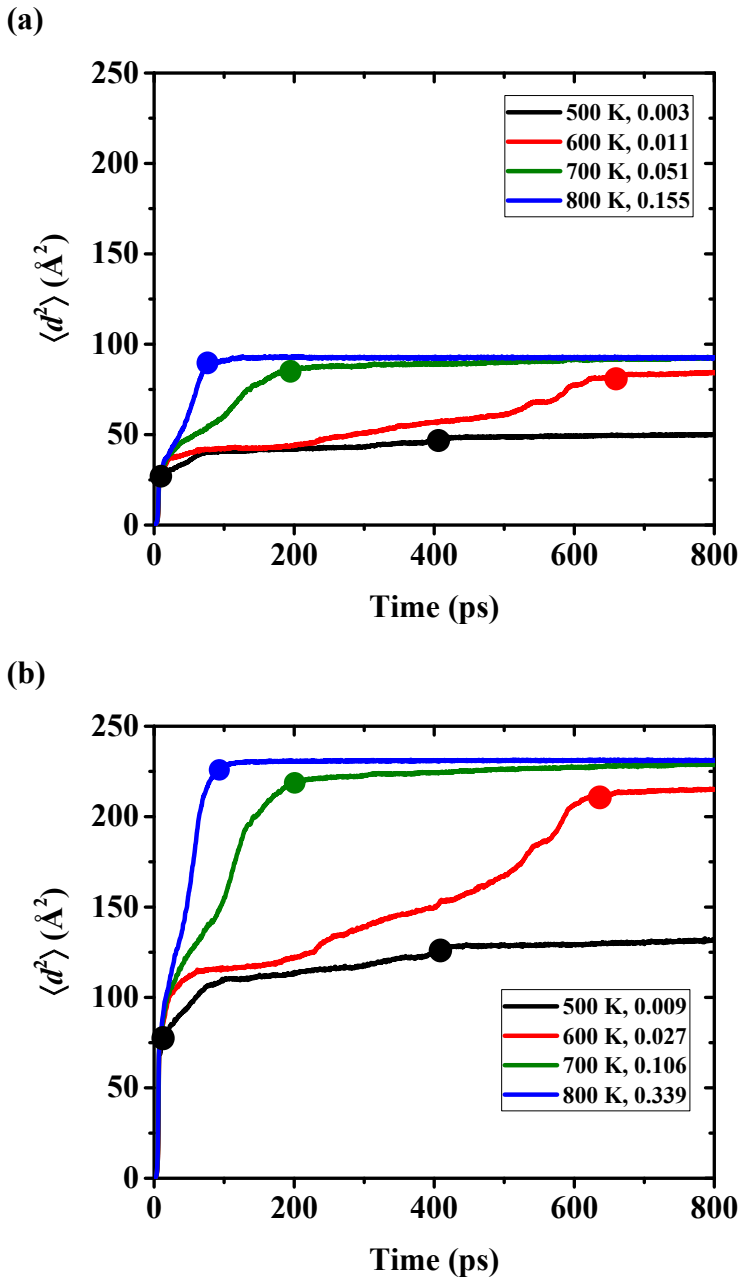

Figure S4: Mean square displacemnt ($\langle d^2 \rangle$) of the **(a)** surface and **(b)** shell atoms during the sintering of multiple $Ag_5Cu_{2.5}$ NPs. The self-diffusivity (in the unit of $Å^2$/ps) obtained by linear fitting is also shown after each T. The dots in each curve represent the starting and ending points, during which the $\langle d^2 \rangle$ is used to calculate the self-diffusivity and activation energy.

