

## Nanoscale Study Gives New Insight Into Heat Transfer in Biological Systems

## October 23 2005

One of the first things we learn in chemistry class is that solids conduct heat better than liquids. But a new study suggests that in nanoscale materials, this is not necessarily the case.

Using computer simulations, researchers at Rensselaer Polytechnic Institute have found that heat may actually move better across interfaces between liquids than it does between solids. The findings, which were published online Oct. 11 in the journal *Nano Letters*, provide insights that could prove useful in fields ranging from computer chip manufacturing to cancer treatment.

Conduction is the movement of heat from a warmer substance to a cooler substance, as when a spoon heats up after sitting in a cup of hot soup. "Liquids generally have low thermal conductivity when compared to solids," says Pawel Keblinski, associate professor of materials science and engineering at Rensselaer and coauthor of the paper. "For example, diamond is one of the best conductors around, with a conductivity of about 5,000 times that of water." Metals also tend to be good conductors, which is why the same spoon would normally feel cold to the touch — it conducts heat away from the hand.

But this conventional wisdom refers only to "bulk" thermal conductivity, which occurs at the macroscale. In nanoscale materials, the conductivity across interfaces plays a major role. "Conductivity at the interface of two materials is controlled by the nature of the interaction between molecules," says Shekhar Garde, associate professor of chemical and



biological engineering at Rensselaer and also coauthor of the paper. "Even if the two substances are good conductors, the nature of the interface could affect heat transfer between them."

Garde and Keblinski performed molecular simulations of a variety of interfaces and found that thermal conductivity between liquid interfaces turns out to be surprisingly high.

The findings could have immediate practical application for cancer therapy, according to Keblinski. "Scientists are developing cancer treatments based on nanoparticles that attach to specific tissues, which are then heated to kill the cancerous cells," he says. "It is vital to understand how heat flows in these systems, because too much heat applied in the wrong spot can kill healthy cells."

Garde's and Keblinski's research also could be important to the electronics industry, because of the growing interest in nanocomposite materials for computer chips, which generate a great deal of heat. Chip designers are increasingly combining solid surfaces with softer organic materials, and understanding heat flow will be a key aspect of continuing to shrink the dimensions of chip components, the researchers say.

The findings also provide more fundamental insights that are extremely important for understanding any system with nanoscale features, which tend to have huge numbers of interfaces, according to the researchers.

Biological systems are a key example. The surfaces of proteins, DNA, and other biomolecules interact with water to form the very basis of life. In water-based solutions, proteins instinctively fold into unique three-dimensional structures, which do much of the work in the body. Misfolded proteins also are implicated in diseases such as Alzheimer's and Parkinson's, and the ability of proteins to function depends on how much they can vibrate in their folded state.



The next step, according to Keblinski and Garde, is to focus on studying heat transfer between proteins and water, which will give them a better understanding of how water governs protein dynamics.

The National Science Foundation provided funding for the project. Harshit Patel, a graduate student in materials science and engineering at Rensselaer, also took part in the research.

Source: Rensselaer Polytechnic Institute

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