Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information for:

Chemical Ordering and Temperature Effect on the Thermal Conductivity of Ag-Au and Ag-Pd Bimetallic Bulk and Nanocluster Systems

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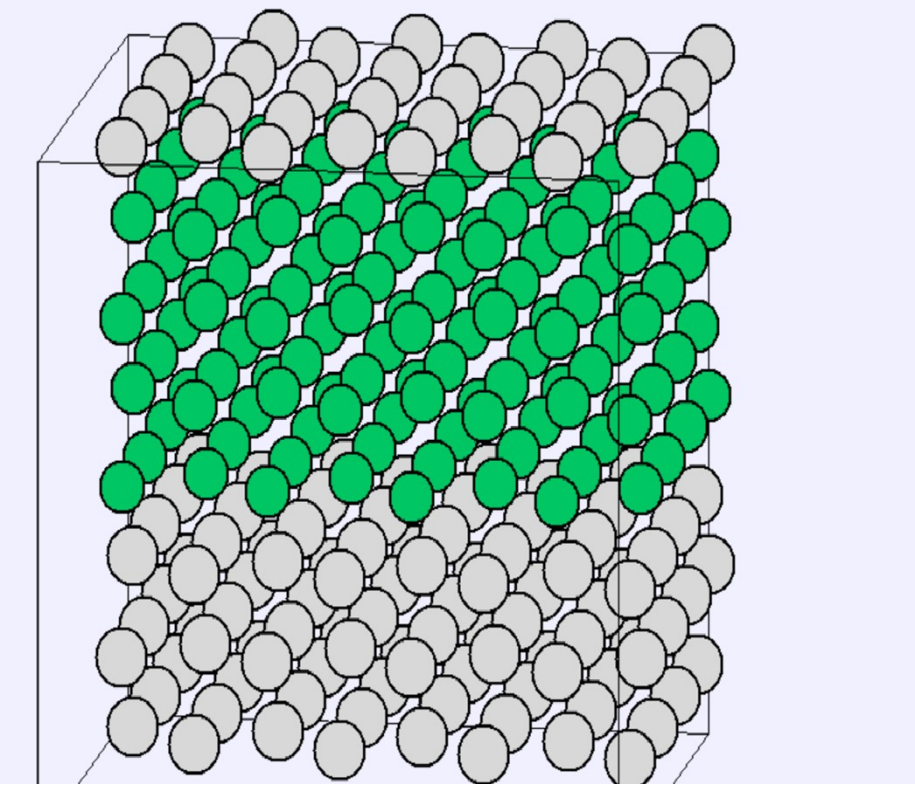


Fig.S1 bulk (Ag0.5-Pd0.5) N=256

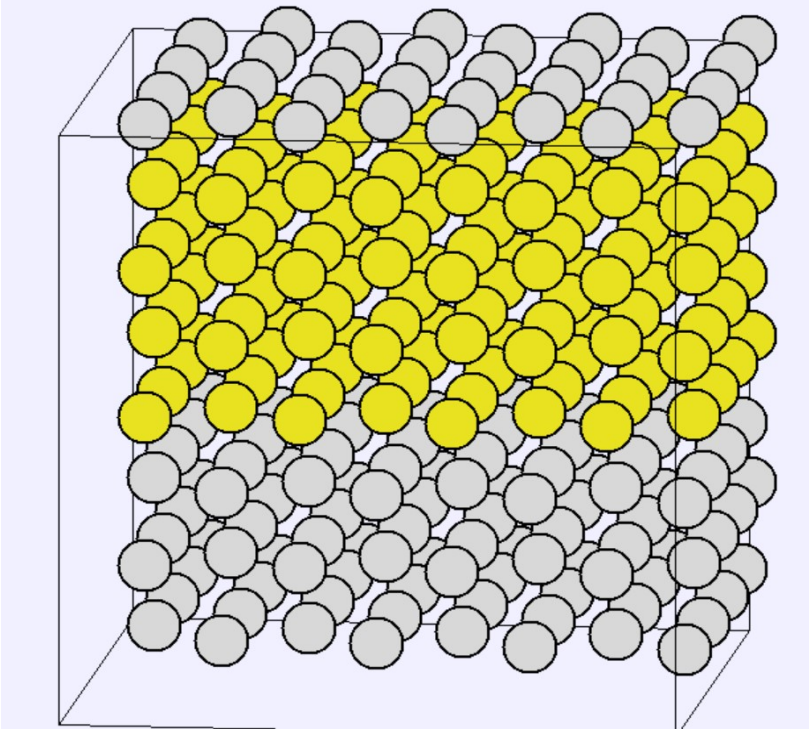
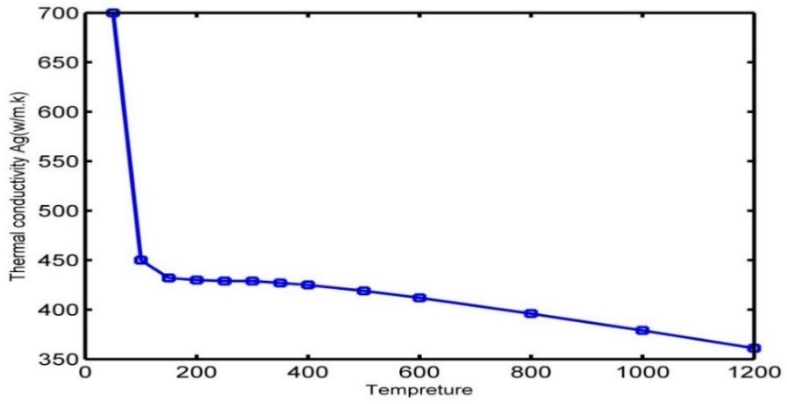
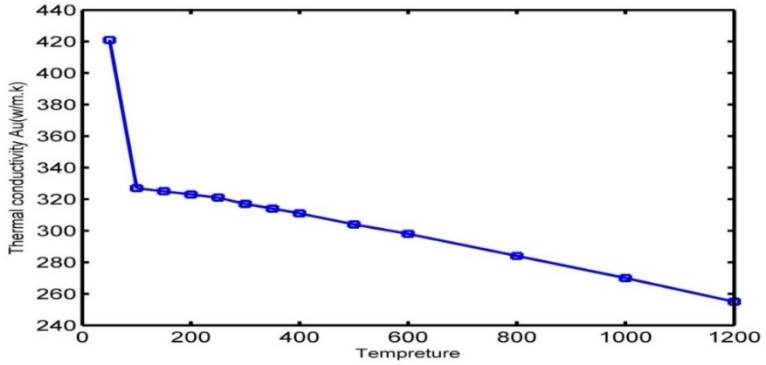


