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

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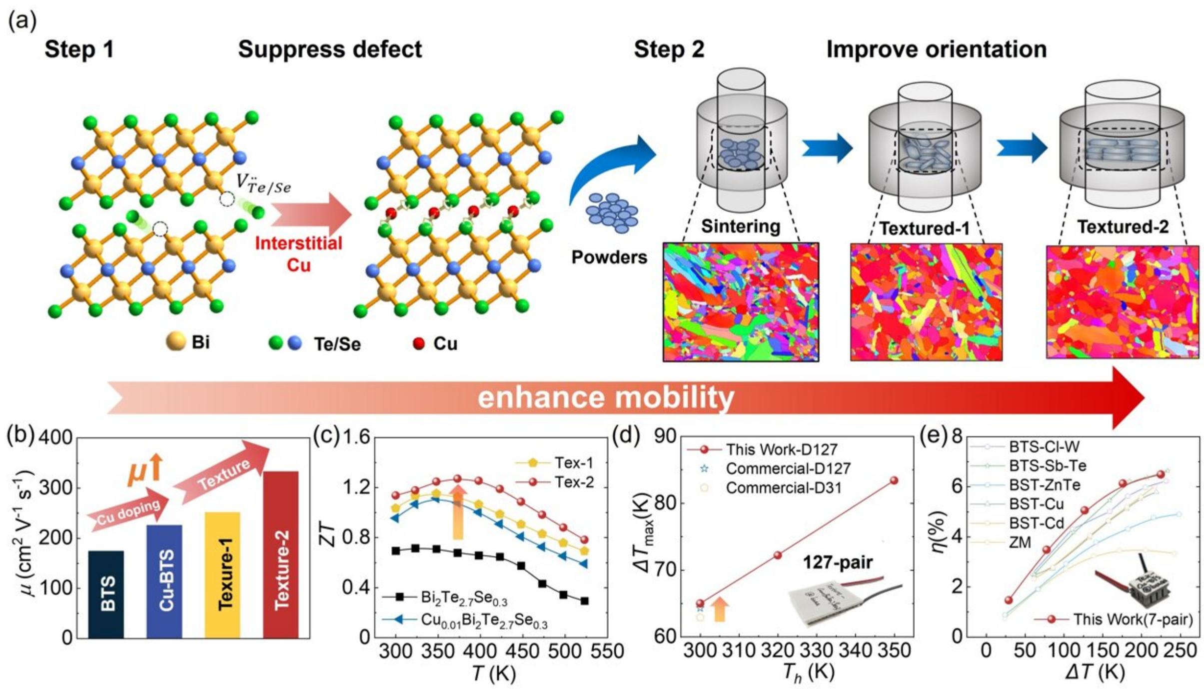

Credit: Science China Press

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 $Bi_2(Te, Se)_3$. 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 $Bi_2Te_{2.7}Se_{0.3}$ to optimize its local defect state, and a two-step hot deformation process was employed to construct the high textured polycrystalline $Bi_2Te_{2.7}Se_{0.3}$ material.

This research reveals that the extra Cu is able to enter the van der Waals gaps between the $Te^{(1)}$-$Te^{(1)}$ layers in $Bi_2Te_{2.7}Se_{0.3}$ matrix, suppressing the formation of the anionic vacancies. This reduction in defect density contributes to lattice plainification in $Cu_{0.01}Bi_2Te_{2.7}Se_{0.3}$, improving the carrier mobility of $Bi_2Te_{2.7}Se_{0.3}$ from 174 $cm^2 V^{-1} s^{-1}$ to 226 $cm^2 V^{-1} s^{-1}$ with the 1% additional Cu, resulting in a maximum ZT of 1.10 at 348 K.

Subsequently, the SPS-sintered $Cu_{0.01}Bi_2Te_{2.7}Se_{0.3}$ 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 $cm^2 V^{-1} s^{-1}$ to 333 $cm^2 V^{-1} s^{-1}$, 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 $Cu_{0.01}Bi_2Te_{2.7}Se_{0.3}$ 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 $Bi_2Te_{2.7}Se_{0.3}$.

Furthermore, a 127-pair thermoelectric cooling device (TEC) was fabricated by using the textured $Cu_{0.01}Bi_2Te_{2.7}Se_{0.3}$ 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 Bi2(Te, Se)3, *Science Bulletin* (2024). DOI: 10.1016/j.scib.2024.04.034

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