Researchers find an unusual way in which a material conducts heat when it is compressed

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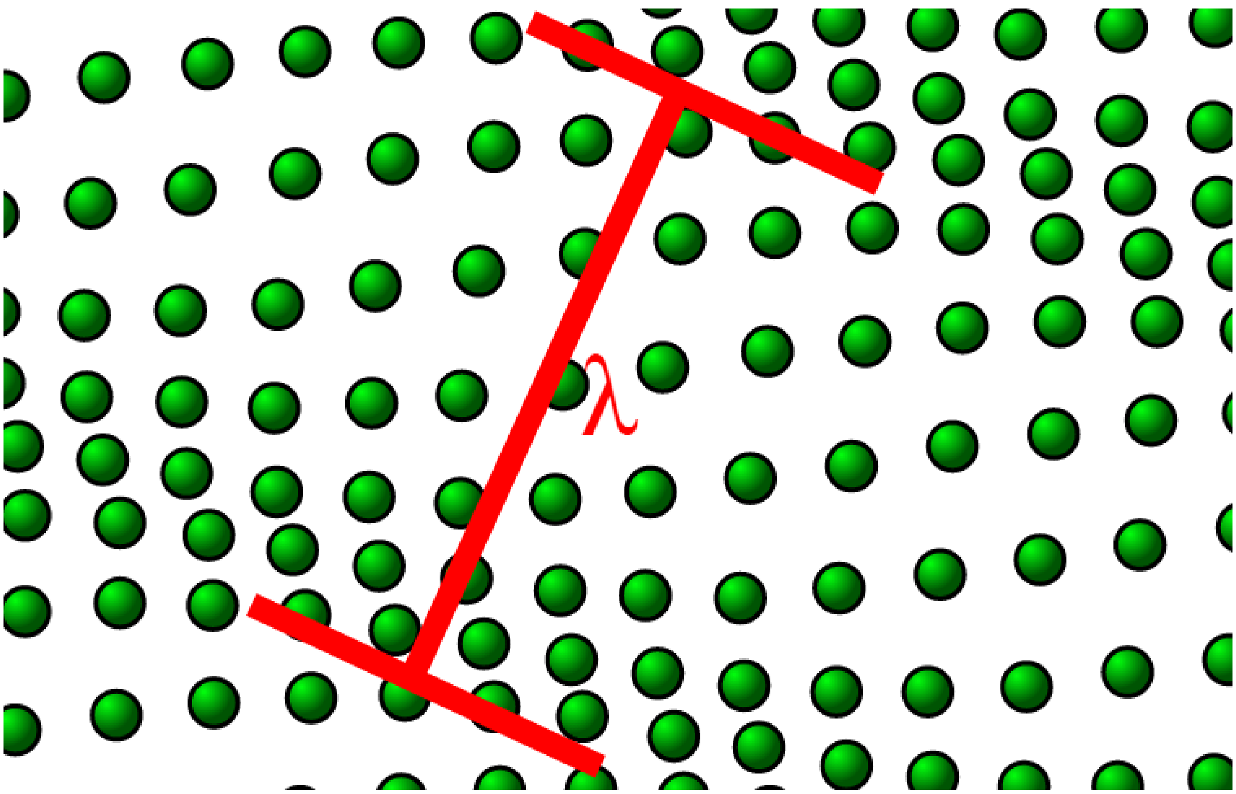

Phonon propagating through a square lattice (atom displacements greatly exaggerated). Credit: Wikipedia

In the latest wrinkle to be discovered in cubic boron arsenide, the unusual material contradicts the traditional rules that govern heat conduction, according to a new report by Boston College researchers in today's edition of the journal *Nature Communications*.

Usually, when a material is compressed, it becomes a better conductor of heat. That was first found in studies about a century ago. In boron arsenide, the research team found that when the material is compressed the conductivity first improves and then deteriorates.

The explanation is based on an unusual competition between different processes that provide heat resistance, according to the co-authors Professor David Broido and Navaneetha K. Ravichandran, a post-doctoral fellow, of the Department of Physics at Boston College. This type of behavior has never been predicted or observed before.

The findings are consistent with the unconventional high thermal conductivity that Broido, a theoretical physicist, and colleagues have previously identified in cubic boron arsenide.

Ravichandran's calculations showed that upon compression, the material first conducts heat better, similar to most materials. But as compression increases, the ability of boron arsenide to conduct heat deteriorates, the co-authors write in the article, titled "Non-monotonic pressure dependence of the thermal conductivity of boron arsenide."

Such odd behavior stems from the unusual way in which heat is transported in boron arsenide, an electrically insulating crystal in which heat is carried by phonons—vibrations of the atoms making up the crystal, Broido said. "Resistance to the flow of heat in materials like boron arsenide is caused by collisions occurring among phonons," he added.

Quantum physics shows that these collisions occur between at least three phonons at a time, he said. For decades, it had been assumed that only collisions between three phonons were important, especially for good heat conductors.

Cubic boron arsenide is unusual in that most of the heat is transported by phonons that rarely collide in triplets, a feature predicted several years ago by Broido and collaborators, including Lucas Lindsay at Oak Ridge National Laboratory and Tom Reinecke of the Naval Research Lab.

In fact, collisions between three phonons are so infrequent in boron arsenide that those between four phonons, which had been expected to be negligible, compete to limit the transport of heat, as shown by other theorists, and by Broido and Ravichandran in earlier publications.

As a result of such rare collision processes among phonon triplets, cubic boron arsenide has turned out to be an excellent thermal conductor, as confirmed by recent measurements.

Drawing on these latest insights, Ravichandran and Broido have shown that by applying hydrostatic pressure, the competition between three-phonon and four-phonon collisions can, in fact, be modulated in the material.

"When boron arsenide is compressed, surprisingly, three-phonon collisions become more frequent, while four-phonon interactions become less frequent, causing the thermal conductivity to first increase and then decrease," Ravichandran said. "Such competing responses of three-phonon and four-phonon collisions to applied pressure has never been predicted or observed in any other material,".

The work of the theorists, supported by a Multi-University Research Initiative grant from the Office of Naval Research, is expected to be taken up by experimentalists to prove the concept, Broido said.

"This scientific prediction awaits confirmation from measurement, but the theoretical and computational approaches used have been demonstrated to be accurate from comparisons to measurements on many other materials, so we're confident that experiments will measure behavior similar to what we found." said Broido.

"More broadly, the theoretical approach we developed may also be useful for studies of the earth's lower mantle where very high temperatures and pressures can occur," said Ravichandran. "Since obtaining experimental data deep in the Earth is challenging, our predictive computational model can help give new insights into the nature of heat flow at the extreme temperature and pressure conditions that exist there."

More information: Navaneetha K. Ravichandran et al, Non-monotonic pressure dependence of the thermal conductivity of boron arsenide, *Nature Communications* (2019). DOI: 10.1038/s41467-019-08713-0

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