

Breaking trade-off problem that limits thermoelectric conversion efficiency of waste heat

October 21 2021

Breaking Trade-off Between Thermopower and Conductivity to Improve Thermoelectric Performance

Thermoelectric device can convert waste heat to electricity

Issue: thermoelectric power factor (PF) is limited by trade-off relation between electrical conductivity (σ) and thermopwer (S)

Mott insulator ($c/a < 1$)
Long a
Short c

Tensile strain

Metal ($c/a > 1$)
Short a
Long c

Compressive strain

10²-fold increase of PF by breaking trade-off between σ and S was demonstrated in strained transition metal oxide LaTiO₃

Lattice strain can be used to harness hidden high PF in thermoelectric oxides

Breaking of Thermopower–Conductivity Trade-off in LaTiO₃ Film Around Mott Insulator to Metal Transition
 Katase et al. (2021) | *Advanced Science*

Credit: Tokyo Tech

In recent years, energy consumption in developed countries has been rather wasteful. Nearly two-thirds of the total energy is typically discarded as "waste heat," which ends up contributing to global warming. Finding a way to productively use this heat has been every material researcher's priority of late.

One of the possible ways to recover this [waste heat](#) as electricity is via "[thermoelectric conversion](#)," a process that uses temperature difference in semiconductors to convert waste heat into electric power. The thermopower (S) is a measure of the magnitude of an induced thermoelectric voltage in response to a temperature difference across the material. The electric power is evaluated by [power factor](#) (PF), which is the product of thermopower S squared and electronic conductivity (s). Therefore, the high [electric power](#) (PF) is capable of combining large S with high s in thermoelectric materials.

However, the PF is constrained by a trade-off between S and s . The S and s depend on carrier concentration, and thus the PF is usually maximized by tuning the carrier concentration with the addition of impurity elements—the s increases with increasing impurity concentration but the S decreases. This trade-off limits the PF.

In a recent study published in *Advanced Science*, a team of scientists led by Associate Professor Takayoshi Katase of the Tokyo Tech have discovered a way to break this trade-off. The scientists grew thin films of the Mott insulator oxide LaTiO_3 on different substrates and found a way to introduce epitaxial strain, a strain that is born from a mismatch in

the lattice structures of the substrate and the deposited (epitaxial) film. The artificial compressive strain was able to change LaTiO_3 from the Mott insulator to metal. In the metallic state, increase in both S and s resulted in a hundred-fold increase in PF. "Different from the conventional way of impurity doping, the behaviors of s and S are apparently decoupled in lattice strained LaTiO_3 films, which leads to a spectacular boost in power factor that defies conventional wisdom," says Dr. Katase.

Increasing the epitaxial compressive strain can induce a change in carrier polarity from [p-type](#) to n-type. Dr. Katase and team found that while the absolute value of thermopower increased with increasing carrier concentration under compressive strain, electronic conductivity also increased with increases in carrier mobility due to electronic structure change from Mott insulator to metal. Density functional theory calculation clarified that the Ti 3D band split to form energy gap in p-type LaTiO_3 film, while the energy gap was closed in the n-type film, which led to an unusual simultaneous increase in conductivity and thermopower.

This discovery promises to advance the field of thermoelectric materials. "Our experiments suggest that [epitaxial strain](#) will be a novel tool to harvest large power factors from thermoelectric oxides that are inconspicuous in their bulk by breaking the trade-off problem. Metal chalcogenides such as Bi_2Te_3 have been known as high performance thermoelectric materials, but the chalcogenides have problems with toxic elements, and low thermal and chemical stability, which restrict the large-scale use of thermoelectricity. Contrarily, since oxides are stable in air and even at high temperatures, they are ideal for maintenance-free thermoelectric conversion applications. The thermoelectric conversion efficiency is much lower than that of metal chalcogenides at this stage. But, by greatly improving the thermoelectric performance of oxides beyond the trade-off relationship, thermoelectric conversion is expected

to become widespread as a general energy source," concludes Dr. Katase.

More information: Takayoshi Katase et al, Breaking of Thermopower–Conductivity Trade-Off in LaTiO₃ Film around Mott Insulator to Metal Transition, *Advanced Science* (2021). [DOI: 10.1002/advs.202102097](https://doi.org/10.1002/advs.202102097)

Provided by Tokyo Institute of Technology

Citation: Breaking trade-off problem that limits thermoelectric conversion efficiency of waste heat (2021, October 21) retrieved 25 April 2024 from <https://phys.org/news/2021-10-trade-off-problem-limits-thermoelectric-conversion.html>

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.