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Cool Conductors: Insulating Crystals

by Catherine Nisbett Becker | August 2014

Crystals are known to be excellent conductors of both heat and electricity. The same orderly crystalline structure that allows electric current to flow freely also enables heat energy to spread efficiently through the lattice of atoms. By contrast, glass is a disorderly clutter of atoms. And glasses are insulators — poor conductors of both heat and electricity.

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A crystal is any material in which the atoms are arranged in a three-dimensional, periodic pattern. Crystals are known to be excellent conductors of both heat and electricity. The same orderly crystalline structure that allows electric current to flow freely also enables heat energy to spread efficiently through the lattice of atoms.

But there are crystals, called clathrates and skutterudites, that break this general rule, conducting electricity well but acting as insulators for heat. Until now, it was unclear why. But recently, a European team led by Stéphane Pailhès of the Institute of Light and Matter at the University of Lyon, France, determined—theoretically and experimentally — how one clathrate prevents heat vibrations from spreading while conducting electric current. The team's results were published in *Physical Review Letters* in July 2014.

Why Crystals Conduct

A crystal is any material in which the atoms are arranged in a three-dimensional, periodic pattern. Almost all metals, for instance, can take on a crystalline structure. Crystals also have a large number of "free electrons". These are electrons in the outer orbits of their respective atoms, and when those atoms are joined in a lattice, the electrons can easily jump from one atom to the next. As a rule, crystals are good conductors. For instance, when you hold one end of an iron rod and put the other end into a fire, you

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will soon feel the end in your hand growing hotter. Electrical wire is made of metal because metal has little resistance to the flow of electricity.

The conduction properties of crystals are due to their atomic structure. When part of a crystal is heated, two things happen. First, the atoms near the heat source begin to vibrate. The lattice functions like a series of balls (the atoms) and stiff springs (the bonds between them). When the atoms in a lattice vibrate, they create a compression wave. They push and pull their neighbors, which in turn begin to vibrate, pushing and pulling *their* neighbors, and so on. The atoms' oscillations are "quantized," which means that they are restricted to certain energies. Waves of quantized energy moving through the crystal lattice are called "phonons."

Institute of Light and Matter/University of Lyon

The Institute of Light and Matter at the University of Lyon in France uses sophisticated technology to heat and X-ray crystals.

The second thing that happens when a crystal is heated is that its electrons become energetic. When free electrons become energetic, they move faster and can travel farther. Just as gas molecules near a heater spread through a room, so energetic electrons disperse through a crystal, carrying heat with them.

Electric current is the directional flow of electrons, and the same process that allows heat to move through a crystal allows electricity to move through it as well. If electrons move through a material without colliding with anything and changing direction, we say that the material has low resistance. And in fact, quantum mechanics predicts that in a perfect crystal, electrons would move through the lattice entirely unimpeded — yielding an electric current with no resistance. In practice, however, a perfect crystal does not exist, because all the atoms in the lattice are vibrating to a certain extent with heat energy.

For opposite reasons, ordinary glass is a poor conductor of both electricity and heat. Glasses are disorderly structures, so free electrons are bound to run into something nearby, and will constantly change direction. They cannot efficiently carry heat or a charge from one end of the glass to the other. Thermal vibrations are transmitted from atom to atom chaotically, so phonon waves cannot get very far.