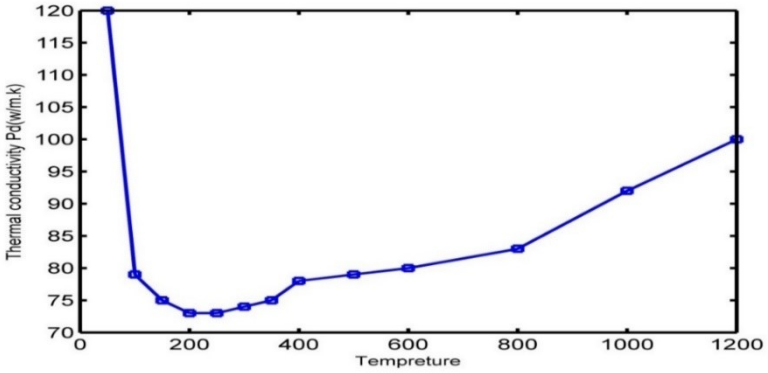
Fig.S2 (Ag0.5-Au0.5) N=256


Thermal conductivity Ag(w/m.k)
Tempreture
700
650
600
550
500
450
400
350
0
200
400
600
800
1000
1200

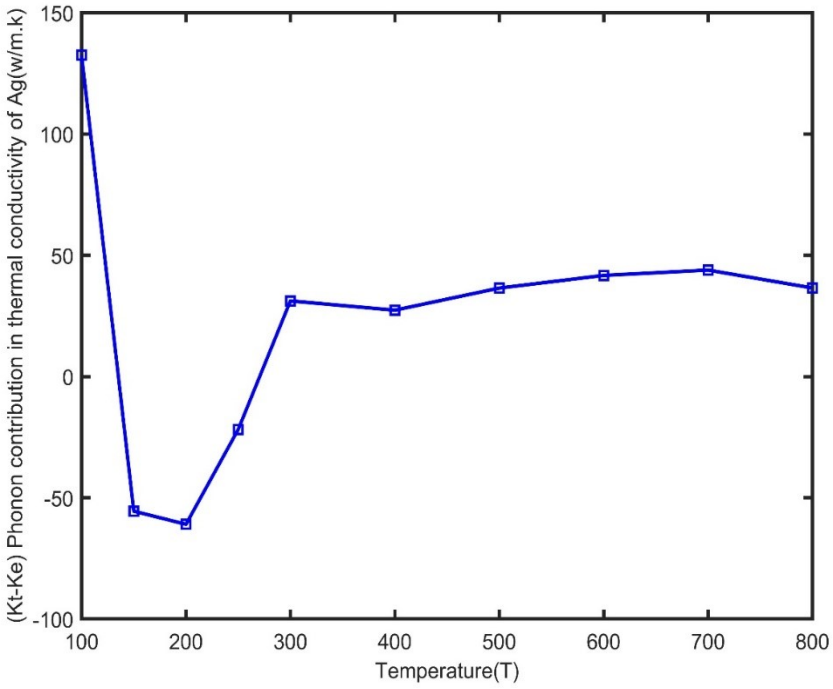
(a)


Thermal conductivity Au(w/m.k)
Tempreture
440
420
400
380
360
340
320
300
280
260
240
0
200
400
600
800
1000
1200

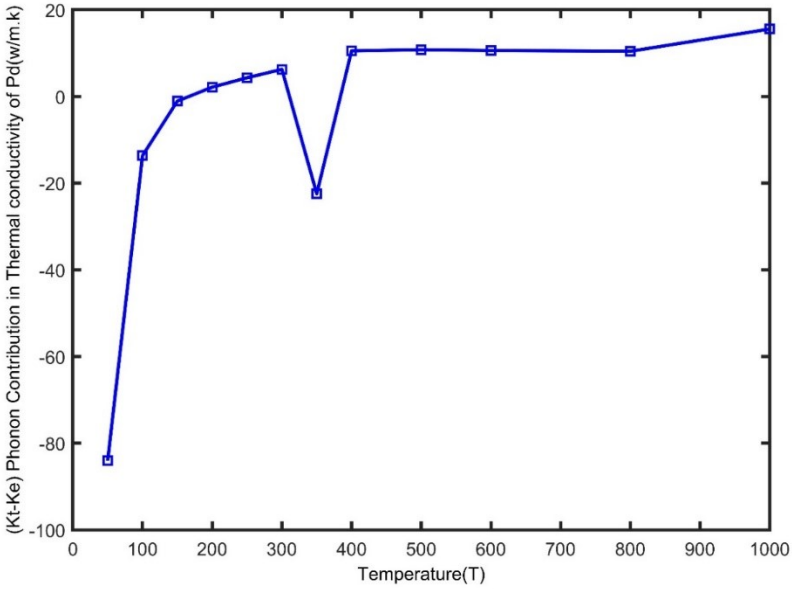
(b)


