Computation helps predict heat transfer in diamond

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(PhysOrg.com) -- Cornell researcher Derek Stewart and collaborators have calculated the exact mechanism by which diamond conducts heat, a breakthrough that could lend insight into many fields, including electronics.

Using computational modeling, Cornell researcher Derek Stewart and collaborators have calculated the exact mechanism by which diamond conducts heat, a breakthrough that could lend insight into fields ranging from heat management in electronics to heat flow in the earth.

The research is described in the Sept. 16 online edition of *Physical Review B* (Vol. 80, Issue 12) and is highlighted by the journal as an "Editor's Suggestion" for its "particular interest, clarity or importance." Stewart, the computational research associate at Cornell NanoScale Science and Technology Facility (CNF), performed the work with researchers at Boston College and the University of Regensburg, Germany.

Thermal conductivity is the measure of how easily a material transfers heat. Diamond, which is also an electrical insulator, has a high thermal conductivity -- about five times that of copper. In insulators, heat is carried by vibrations of atoms in the crystal, called phonons.

Using powerful computing tools at CNF and Boston College, Stewart and his collaborators calculated the interactions between the diamond's phonons and how they scatter off of each other.

By doing so, they precisely solved the scattering term of the long-used Boltzmann Transport Equation, developed by Rudolf Peierls, which scientists had been forced to approximate for 80 years to get a best estimate for exactly how phonons travel across materials. The equation describes how phonons carry heat from hot to cold regions through diffusion, and how the scattering of phonons impedes heat flow.

One of the research team's key breakthroughs, Stewart said, is that they calculated these million or more phonon-phonon interactions directly from first principles, without any experimental data.

"This makes the approach truly predictive," he said.

This ability to "see" how phonons interact in diamond and how this affects heat transfer could be applied to other materials and thus provide insights into what materials might be best for applications in such areas as thermoelectrics.

"If we can do a good job modeling the thermal properties of these materials that people have studied, it puts us in a strong position to look at new candidate structures no one has considered before," Stewart said. "It can also give us ideas of how to manipulate materials on the nanoscale to change their thermal properties."

The researchers have already done similar calculations on traditional semiconductor materials, silicon and germanium.

Study co-authors are Professor David A. Broido and graduate student Alistair Ward of Boston College, and Gernot Deinzer of the University of Regensburg. The National Science Foundation funded the study.

Provided by Cornell University (news : web)