An unlikely competitor for diamond as the best thermal conductor

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An unlikely material, cubic boron arsenide, could deliver an extraordinarily high thermal conductivity – on par with the industry standard set by costly diamond – researchers report in the current issue of the journal *Physical Review Letters*.

The discovery that the chemical compound of boron and arsenic could rival diamond, the best-known thermal conductor, surprised the team of theoretical physicists from Boston College and the Naval Research Laboratory. But a new theoretical approach allowed the team to unlock the secret to boron arsenide's potentially extraordinary ability to conduct heat.

Smaller, faster and more powerful microelectronic devices pose the daunting challenge of removing the heat they generate. Good thermal conductors placed in contact with such devices channel heat rapidly away from unwanted "hot spots" that decrease the efficiency of these devices and can cause them to fail.

Diamond is the most highly prized of gemstones. But, beyond its brilliance and beauty in jewelry, it has many other remarkable properties. Along with its carbon cousins graphite and graphene, diamond is the best thermal conductor around room temperature, having thermal conductivity of more than 2,000 watts per meter per Kelvin, which is five times higher than the best metals such as copper. Currently, diamond is widely used to help remove heat from computer chips and other electronic devices. Unfortunately, diamond is rare and expensive, and high quality synthetic diamond is difficult and costly to produce. This has spurred a search for new materials with ultra-high thermal conductivities, but little progress has been made in recent years.

The high thermal conductivity of diamond is well understood, resulting from the lightness of the constituent carbon atoms and the stiff chemical bonds between them, according to co-author David Broido, a professor of physics at Boston College. On the other hand, boron arsenide was not expected to be a particularly good thermal conductor and in fact had been estimated – using conventional evaluation criteria – to have a thermal conductivity 10 times smaller than diamond.

The team found the calculated thermal conductivity of cubic boron arsenide is remarkably high, more than 2000 Watts per meter per Kelvin at room temperature and exceeding that of diamond at higher temperatures, according to Broido and co-authors Tom Reinecke, senior scientist at the Naval Research Laboratory, and Lucas Lindsay, a post-doctoral researcher at NRL who earned his doctorate at BC.

Broido said the team used a recently developed theoretical approach for calculating thermal conductivities, which they had previously tested with many other well-studied materials. Confident in their theoretical approach, the team took a closer look at boron arsenide, whose thermal conductivity has never been measured.

Unlike metals, where electrons carry heat, diamond and boron arsenide are electrical insulators. For them, heat is carried by vibrational waves of the constituent atoms, and the collision of these waves with each other creates an intrinsic resistance to heat flow. The team was surprised to find an unusual interplay of certain vibrational properties in boron arsenide that lie outside of the guidelines commonly used to estimate the thermal conductivity of electrical insulators. It turns out the expected collisions between vibrational waves are far less likely to occur in a certain range of frequencies. Thus, at these frequencies, large amounts heat can be conducted in boron arsenide.

"This work gives important new insight into the physics of heat transport in materials, and it illustrates the power of modern computational techniques in making quantitative predictions for materials whose thermal conductivities have yet to be measured," said Broido. "We are excited to see if our unexpected finding for boron arsenide can be verified by measurement. If so, it may open new opportunities for passive cooling applications using boron arsenide, and it would further demonstrate the important role that such theoretical work can play in providing useful guidance to identify new high thermal conductivity materials."

Provided by Boston College

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