Thermal conductivity Pd(w/m.k)
Tempreture
120
115
110
105
100
95
90
85
80
75
70
0
200
400
600
800
1000
1200

(c)

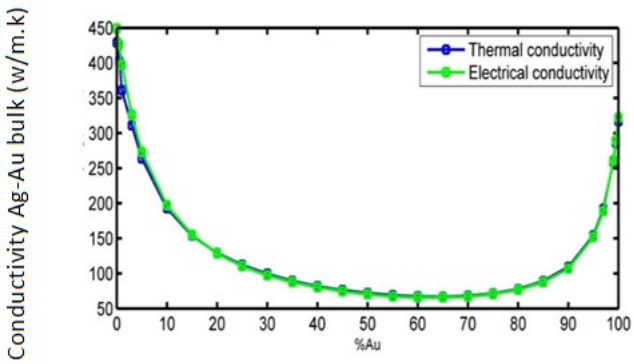


(d)

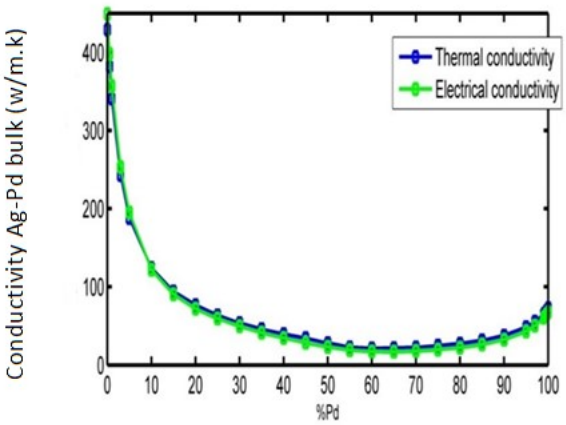


(e)

Fig.S3. (a-c) Experimental thermal conductivity of bulk metals as a function of temperature: (a) Ag, (b) Au, and (c) Pd, respectively. (d-e) Phonon contribution to the thermal conductivity of bulk metals as a function of temperature: (d) Ag, and (e) Pd [51].



(a)



(b)

Fig.S4. Comparison of experimental thermal [51] and electronic conductivity based on the Weidman-Franz equation for bulk metals alloys at 300 K as a function of doping (Au or Pd content): (a) Ag-Au, and (b) Ag-Pd.

FigS5.a

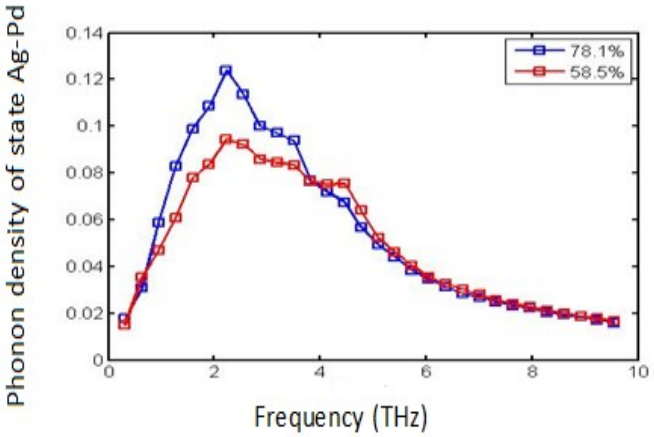


Fig.S5.b

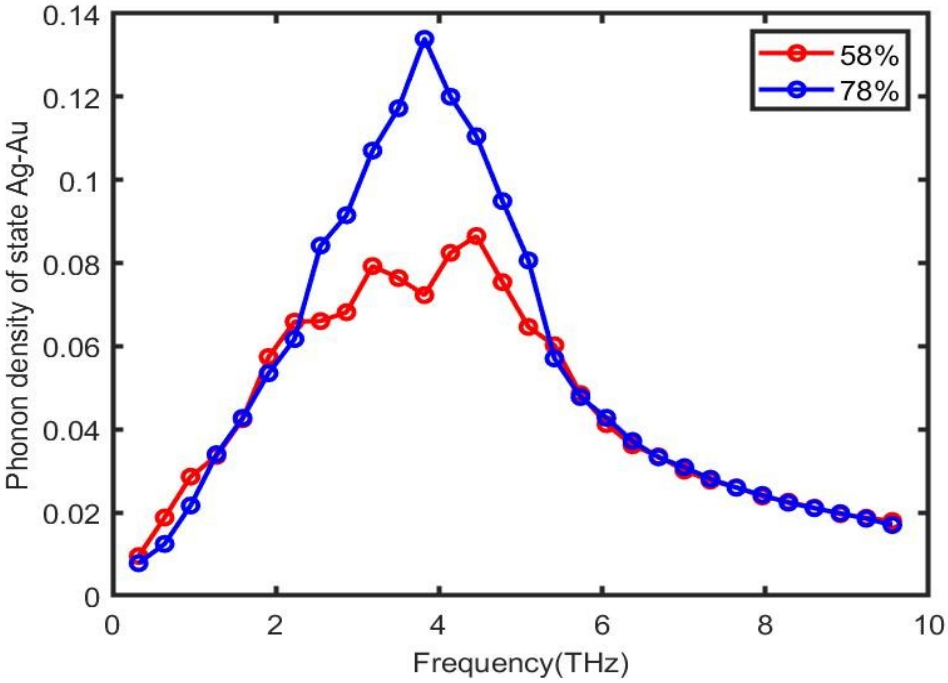
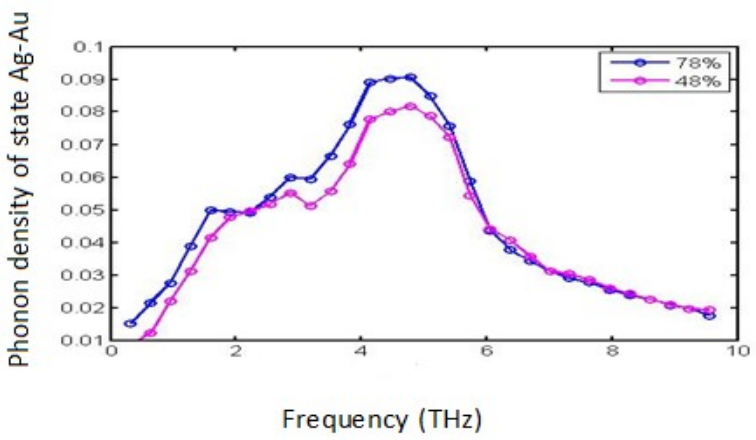
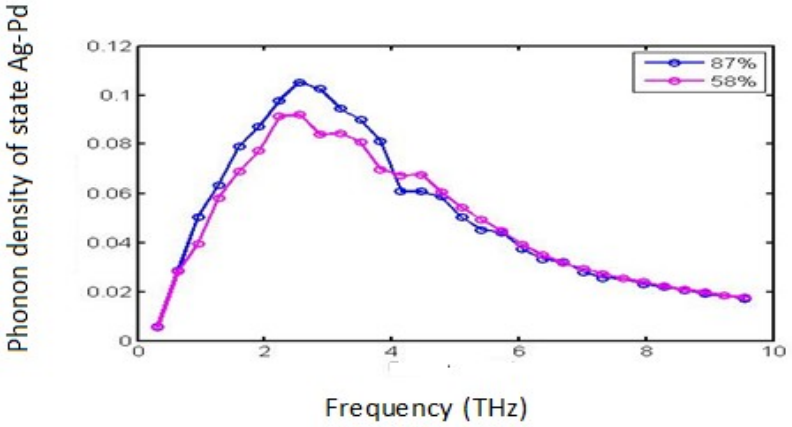