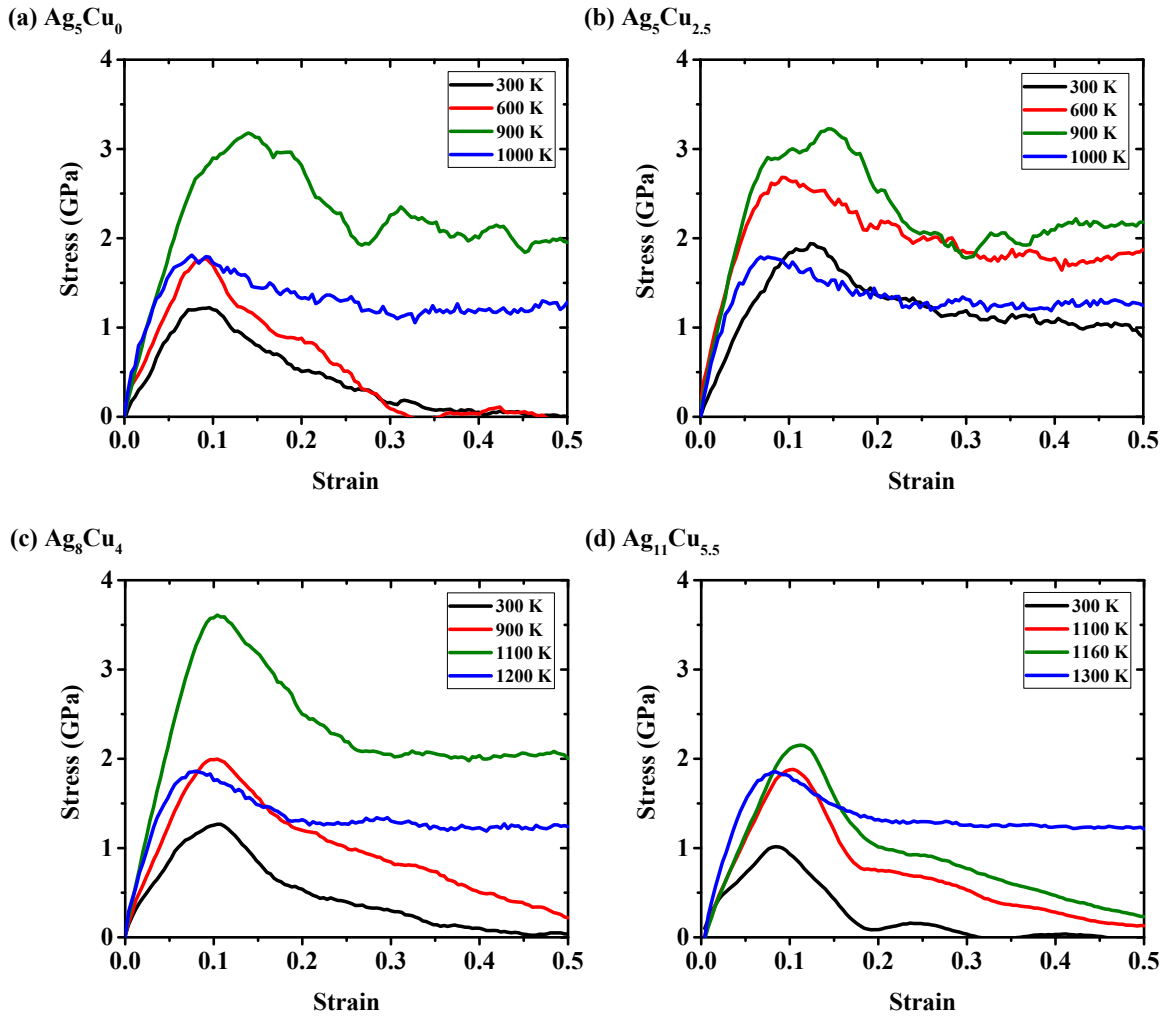

Figure S5: Stress-strain plots for structures sintered by multiple NPs **(a)** Ag_5Cu_0, **(b)** $Ag_5Cu_{2.5}$, **(c)** Ag_8Cu_4, and **(d)** $Ag_{11}Cu_{5.5}$ at different *T*'s. Note that all tensile simulations are performed at 300 K, i.e., the final sintered structures are quenched to 300 K before executing the tensile simulations.

