Electronic Supplemently Information

Multiple Heteroatoms Induced Carrier Engineering and Hierarchical Nanostructure for High Thermoelectric Performance of Polycrystalline $In_4Se_{2.5}$

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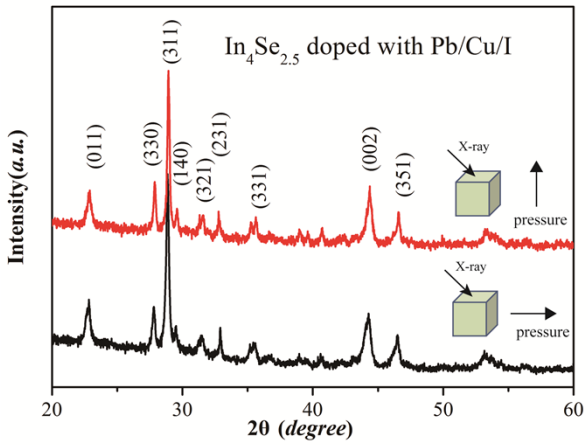

Figure S1:XRD patterns of the sintered samples (M=Pb+Cu+I) from sections parallel and perpendicular to the pressing dirction.

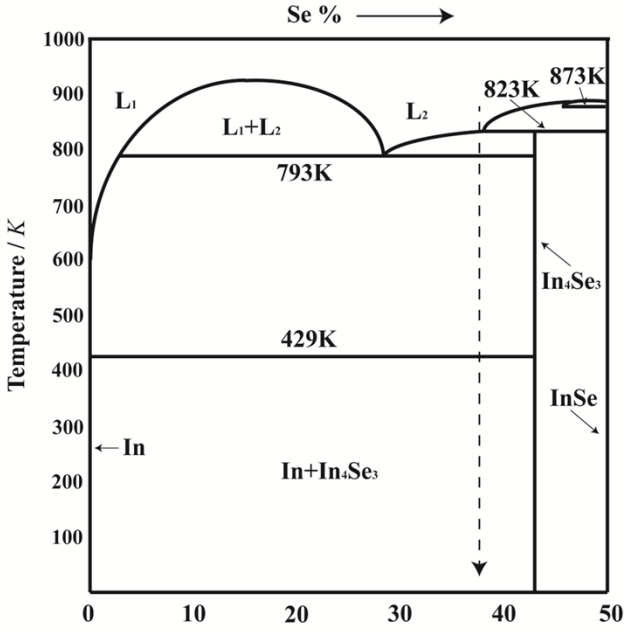

Figure S2: The In-Se binary phase diagram

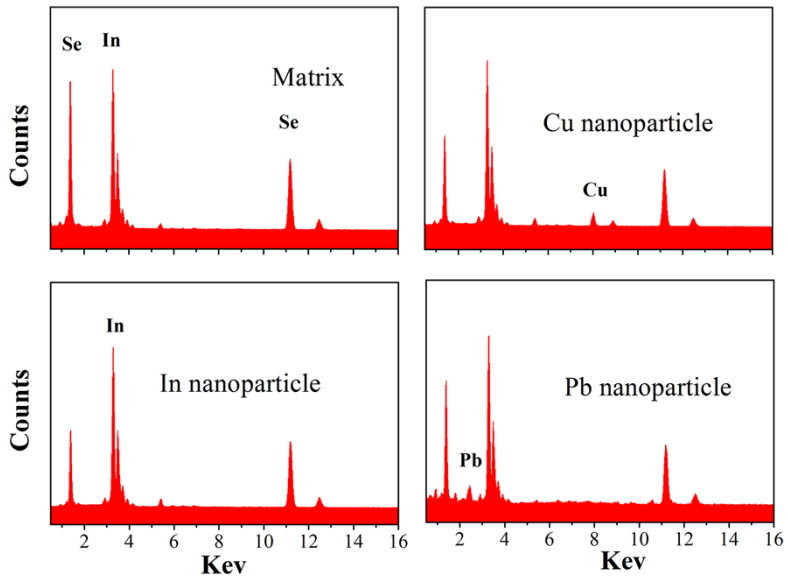

Figure S3: the EDS results for Matrix, Cu, Pb and In nanoparticles

SI4: the calculation of Lorenz number of all the samples

The Lorenz number (L) is estimated by the follow equation:

$$L = \left(\frac{k_B}{e}\right)^2 \left(\frac{(r+7/2)F_{r+5/2}(\varphi)}{(r+3/2)F_{r+1/2}(\varphi)} - \left(\frac{(r+7/2)F_{r+3/2}(\varphi)}{(r+3/2)F_{r+1/2}(\varphi)} \right)^2 \right)$$

Here, $F_n(\varphi)$ is the Fermi integration: $F_n(\varphi) = \int_0^\infty \frac{x^n}{1+e^{x-n}} dx$, r is the scattering parameter (typical r=-1/2 for acoustic phonon scattering near room temperature) and φ is the reduced Fermi energy $\varphi = E_F / k_B T$ and which can be derived from the measured S on the basis of single band approximation:

$$S = \pm \frac{k_B}{e} \left(\frac{(r+5/2)F_{r+3/2}(\varphi)}{(r+3/2)F_{r+1/2}(\varphi)} - \varphi \right)$$

Finally, the calculated L for $In_4Se_{2.5}$, Pb, Pb/I, Pb/Cu, Cu/I and Pb/Cu/I doped samples are1.57×10^{-8} $W\Omega K^{-2}$, 1.81×10^{-8} $W\Omega K^{-2}$, 1.77×10^{-8} $W\Omega K^{-2}$, 1.68×10^{-8} $W\Omega K^{-2}$, 1.66×10^{-8} $W\Omega K^{-2}$ and 1.67×10^{-8} $W\Omega K^{-2}$, respectively.

SI Table 1: Parameters used to calculate the lattice thermal conductivity

Parameters	
Lattice constant	a=12.308Å b=15.296Å C=4.081Å
Volume per atom	$26.37\times10^{-30}m^3$
Mass per atom	$1.65\times10^{-22}g$
Gruneisen parameter	γ=1.82
Sound velocity	2045m/s
Debye temperature	260K
Density of mass	$6.02g/m^3$