Curious compound: Tin selenide may hold the key for thermoelectric solutions

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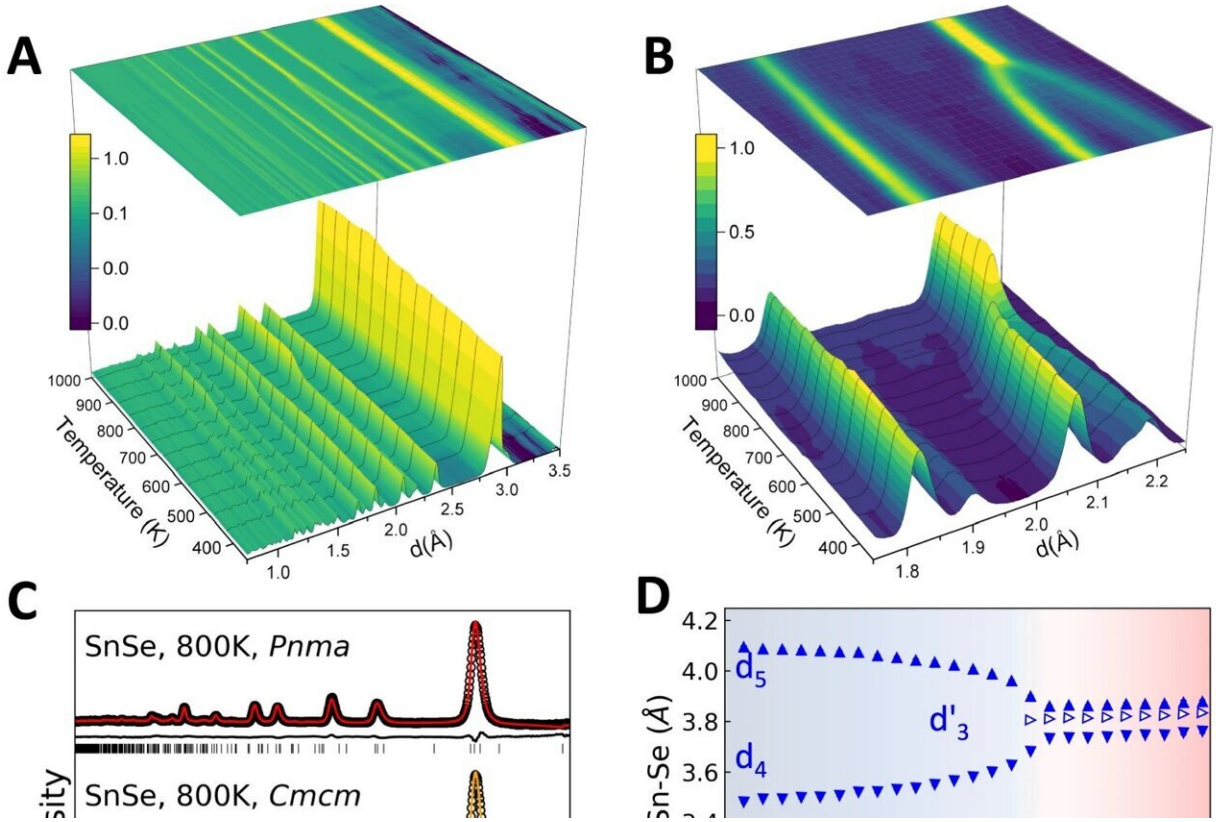

Average structure of SnSe. **A** 3D surface maps with projection of neutron diffraction data as a function of temperature, with **B** a close-up view of several peaks. **C** Results of Rietveld refinement of the data for 800 K (completed with both GeS-type (*Pnma*) and TlI-type (*Cmcm*) models) and 400 K (completed with GeS-type (*Pnma*) model), with data shown as black circles, model fits shown as red/orange/cyan lines, and difference curves shown as black lines (offset below data and fits). **D** Evolution of Sn-Se bond distances as a function of temperature from the Rietveld fits; values resulting from *Pnma* and *Cmcm* models are

indicated with solid and hollow symbols, respectively. Error bars have been included but are smaller than the data symbols. The colored backgrounds indicate the boundary of the phase transition temperature. Rietveld refinement of the 800 K data in *Cmcm* space group yields the structure model shown in **E** compared with the *Pnma* refined structure model in **F**. First coordination polyhedron of SnSe (**G**) at 800 K using the *Pnma* model. Models employ 80% probability ellipsoids to emphasize the ADP obtained. Source data are provided as a Source Data file. Credit: *Nature Communications* (2023). DOI: 10.1038/s41467-023-38454-0

Researchers at the FAMU-FSU College of Engineering and the National High Magnetic Field Laboratory discovered that atomic-level structural changes occur when the compound tin selenide heats up—changes that help it to conduct electricity but not heat.

The study provides information that could lead to new technologies for applications such as refrigeration or waste heat recovery from cars or nuclear power plants. The research was published by *Nature Communications*.

"Tin selenide is a curious compound," said Theo Siegrist, a chemical and biomedical engineering professor at the FAMU-FSU College of Engineering. "It has gotten a lot of interest for its special high-temperature thermoelectric properties. Optimizing those characteristics may lead to viable options for sustainable power generation and other uses in the future."

Scientists already knew that tin selenide had a high thermoelectric coefficient at elevated temperatures, meaning it can create a strong electric current from a temperature gradient. The question was why and how.

The researchers found that as the compound heated up, the bonds between tin and selenium remained mostly unchanged, still connected by three short and several long bonds. But the tin atoms in the compound began to move around, changing from a fully ordered lattice structure into a partially disordered one.

"The initial idea about this change was that the atoms were displaced, but we found that it is an order-disorder phase transition that was actually what was happening," Siegrist said. "The tin atom was flopping around, so to speak. That was what allowed tin selenide to scatter the energy waves that conduct heat."

A good thermoelectric material needs strong electrical conductivity but thermal conductivity that is as low as possible. In tin selenide, this is achieved by a dynamic partial disorder of the tin atoms at elevated temperatures that results in a reduction of the heat conductivity.

Siegrist collaborated on the work with researchers from Oak Ridge National Laboratory, or ORNL, and the University of Tennessee, Knoxville. They used a type of particle accelerator at ORNL called a spallation neutron source to test the material. The accelerator shoots protons onto a target to generate bursts of neutrons, allowing scientists to analyze that target's crystal structure.

By examining what is happening at the atomic scale, researchers can understand what is driving certain properties that engineers may want to optimize.

"This is fundamental research, and we are interested in the mechanism and influence of the material to get it to do what we want in a thermoelectric device," Siegrist said. "All these ideas can improve energy conversion devices by making them more efficient."

More information: Bo Jiang et al, The curious case of the structural phase transition in SnSe insights from neutron total scattering, *Nature Communications* (2023). DOI: 10.1038/s41467-023-38454-0

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