Direct ink writing of 3D thermoelectric architectures for fabrication of micro power generators

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Supplementary Discussion

Calculation of the lattice & bipolar thermal conductivities

The p-type sample exhibited a positive temperature dependence of thermal conductivity, whereas the n-type sample exhibited an almost constant value. To understand the temperature dependence, we calculated the lattice and bipolar thermal conductivities according to the relationship $\kappa = \kappa_e + \kappa_l + \kappa_{bi}$. Based on the Wiedemann–Franz law, $\kappa_e$ was estimated as $\kappa_e = L\sigma T$, where $T$ is the absolute temperature, $\sigma$ is the electrical conductivity, and $L$ is the Lorenz number. For each sample, $L$ was calculated from the experimentally determined Seebeck coefficient using the single parabolic model proposed by Kim et al.$^{S2}$: $L = 1.5 + (\exp{\frac{|S|}{116}}$).

After the electronic contribution $\kappa_e$ was subtracted, $\kappa$ decreased with the temperature in the low-temperature range and stabilised or increased at higher temperatures, where the bipolar contribution, $\kappa_{bi}$, became significant (Supplementary Fig. 13).

Above the Debye temperature ($\theta_D$), which is 165 K for Bi$_2$Te$_3$ and approximately 160 K for Bi$_{0.5}$Sb$_{1.5}$Te$_3$, phonon scattering by the Umklapp mechanism leads to the $T^{-1}$ dependence of the lattice thermal conductivity, $\kappa_l$. On the other hand, $\kappa_{bi}$ exhibits an exponential dependence on the temperature and material bandgap, $E_g$:

$$\kappa_{bi} \propto \exp\left(-\frac{E_g}{2k_BT}\right)$$

To estimate $\kappa_{bi}$, we linearly fitted ($\kappa - \kappa_e$) vs. $T^{-1}$ in the low-temperature range and extrapolated the data to higher temperatures (Supplementary Fig. 13). The band gap of the n-type sample ($E_g = 0.126$ eV) was larger than that of the p-type sample ($E_g = 0.184$ eV). The band gap can be estimated from the value of $S_{max}$ at $T_{max}$:

$$E_g = 2eS_{max}T_{max}$$
The band gap of the n-type sample was relatively wide (0.184 eV), leading to the suppression of the bipolar effect, whereas that of the p-type sample was relatively narrow (0.126 eV), which was responsible for the increase in the bipolar contribution at elevated temperatures. The temperature dependence of thermal conductivities was caused by the different bipolar contributions.
Supplementary References