Fig.S5. a) Calculated phonon density of states as a function of frequency for bulk Ag-Pd alloy with different doping levels at 300 K. b) Calculated phonon density of states as a function of frequency for bulk Ag-Au alloy with different doping levels at 300 K

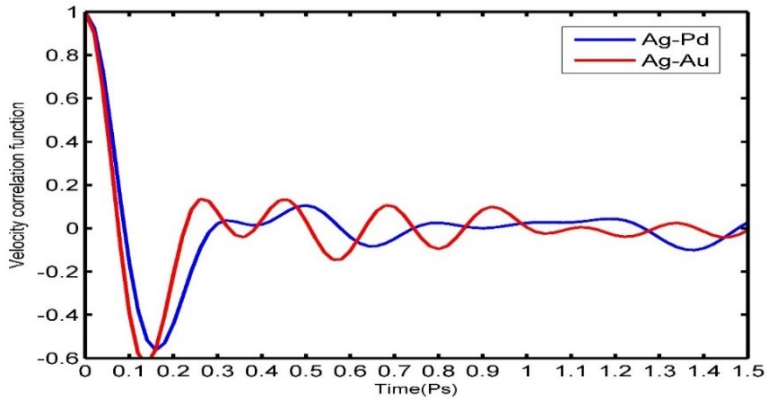


(a)

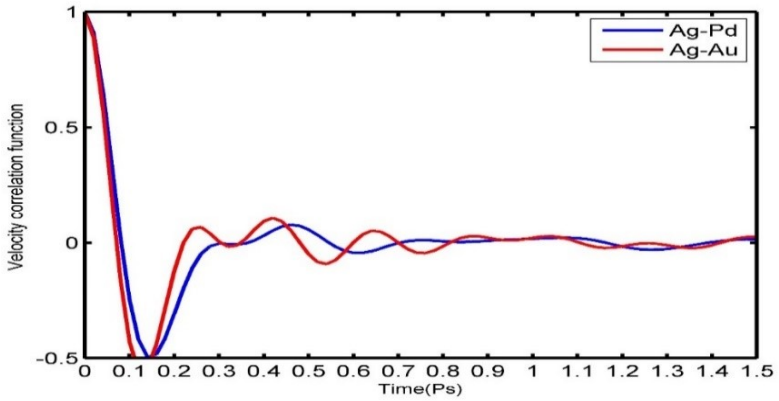


(b)

FigS6. Calculated phonon density of states as a function of frequency for bulk metal alloys with different doping levels at 700 K: (a) Ag-Au, and (b) Ag-Pd.

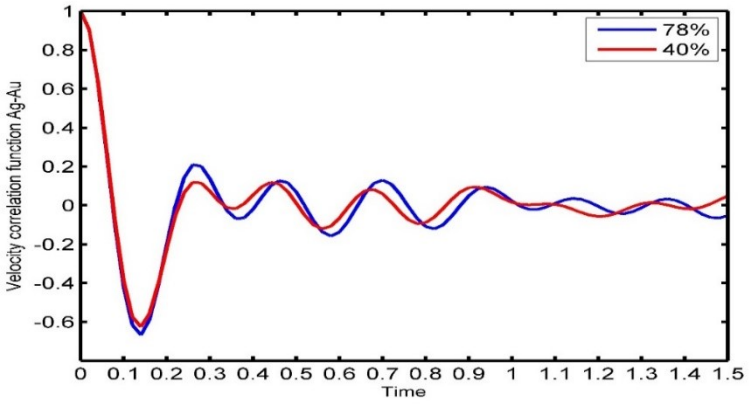


(a)