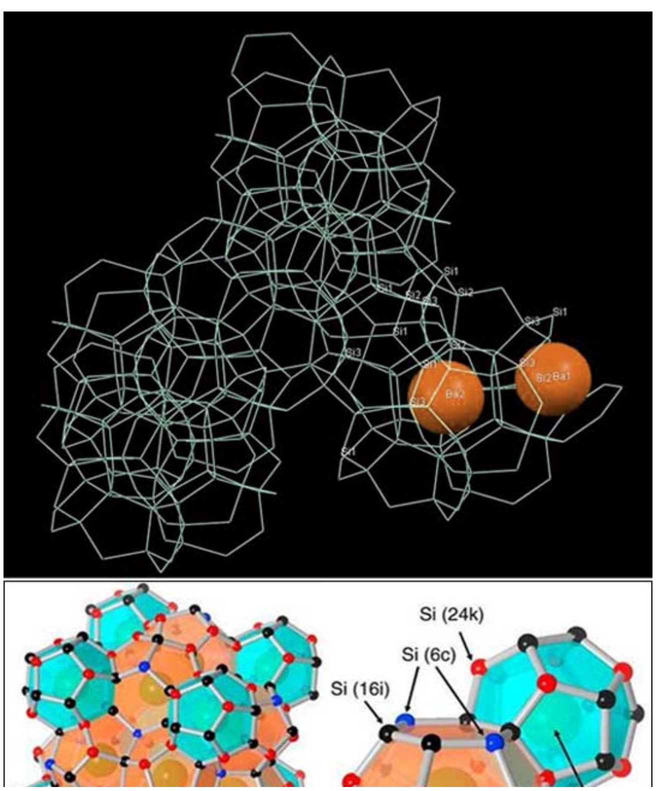
Cool, Charged Crystals

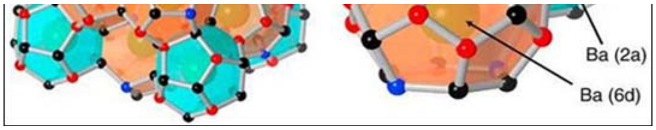
There are a couple of exceptions. Crystals that are “doped” with “impurities” will conduct electricity well, but heat poorly. In such crystals, impurity atoms are randomly distributed throughout the lattice structure. There aren’t enough of them to significantly impede the movement of electrons, so electric current will flow through the material. However, the impurities act like a breakwater to phonons of heat energy. They vibrate irregularly, preventing oscillating lattice atoms from transferring motion to their neighbors.

Since the 1990s, engineers have believed that a special class of crystals called clathrates would behave similarly, though lacking true impurities. In a clathrate, cage-like lattices of heavier atoms surround lighter, “guest” atoms inside. Unlike impurities, which are randomly distributed, these guest atoms are a regularly recurring, integral part of the clathrate’s crystal structure. It was thought that when atoms in the cage lattice began to vibrate, the trapped guest atoms would behave like the impurities in doped crystals and vibrate randomly rather than regularly. Clathrates, then, would act as a crystal for electricity, but as a glass for heat.

Phonon Conversion

According to Pailhès and his team, the truth is more complicated than that. Instead of acting as a glass for heat, clathrates are “thermoelectric”; they can actually change one form of vibration (heat) into another (electricity).





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In order to figure out how clathrates conducted heat, Pailhès and his team painstakingly synthesized a soccer-ball-shaped clathrate, Ba_8Si_{46} (a barium and silicon compound). The silicon formed the outer, soccer-ball shape, and the barium was trapped inside. They verified that the clathrate was pure, and then used X-rays to measure the phonons.

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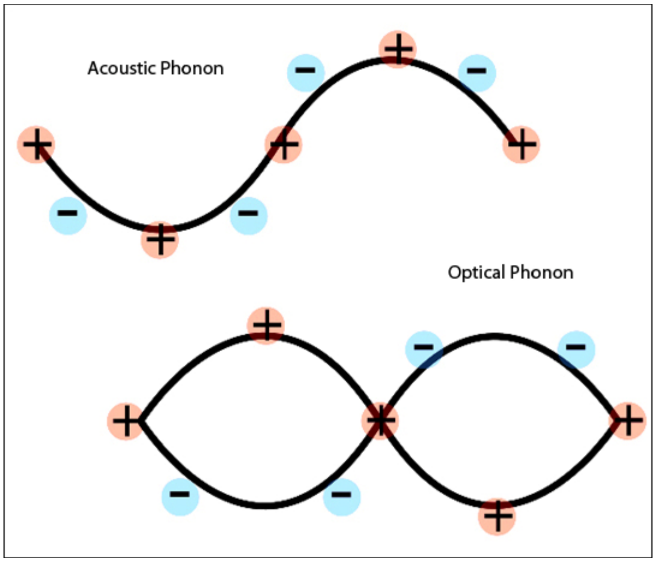
Phonons come in two types. "Acoustic phonons" act much like sound waves. They move through the lattice at fixed speeds, regardless of their wavelength, and they transmit heat. The simplest acoustic phonon occurs when all the atoms in a lattice move back and forth together. The second type, "optical phonons", are higher-energy phonons than acoustic phonons. Optical phonons are slower and don't transmit much heat. The simplest optical phonon occurs when adjacent atoms oscillate in opposite directions.