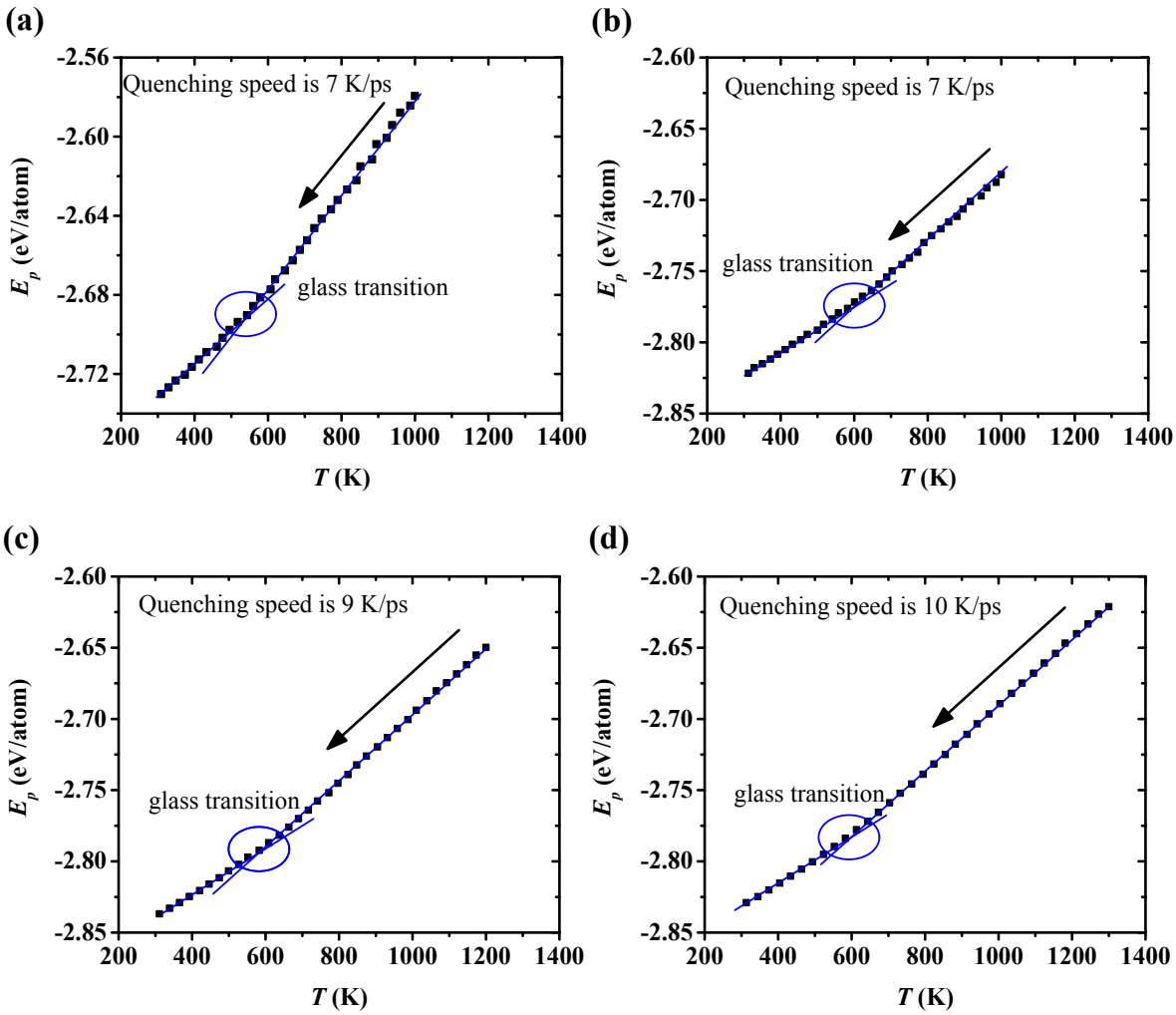

Figure S6: Potential energy (E_p) evolution during the quenching process of the sintered structures of multiple NPs **(a)** Ag_5Cu_0, **(b)** $Ag_5Cu_{2.5}$, **(c)** Ag_8Cu_4, and **(d)** $Ag_{11}Cu_{5.5}$. No steep decrease of E_p is observed in these curves, indicating the formation of metallic glass after the quenching process.