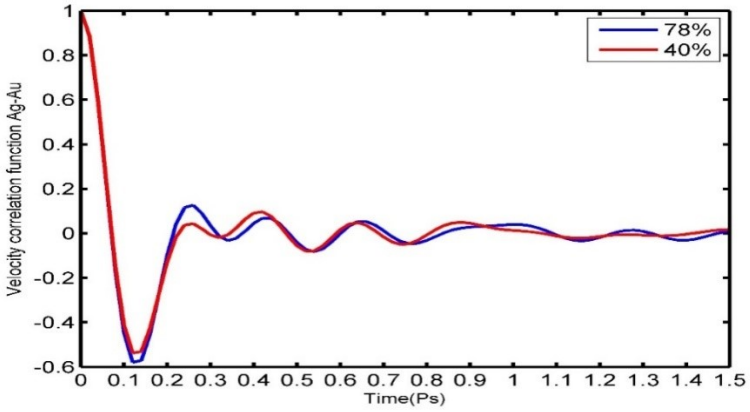
(b)

Fig.S7. Comparison of Velocity Correlation Function of Ag-Au and Ag-Pd in (a) 300K and (b) 700 K temperature



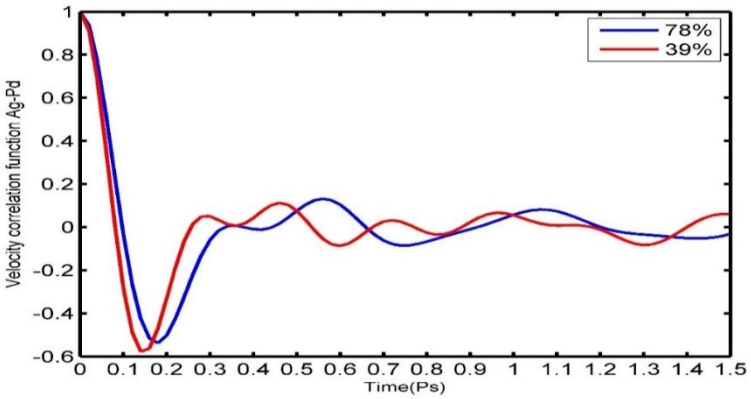
(a)

Fig. S8a. Velocity Correlation Function of Ag-Au bulk (78%,40%) at 300K



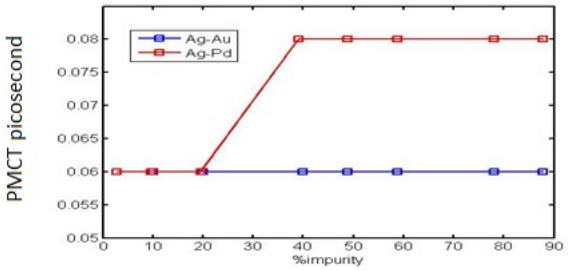
(b)

Fig.S8b. Velocity Correlation Function of Ag-Au bulk (78%,40%) at 700 K



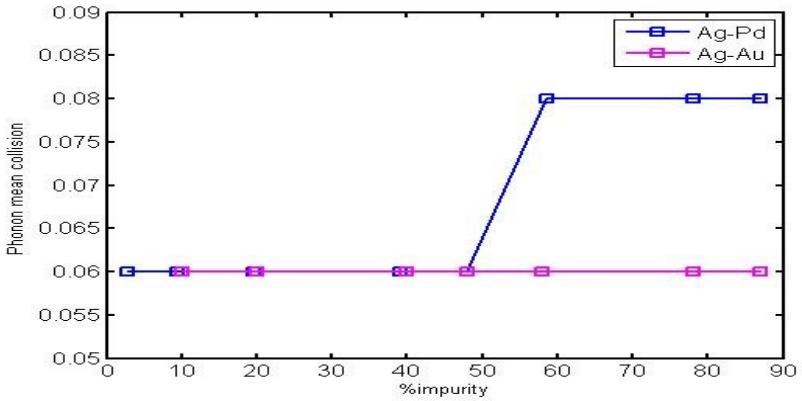
(c)

Fig. S8c. Velocity Correlation Function of Ag-Pd (78%,39%) 300K



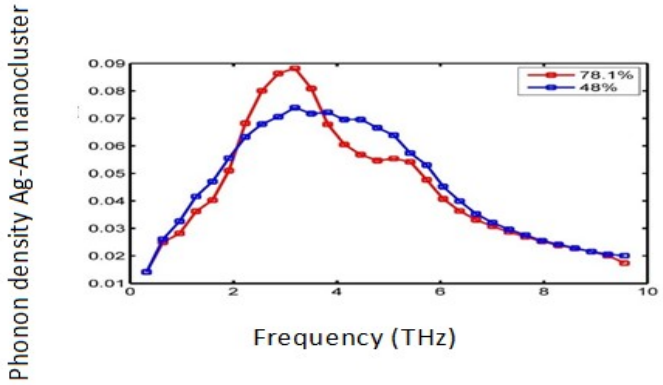
(a)

Fig.S9.a. Phonon mean collision time (PMCT) Ag-Au and Ag-Pd bulk in 300 K



(b)

Fig.S9.b Phonon mean collision time Ag-Au and Ag-Pd bulk in 700 K



(a)

Fig.S10a. a) Phonon density of state for Ag-Au nanoalloy with impurity 78% and 48% Au in Ag

