Nano Focus

Theoretical thermocrystals control heat like sound

Martin Maldovan of the Massachusetts Institute of Technology has produced a theoretical framework that could lead to improved control of heat flow in materials. Thermocrystals, comprising alloys containing nanoparticles, are materials that can manipulate thermal energy flow by exploiting the coherent reflections of phonons from internal surfaces. Potential applications including heat waveguides, heat lensing, thermal diodes, and thermal cloaking may become possible.

"The theory outlines a completely new way of manipulating heat," Maldovan says. "When they created photonic crystals, it was a completely new way of manipulating light. Then, they created phononic crystals as a completely new way to manipulate sound. This is equivalent to that, but for heat."

The key to the theory, as reported in the January 11 issue of *Physical Review Letters* (025902; DOI: 10.1103/PhysRevLett.110.025902), is to transfer thermal energy flow from standard short wavelength particle transport to long wavelength wave transport—to make "heat behave like light," according to Maldovan. Particle transport occurs when a phonon hits an interface and scatters diffusely in all directions. Wave transport happens when a phonon hits an interface and reflects and transmits coherently, like light in a mirror. Most of the time, heat phonons are scattered diffusely when they encounter an interface because their wavelengths are so small. For coherent scattering to occur, the interface has to be almost perfect (defect-free), rendering it almost impossible to make.

Instead of trying to make the perfect interface, Maldovan decided to try to make the phonon wavelength larger by reducing its frequency. Such phonons should transmit and reflect like light from even an imperfect interface.

From previous experience, Maldovan knew that in thermoelectrics, researchers use alloys and nanoparticles in order to block *all* frequencies of phonons. In this work, he used $Si_{1-x}Ge_x$ alloys with Ge nanoparticles to block only select frequencies. The mass-difference scattering in the alloy blocks some high-frequency phonons, and the nanoparticles block another portion. "I use the nanoparticles in such a way to kill only the really high-frequency phonons," he says, "so the nanoparticles in my case must be very, very small." In this work, he considered Ge nanoparticles with 1 nm diameter.

After killing the high-frequency phonons, Maldovan's theory was still left with a large number of wavelengths of heat that it could not handle, so he decided to narrow the frequency range by requiring the material to be a thin film, which kills the very low phonon frequencies. Having chopped off the highest and lowest frequencies, the heat that was left was concentrated into a narrow, intermediate band of wavelengths. Specifically, for $Si_{90}Ge_{10}$ thermocrystal thin films containing Ge nanoparticles, the heat spectrum was concentrated into a relatively narrow, low frequency window between 0.1 THz and 2.0 THz. Up to 40% of this heat was restricted to a narrow hypersonic range of 100–300 GHz.

Next, Maldovan investigated the design of periodic structures in the thin films to better manage the flow of this narrow range of heat frequencies, effectively engineering the thermal bandgap of these materials to match the heat frequency range. He found that by patterning the film periodically with lattice constants of 10 nm and 20 nm, the material could be tuned so that up to 23% (for two-dimensional patterning) of the thermal transport could be carried by phonons with frequencies in the engineered thermal bandgaps.

"The idea was that once I had the heat concentrated in a window, I wanted to match those frequencies for heat to the bandgap of a phononic crystal," Maldovan says. "Then I can control heat as if it is sound."

Future work will include collaborating with experimental materials scientists to try to produce thin films that might verify this theory. Maldovan says that although he focused on Si in this article, the theory is applicable to a wide range of materials, which he hopes experimentalists will be interested in exploring.

Tim Palucka

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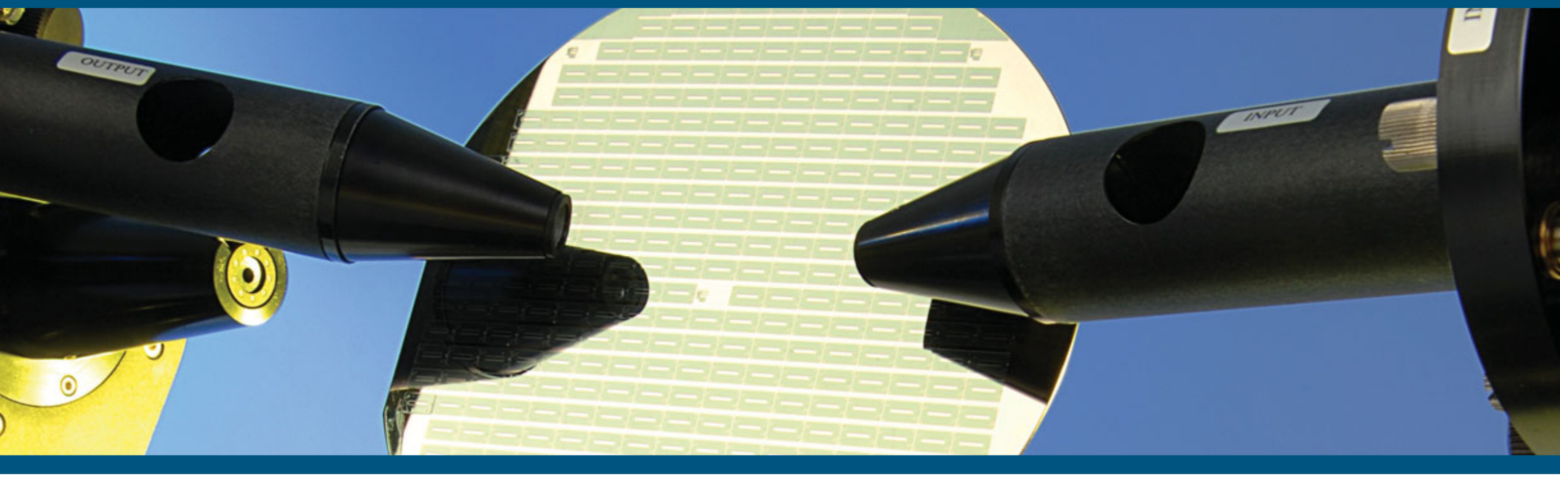

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