Physics Colloquium

Thursday, Sep 22nd at 3:30 pm in SC 234

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Phonons, defects, and heat flow control in (covalent) materials

Defects in materials impede the flow of heat. Almost 100 years ago, Rudolf Peierls proposed that defects scatter lattice waves (the word 'phonon' did not exist then). A few years later, Hendrik Casimir similarly argued that surfaces scatter lattice waves. Today, phonon scattering by impurities, grain boundaries, interfaces, surfaces, and other defects is the accepted way to think about the interactions between thermal phonons and any disruption to the perfect crystalline order. This implies that when (incoming) phonons encounter a defect, the interactions somehow generate new (outgoing) phonons whose momentum is equal (or at least related) to the momentum of the incoming ones.

However, defects have their own degrees of freedom. Some defect-related vibrational modes are visible in infrared absorption, Raman, or photoluminescence spectra, but most are not easily detected. However, they can be calculated. Defect-related modes exhibit two fundamental properties. First, they are localized in space; second, once optically or thermally excited, their vibrational lifetimes are much longer than those of bulk modes. Thus, defects trap small amounts of vibrational energy and this must play a role. But how significant is this 'phonon trapping' compared to phonon scattering? Recent ab-initio MD simulations show that phonon trapping is the only process taking place and that no scattering occurs at all. Further, the outcome of phonon-defect interactions depends on the temperature window and can be predicted. If it can be predicted, then it can also be controlled. Is the accepted knowledge incorrect?

Refreshments at 3:00 pm in SC 103