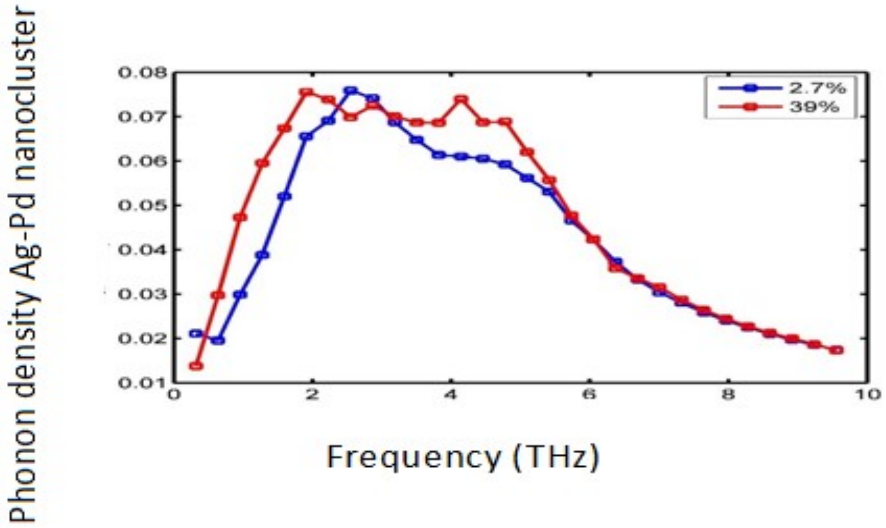


Fig.S10.b) Phonon density of state for Ag-Pd nanoalloy with impurity 2.7% and 39% Pd in Ag

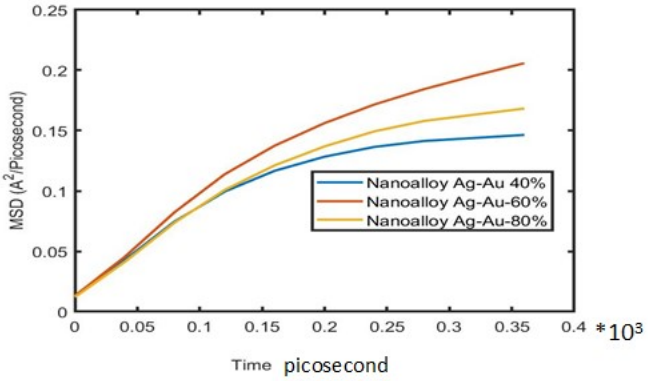


Fig.S11. MSD calculation for Ag-Au nanoalloy versus time for different composition

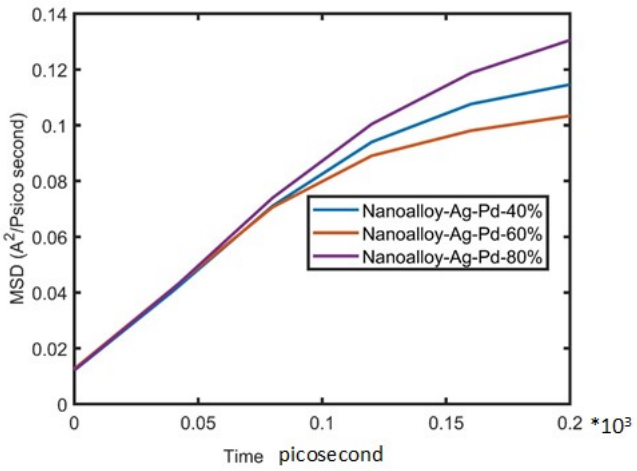


Fig.S12. MSD calculation for Ag-Au nanoalloy versus time for different composition

S1. Comparison theoretical phonon contribution result with experimental result

The total thermal conductivity of Ag-Au and Ag-Pd alloy was subtracted from the electronic contribution to thermal conductivity which was obtained based on the Wiedemann−Franz equation. The obtained difference

was compared with our calculated phonon contribution to thermal conductivity of Ag-Au and Ag-Pd alloys. The result of calculated phonon contribution to thermal conductivity and the difference between experimental total thermal conductivity and its electronic contribution by using the Wiedemann−Franz equation for Ag-Au and Ag-Pd alloys versus doping at two different temperature 300K and 700K are presented in Fig.S13.a-d respectively.

Fig.S13.a

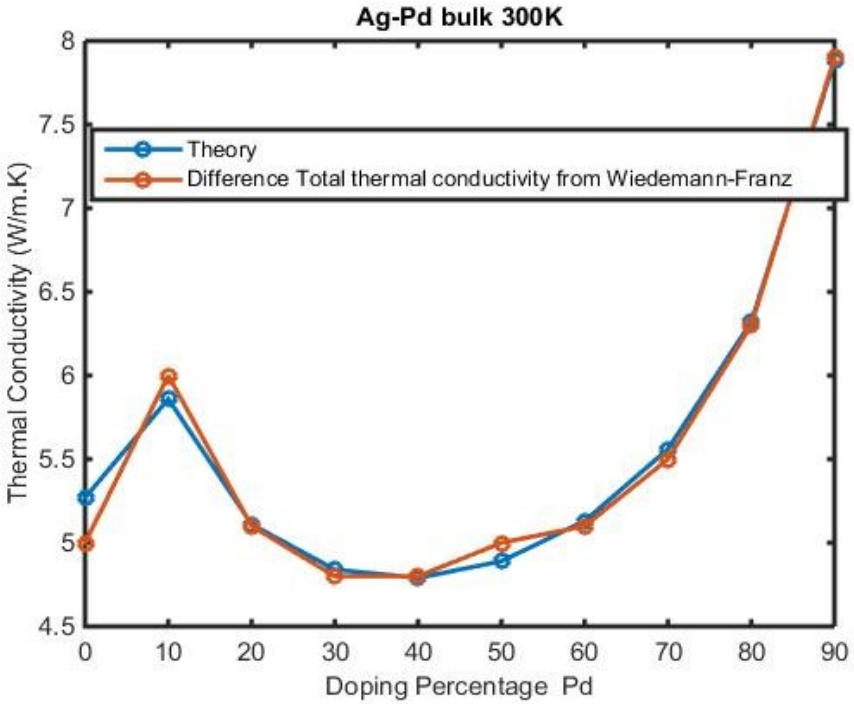
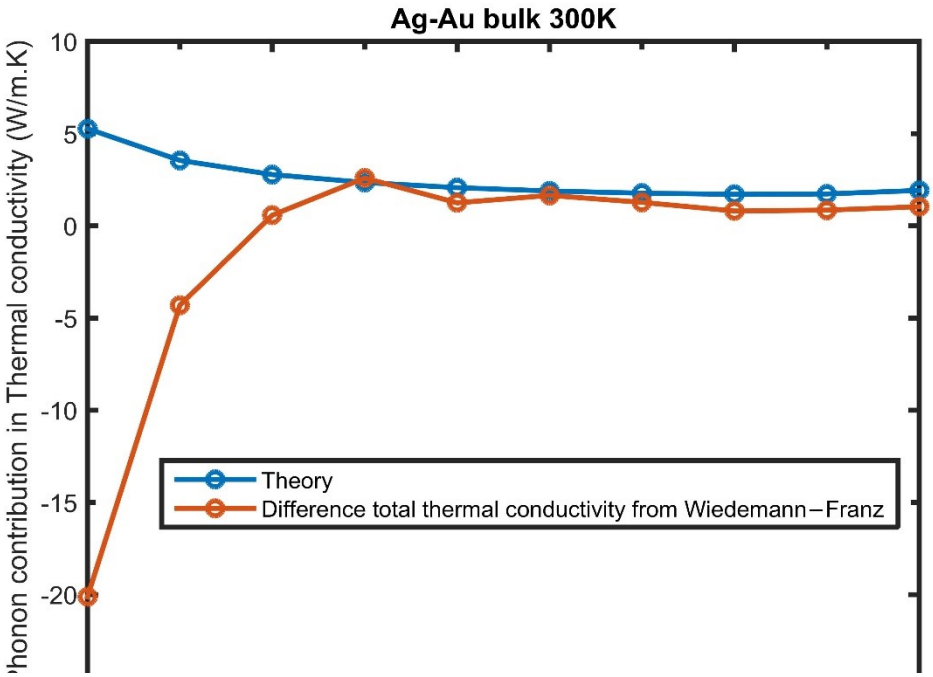