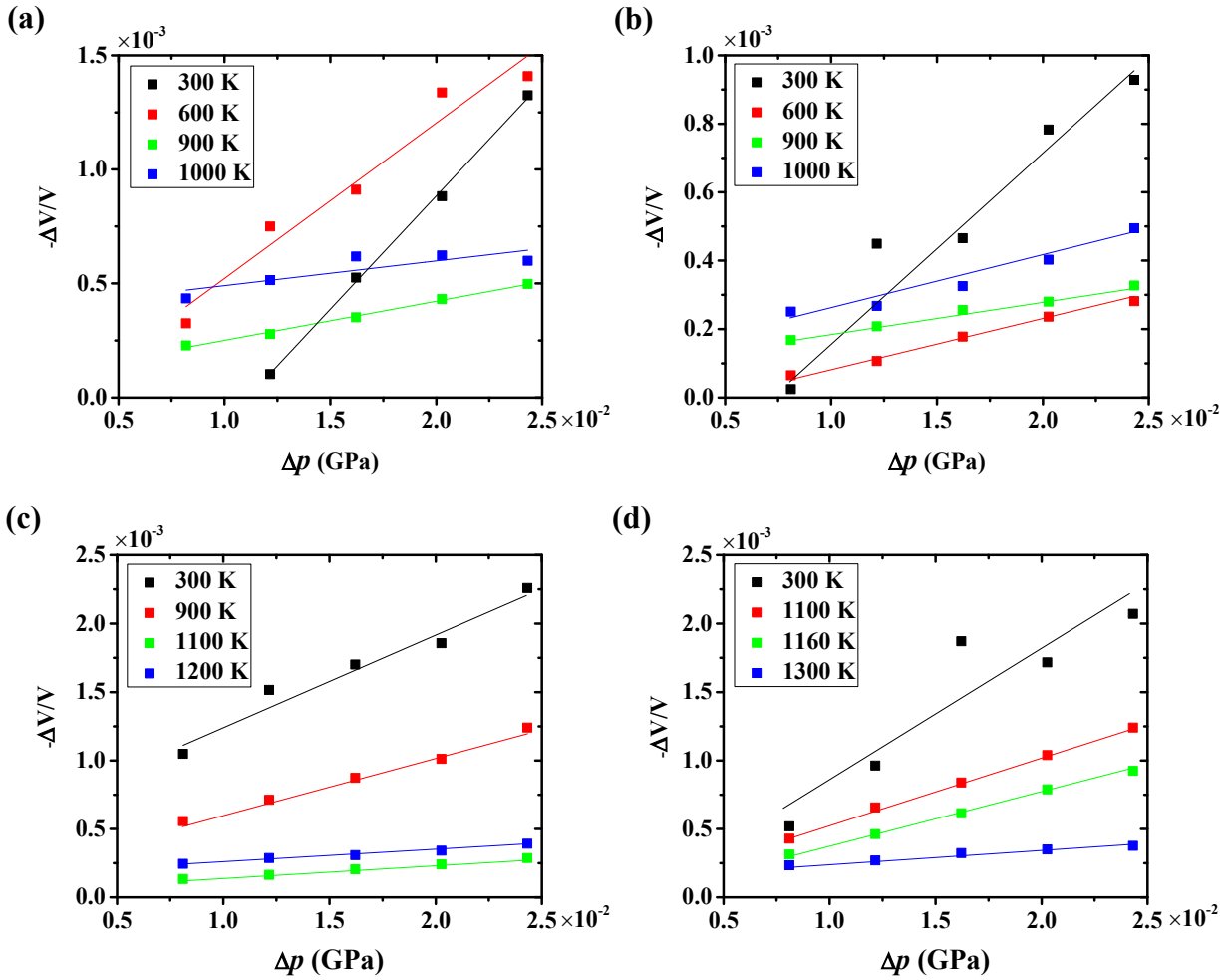

Figure S7: Plots of ($-\Delta V/V_0 - \Delta p$) of structures sintered by multiple NPs **(a)** Ag_5Cu_0, **(b)** $Ag_5Cu_{2.5}$, **(c)** Ag_8Cu_4, and **(d)** $Ag_{11}Cu_{5.5}$ at different T's. Isothermal compressibility is the slope of the linear fitting lines.

