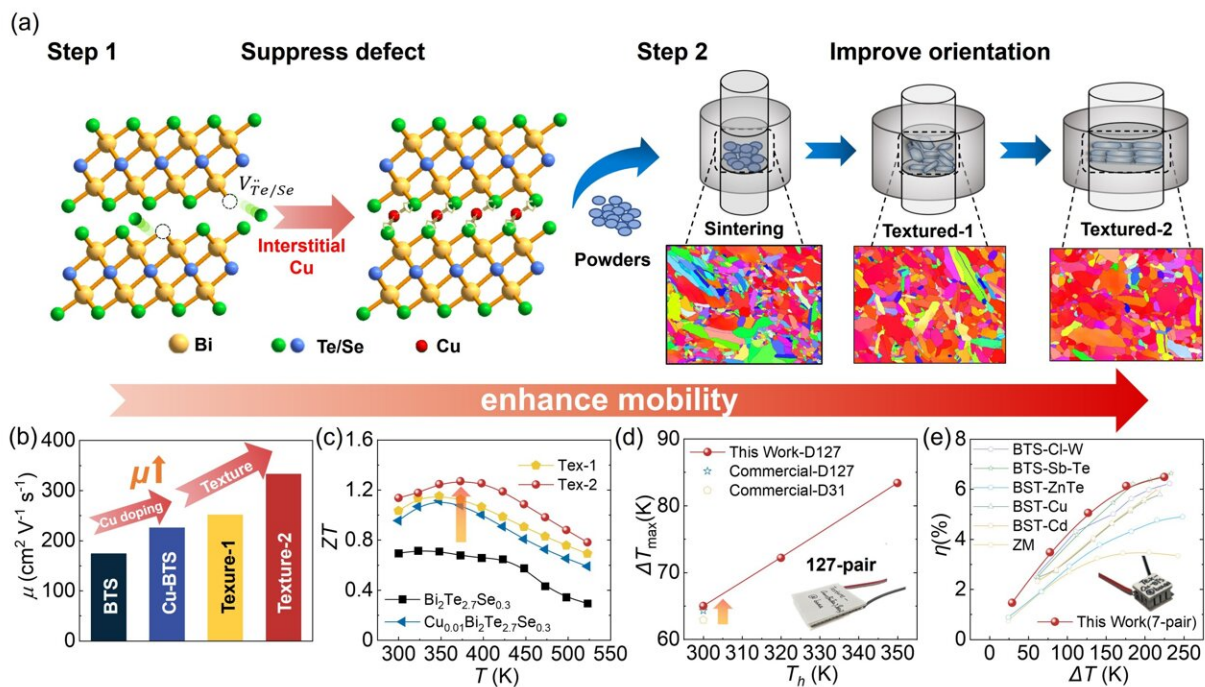


Study indicates interstitial Cu reduces the defect density in matrix and suppresses the donor-like effect

May 22 2024



Credit: Science China Press

Due to the capacity to directly and reversibly convert heat into electricity, thermoelectric (TE) material has potential applications in solid-state heat pumping and exhaust heat recuperation, thus attracting worldwide attention. Bi_2Te_3 stands out for its excellent thermoelectric

properties and has been used in commercial thermoelectric devices.

However, the development of Bi_2Te_3 -based thermoelectric devices is seriously hindered by the weak mechanical properties and low TE properties of n-type $\text{Bi}_2(\text{Te}, \text{Se})_3$. Therefore, it is important to develop a high-performance n-type Bi_2Te_3 polycrystalline material.

To address this issue, a study, [published](#) in the journal *Science Bulletin*, introduced extra Cu into the classical n-type $\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$ to optimize its local defect state, and a two-step hot deformation process was employed to construct the high textured polycrystalline $\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$ material.

This research reveals that the extra Cu is able to enter the van der Waals gaps between the $\text{Te}^{(1)}\text{-Te}^{(1)}$ layers in $\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$ matrix, suppressing the formation of the anionic vacancies. This reduction in defect density contributes to lattice plainification in $\text{Cu}_{0.01}\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$, improving the carrier mobility of $\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$ from $174 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ to $226 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ with the 1% additional Cu, resulting in a maximum ZT of 1.10 at 348 K.

Subsequently, the SPS-sintered $\text{Cu}_{0.01}\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$ bulk material underwent a two-step hot deformation process. Since the interstitial Cu can stabilize the lattice and effectively suppress the donor-like effect. The carrier concentration of hot deformation sample remains almost unchanged, while its grain orientation and [grain size](#) have significantly increased, which dramatically boosts the carrier mobility, from the initial $174 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ to $333 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, representing a 91% increase after the hot deformation process.

This significant improvement in [electronic properties](#) contributes to a substantial enhancement in ZT for hot deformation sample. The ZT_{max} of the textured $\text{Cu}_{0.01}\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$ reaches 1.27 at 373 K, and its average ZT value is 1.22 in the range of 300-425 K, nearly twice as much as the initial $\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$.

Furthermore, a 127-pair thermoelectric cooling device (TEC) was fabricated by using the textured $\text{Cu}_{0.01}\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$ sample coupled with commercial p-type BST. The TEC module achieved cooling temperature differentials of 65 K and 83.4 K at hot-end temperatures (T_h) of 300 K and 350 K, respectively, which is superior to the commercial Bi_2Te_3 -based TEC modules. And a 7-pair thermoelectric generator module (TEG) was constructed by using the same materials.

The TEG module demonstrated a significantly high conversion efficiency of 6.5% at a temperature different of 225 K, which is comparable to other state-of-the-art Bi_2Te_3 -based TEG modules.

More information: Yichen Li et al, Realizing high-efficiency thermoelectric module by suppressing donor-like effect and improving preferred orientation in n-type $\text{Bi}_2(\text{Te}, \text{Se})_3$, *Science Bulletin* (2024).

[DOI: 10.1016/j.scib.2024.04.034](https://doi.org/10.1016/j.scib.2024.04.034)

Provided by Science China Press

Citation: Study indicates interstitial Cu reduces the defect density in matrix and suppresses the donor-like effect (2024, May 22) retrieved 21 June 2024 from

<https://phys.org/news/2024-05-interstitial-cu-defect-density-matrix.html>

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