Fig.S13. a) Calculated Phonon contribution in thermal conductivity bulk Ag-Pd versus Pd doping at 300K by using molecular dynamics and compare to experimental result, which is obtained by subtraction total thermal conductivity from electronic contribution based on Wiedemann-Franz equation.

Fig.S13.b

Fig.S13.b) Calculated Phonon contribution in thermal conductivity bulk Ag-Au versus Au doping at 300K by using molecular dynamics and compare to experimental result.



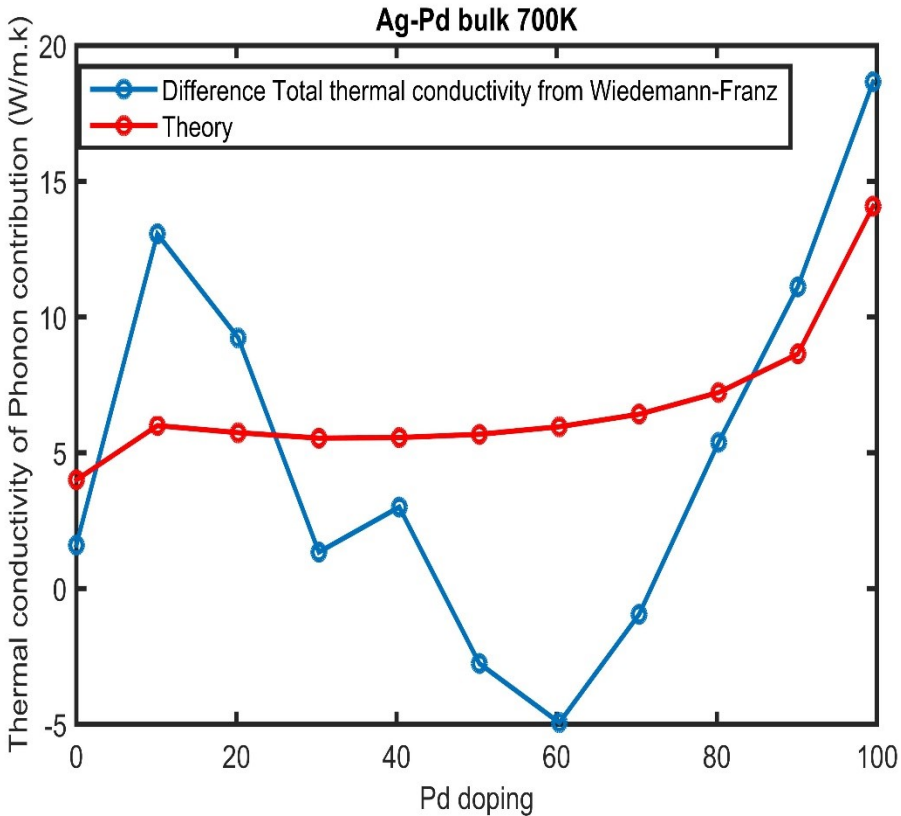


Fig.S13.c

Fig.S13.C) Same as Fig.S13.a Phonon contribution in thermal conductivity for bulk Ag-Pd versus Pd at 700K.

