New approach boosts performance in thermoelectric materials

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Thermoelectric materials are considered a key resource for the future - able to produce electricity from sources of heat that would otherwise go to waste, from power plants, vehicle tailpipes and elsewhere, without generating additional greenhouse gases. Although a number of materials with thermoelectric properties have been discovered, most produce too little power for practical applications.

A team of researchers - from universities across the United States and China, as well as Oak Ridge National Laboratory - is reporting a new mechanism to boost performance through higher carrier mobility, increasing how quickly charge-carrying electrons can move across the material. The work, reported this week in the *Proceedings of the National Academy of Science*, focused on a recently discovered n-type magnesium-antimony material with a relatively high thermoelectric figure of merit, but lead author Zhifeng Ren said the concept could also apply to other materials.

"When you improve mobility, you improve electron transport and overall performance," said Ren, M.D. Anderson Chair professor of physics at the University of Houston and principal investigator at the Texas Center for Superconductivity at UH.

Thermoelectric materials produce electricity by exploiting the flow of heat current from a warmer area to a cooler area, and their efficiency is calculated as the measure of how well the material converts heat into power. However, because waste heat is both an abundant and free source of fuel, the conversion rate is less important than the total amount of power that can be produced, Ren said. That has prompted researchers to look for ways to improve the power factor of thermoelectric materials.

Paul Ching-Wu Chu, TLL Temple Chair of Science, founding director and chief scientist of the Texas Center for Superconductivity, noted that Ren previously had demonstrated the importance of a material's power factor in determining how well it will work in a thermoelectric device. Chu is a co-author for this most recent work, which he said "demonstrates in the n-type magnesium-antimony-based materials that the power factor can indeed be enhanced by properly tuning the carrier scattering in the material."

"That provides a new avenue to more powerful thermoelectric devices," he added.

Thermoelectric semiconductors come in two variations, n-type, created by replacing an element resulting in a "free" electron to carry the charge, and p-type, in which the replacing element has one fewer electron than the element which it replaced, leaving a "hole" that facilitates movement of energy as the electrons move across the material to fill the vacant spot.

The work reported in *PNAS* addresses the need for a more powerful n-type magnesium-antimony compound, expanding its potential as a thermoelectric material that can be paired with an effective p-type magnesium-antimony material, which had been previously reported.

The material's power factor can be boosted by increasing carrier mobility, the researchers said. "Here we report a substantial enhancement in carrier mobility by tuning the carrier scattering mechanism in n-type Mg3Sb2-based materials," they wrote. "... Our results clearly demonstrate that the strategy of tuning the carrier scattering mechanism is quite effective for improving the mobility and should also be applicable to other material systems."

The researchers replaced a small fraction of magnesium in the compound with a variety of transition-metal elements, including iron, cobalt, hafnium and tantalum, to determine how best to boost carrier mobility and, through that, the material's power factor.

"Our work," the researchers conclude, "demonstrates that the carrier scattering mechanism could play a vital role in the thermoelectric properties of the material, and the concept of tuning the carrier scattering mechanism should be widely applicable to a variety of material systems."

More information: Jun Mao el al., "Manipulation of ionized impurity scattering for achieving high thermoelectric performance in n-type Mg3Sb2-based materials," *PNAS* (2017). www.pnas.org/cgi/doi/10.1073/pnas.1711725114

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