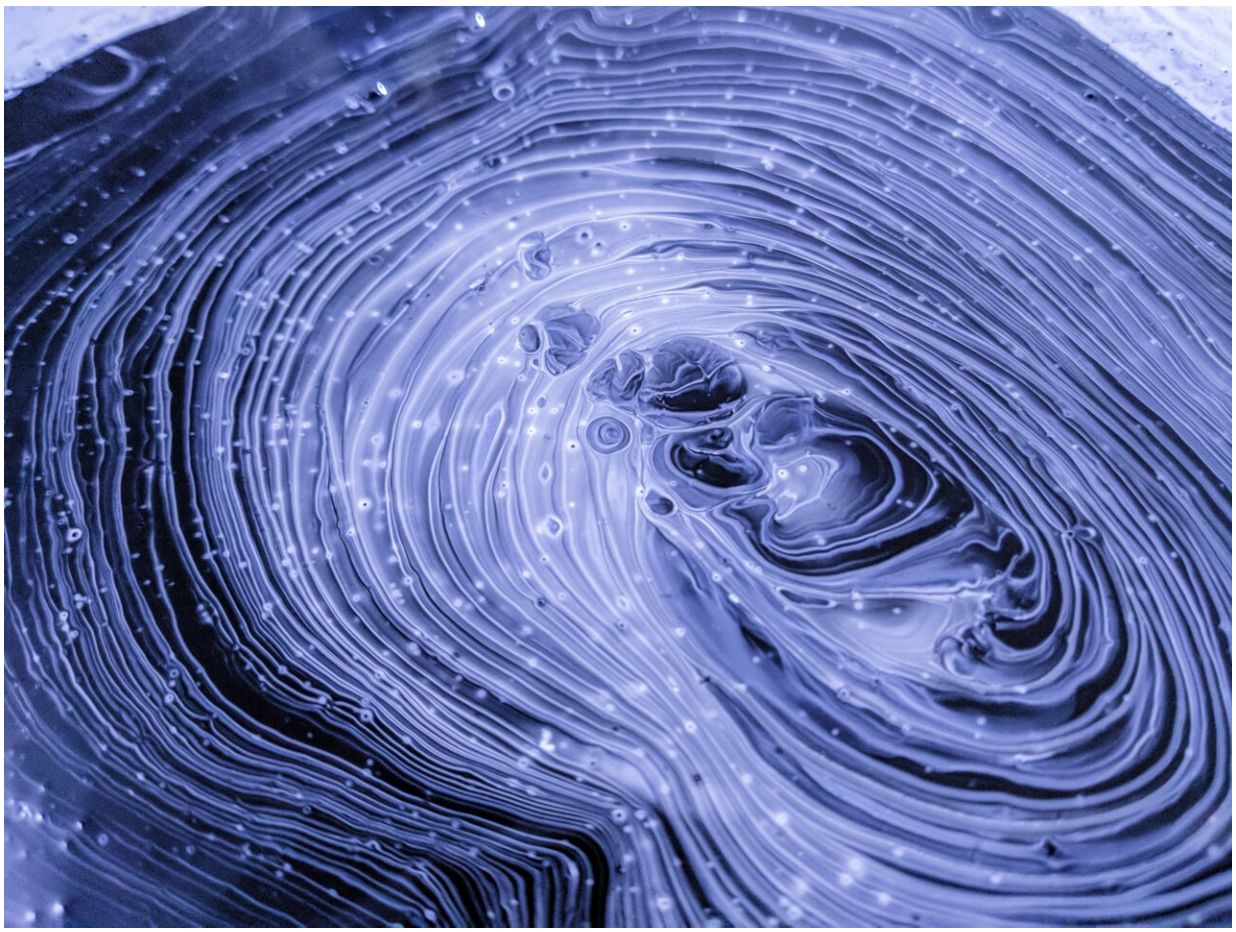
Calculations reveal how mixtures of different elements can control the thermal properties of nanowires

April 1 2015



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A mathematical model of heat flow through miniature wires could help develop thermoelectric devices that efficiently convert heat—even their own waste heat—into electricity.

Developed at A*STAR, the model describes the movement of vibrations called phonons, which are responsible for carrying heat in insulating materials. Phonons typically move in straight lines in nanowires—threads barely a few atoms wide. Previous calculations suggested that if parts of a nanowire contained random arrangements of two different types of atoms, phonons would be stopped in their tracks. In actual alloy nanowires, though, atoms of the same element might cluster together to form short sections composed of the same elements.

Now, Zhun-Yong Ong and Gang Zhang of the A*STAR Institute of High Performance Computing in Singapore have calculated the effects of such short-range order on the behavior of phonons. Their results suggest that heat conduction in a nanowire does not just depend on the relative concentrations of the alloy atoms and the difference in their masses; it also depends on how the atoms are distributed.

Their model simulated an 88-micrometer-long nanowire containing 160,000 atoms of two different elements. They found that when the nanowire was more ordered—containing clusters of the same elements—low-frequency phonons struggled to move. In contrast, high-frequency phonons could travel much further than the average length of the ordered regions in the alloy. "The high-frequency phonons were more mobile than we imagined," says Ong.

The researchers used their model to study the thermal resistance of a nanowire containing an equal mix of silicon and germanium atoms. Short-range ordering of the atoms allowed high-frequency phonons to travel freely through the wire, giving it a relatively low thermal resistance. In contrast, a random distribution of alloy atoms resulted in a higher resistance—over triple that of the ordered case for a 2.5-micrometer-long wire. "If this disorder can be realized in real composite materials then we could tailor the thermal conductivity of the system," says Ong.

Understanding the relative contribution of low- and high-frequency phonons to heat conduction could also help researchers tune the thermal properties of nanowires in the laboratory. "For instance, the surface roughening of nanowires is known to reduce the thermal conductivity contribution of high-frequency phonons," says Ong.

The researchers hope their model will help scientists design composite materials with low thermal conductivity. One attractive application is thermoelectric devices, explains Ong. "As these devices rely on a thermal differential, a low thermal conductivity is desirable for optimal performance."

More information: Ong, Z.-Y. & Zhang, G. "Enhancement and reduction of one-dimensional heat conduction with correlated mass disorder." *Physical Review B* 90, 155459 (2014). dx.doi.org/10.1103/PhysRevB.90.155459

Provided by Agency for Science, Technology and Research (A*STAR), Singapore