Fig.S13.d

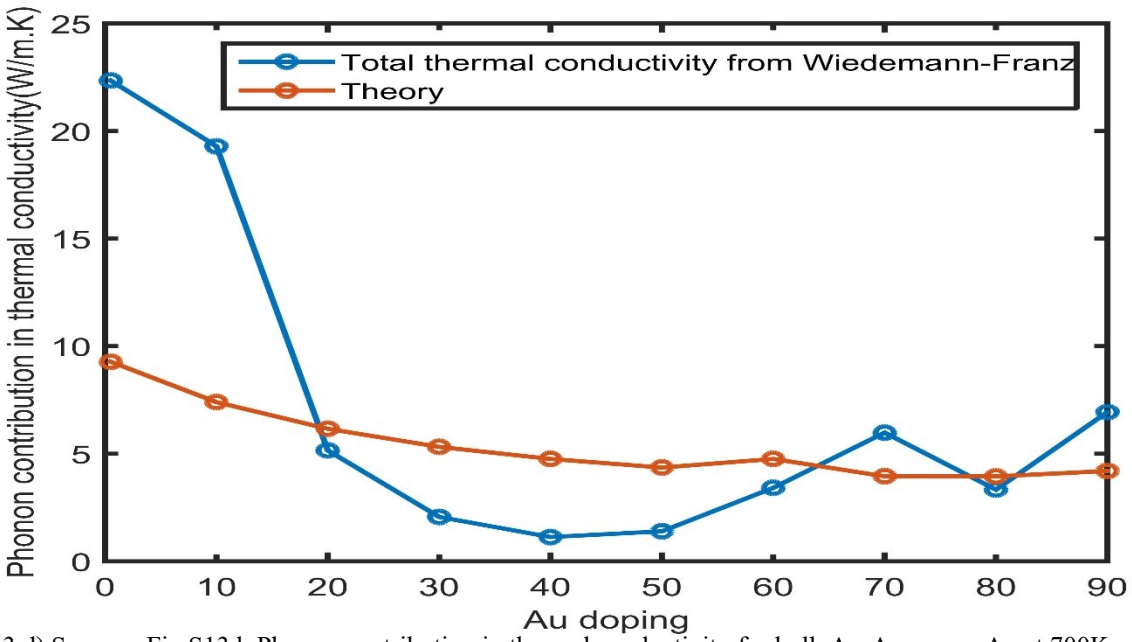


Fig.S13.d) Same as Fig.S13.b Phonon contribution in thermal conductivity for bulk Ag-Au versus Au at 700K

According to Fig.S13.a and Fig.S13.b, for most doping values in Ag-Au and Ag-Pd alloys, the calculated phonon contribution at 300K is agreement to the experimental data. Results of phonon contribution to thermal conductivity for Ag-Au and Ag-Pd alloy versus doping at 700K are shown in Fig.S13.c and Fig.S13.d. FigS13.c and Fig.S13.d show that there is a little difference between the calculated phonon contribution to thermal conductivity and the phonon contribution estimated from subtracting from the total experimental thermal conductivity its electronic contribution by using the Wiedemann−Franz equation.

S2. Convergence of thermal conductivity with system size

In previous literature, the effect of finite size on thermal conductivity has been investigated[70]. Thermal conductivity as a function of system size has been investigated in our MD simulation. We have chosen cubic boxes with three sizes (10*a, 15*a, 20*a) with a=0.41 nm as a lattice constant in our MD simulation. Result of thermal conductivity for bulk Ag-Pd at 300K with the mentioned three sizes are presented in Fig.S14. Fig.S14 shows that thermal conductivity convergences with the system size. In all MD simulations the system size has been chosen as 15*a.

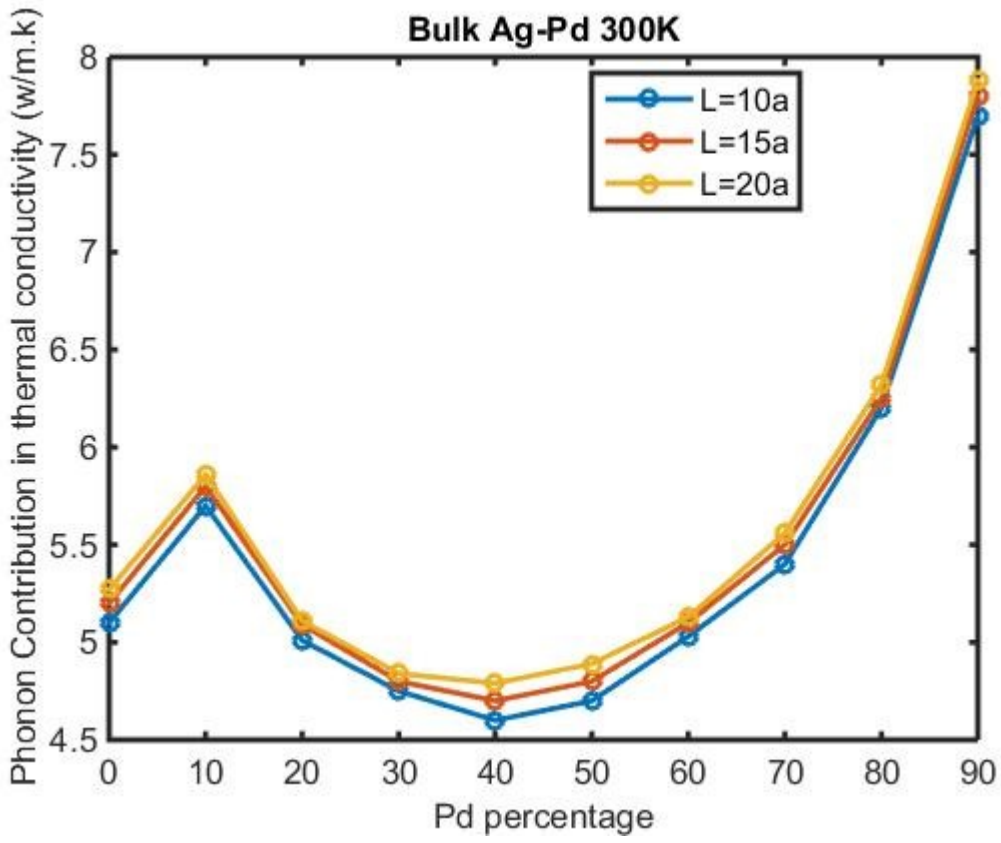


Fig.S14 . Thermal conductivity of bulk Ag-Pd at 300K at different system size, (10*a,15*a,20*a, a=0.41nm)