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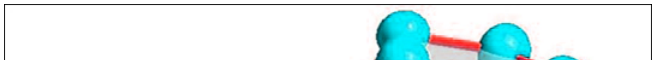
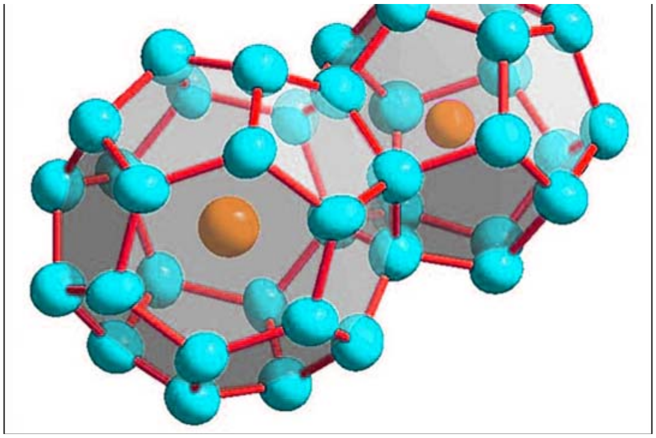
Phonons come in two types: acoustic phonons and optical phonons. In acoustic phonons, both positive and negative ions swing together. In optical phonons, positive and negative phonons swing against each other.

The team varied the energy of the acoustic phonons, bringing it up to the range of the optical phonons. They wanted to see whether their clathrate acted as a glass for acoustic phonons, with the guest atoms vibrating independently from the cages, thus preventing the wave from spreading. If individual, caged barium atoms were acting as breakwaters to the heat waves, one would expect the acoustic phonons to die off more quickly and their energy to be more variable. That was not what happened. As the energy increased to a critical point, the motion of the phonon was transferred from the silicon cages to the barium atoms, until the silicon stood still and the barium atoms moved back and forth together. The acoustic phonons became stationary optical phonons.





S. Pailhès/U. Lyon and M. de Boissieu/INP Grenoble

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The team's theoretical model and its experimental observation of clathrate behavior both bear out this result. The next step is for researchers to test other, more complicated clathrates. Scientists also want to know if skutterudites, a similar class of crystals, behave in the same way. Like clathrates, skutterudites have cage lattices with guest atoms, but the number of guest atoms in each cage varies.

Eventually, when they are better understood, clathrates and skutterudites might be used to help cell phones and other electronics stay cool. Or, they may be used to recapture the heat exhaust from a car and convert it into electricity.

Discussion Questions

Clathrates change heat into electricity, according to this study. What are other contexts in which this transformation occurs? How would you compare the phenomenon described here to piezoelectricity? Would you expect skutterudites to behave like clathrates?

Journal Abstracts and Articles

(Researchers' own descriptions of their work, summary or full-text, on scientific journal websites).

Pailhès, Stéphane, et al. "Localization of Propagative Phonons in a Perfectly Crystalline Solid." *Physical Review Letters* (July 1, 2014) [accessed July 9, 2014]: journals.aps.org/prl/abstract/10.1103/PhysRevLett.113.025506.

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