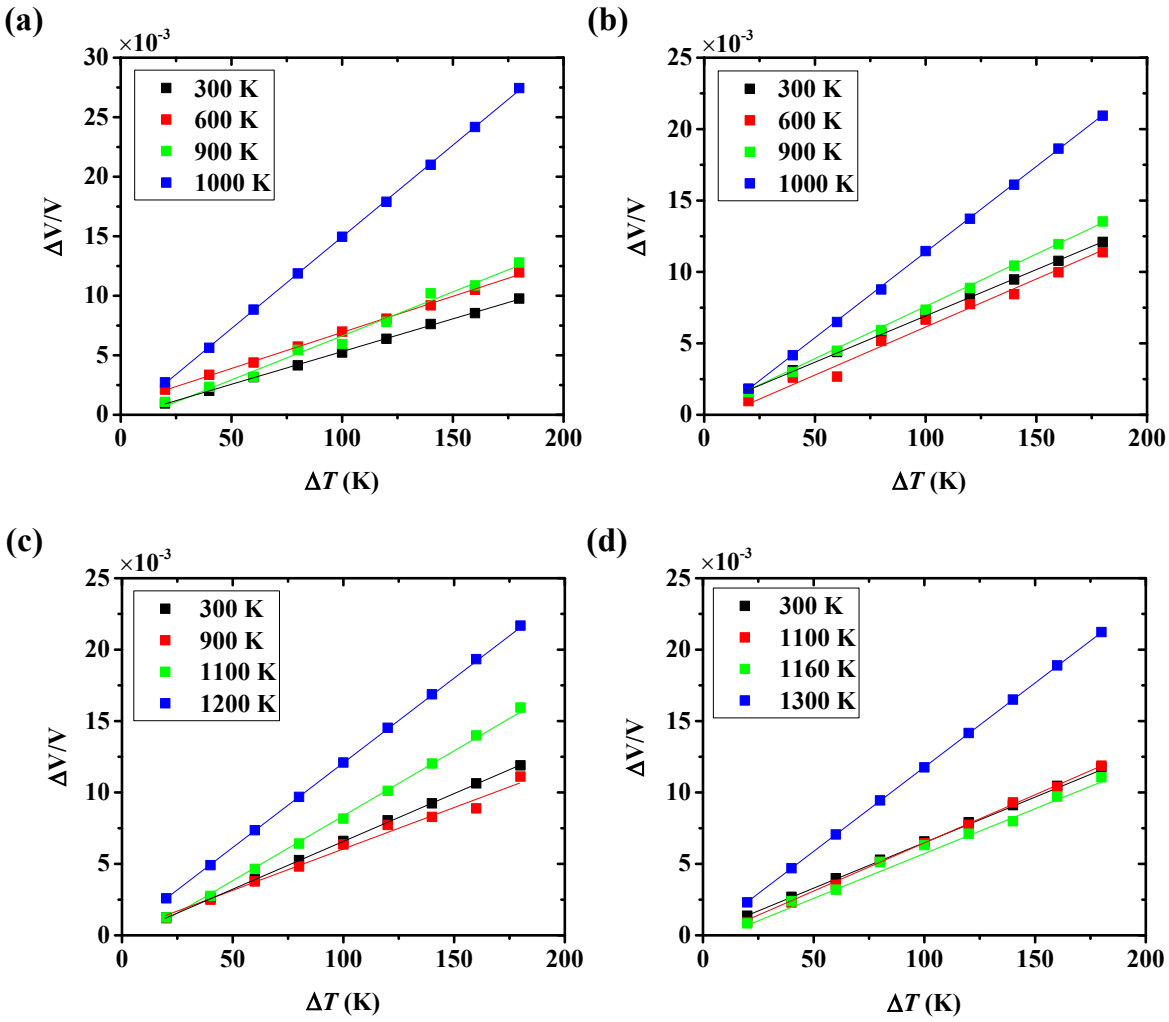

Figure S8: Plots of ($\Delta V/V_0 - \Delta T$) of structures sintered by multiple NPs **(a)** Ag_5Cu_0, **(b)** $Ag_5Cu_{2.5}$, **(c)** Ag_8Cu_4, and **(d)** $Ag_{11}Cu_{5.5}$ at different T's. Coefficient of thermal expansion is the slope of the linear fitting lines.