Exotic alloys for potential energy applications

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The search for thermoelectrics, exotic materials that convert heat directly into electricity, has received a boost from researchers at the California Institute of Technology and the University of Tokyo, who have found the best way to identify them.

In the new open-access journal *APL Materials*, the team shows that a relatively simple technique called the "rigid band approximation" can predict a material's properties more accurately than a competing, more complicated method.

"The rigid band approach still supplies the simple, predictive engineering concepts we need for discovering fruitful thermoelectric material compositions," says G. Jeffrey Snyder, a Caltech faculty associate in materials science, who led the research.

Thermoelectrics have been used since the 1950s to power spacecraft by converting the heat from radioactive decay into electricity. Their unusual properties arise from complex interactions between the many electrons associated with the atoms in alloys of heavy metals such as lead, bismuth, tellurium and antimony.

With no moving parts, thermoelectric generators are quiet and extremely reliable, requiring minimal maintenance. However, the generators are relatively inefficient (typically less than 10 percent) and the materials needed to build them are expensive—factors that have prevented their widespread use and limited thermoelectrics to niche applications such as spacecraft or wine refrigerators.

In recent years, however, the need for increased energy efficiency and non-carbon-based power generation has sparked renewed interest in thermoelectrics. With improvements, researchers believe the materials could generate cheap electricity from otherwise wasted heat produced by engines and factory furnaces.

"If we could double their efficiency, then thermoelectric modules incorporated into an automobile engine's exhaust system could generate enough power to replace the alternator, which would increase the car's gas mileage," said Snyder.

The challenge for scientists is to choose alloy compositions, crystal sizes and additives, (also called dopants), which would yield high thermoelectric efficiency. With an exhaustive number of possible combinations to choose from, scientists use theoretical calculations to guide their search for promising materials. The materials' extreme complexity, however, requires theorists to make various assumptions that have each led to different approaches.

The most common approach is the "rigid band" approximation, which provides a relatively simple model of a material's electronic structure, and the more complex "supercell" approach, which gives a detailed picture of its ideal atomic arrangement. Some scientists have said the rigid band approach is too simple and inaccurate to be useful.

Snyder's team reported exactly the opposite result. Their calculations showed that the rigid band approach was actually more accurate than the supercell method in predicting the observed properties of a popular thermoelectric – lead telluride – doped with a small amount of sodium, potassium or thallium.

"Supercell approaches are accurate for very specific dopant cases, but they do not take into account the various defects present in real materials," Snyder said. By using the simpler rigid band model, he added, scientists should be able to more quickly identify promising new and more-efficient thermoelectric compositions.

More information: dx.doi.org/10.1063/1.4809545

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