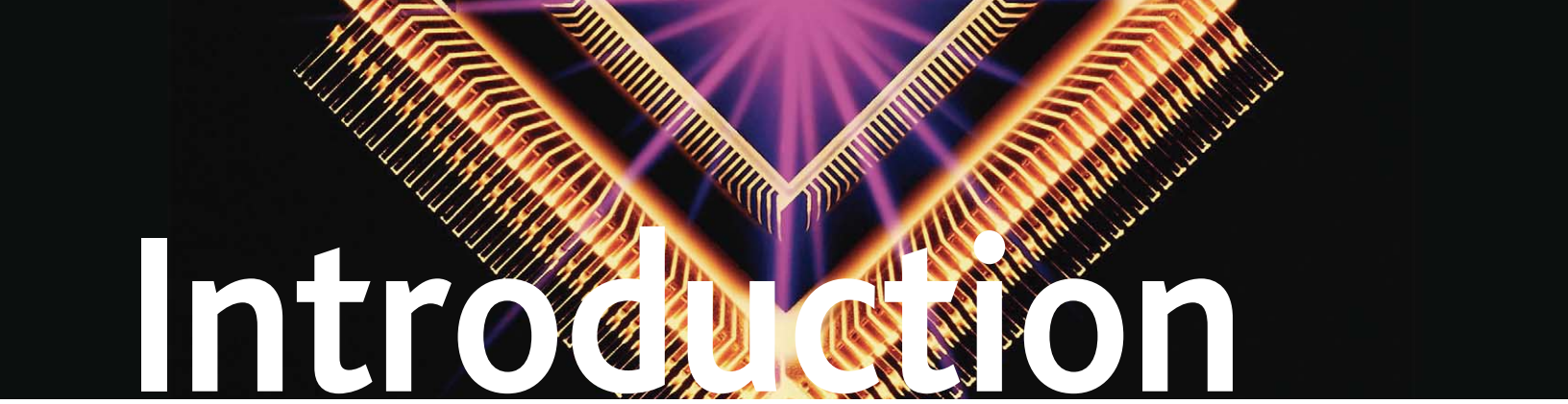

Introduction to thermal transport

by Simon R. Phillpot[†] and Alan J. H. McGaughey[‡]

The relentless increase in the thermal loads imposed on devices and materials structures is driving renewed interest among materials scientists and engineers in the area of thermal transport. Applications include thermal barrier coatings on turbine blades, thermoelectric coolers, high-performance thermal-transfer liquids, and heat dissipation in microelectronics. These, and other applications, demand not only ever more efficient thermal management, but also a better fundamental understanding of the underlying physical mechanisms.

This task is made more challenging because increased thermal-management performance must typically be accompanied by corresponding advances in other properties, such as electrical and mechanical behavior. This drive to higher performance is made yet more difficult by the decrease in dimensions of structures to the nanoscale and the increase in operating frequencies to the gigahertz range. Thermal transport in these regimes remains a largely unexplored research frontier. By giving a brief overview of thermal-transport mechanisms, this introductory article aims to set the context for the following three Review Features, which explore different aspects of nanoscale thermal transport. More detailed descriptions of the relevant theory can be found in the references listed at the end.

Heat can be transported by conduction, convection, and radiation, with the heat carriers typically being electrons, photons, phonons, atoms, or molecules. While conduction dominates in solids, both conduction and convection can play important roles in fluids. Radiation is most relevant to the study of gases, gas-solid mixtures, and porous materials, but can be appreciable in solids at high temperatures (e.g. in thermal barrier coatings). The Review Features presented here deal with thermal transport in solids and liquids, and so we focus on conduction and convection. Moreover, the solids discussed are generally electrical insulators in which phonons, i.e. atomic vibrations, dominate and conduction by electrons is negligible.

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Conduction

In 1811, based on experimental results, Fourier proposed the law that still forms the basis for analysis of heat conduction. Fourier's Law may be written as:

$$J_Q = -\kappa \, dT/dz \quad (1)$$

where J_Q, dT/dz, and κ are the z-direction heat flux (in units of W/m^2), temperature gradient (K/m), and thermal conductivity (W/mK), respectively. Generally, Fourier's Law is a vector equation, and the thermal conductivity is a second-order tensor (i.e. it may have a directional dependence). This relation defines the thermal conductivity. The thermal conductivities of a selection of materials between temperatures of 1 K and 1000 K are shown in Fig. 1. At very low temperatures, thermal conductivities of the order of 10 000 W/mK are found in some metals (e.g. Sn, Cu, and Ag) and dielectrics (e.g. alumina). At room temperature, values for dense solids range from ~1 W/mK (for amorphous materials) to 2300 W/mK (diamond). This range of values is much less than that for electrical conductivity, which spans more than 20 decades. As a result, the exploration of the high and low limits of thermal conductivity is of great technological and conceptual interest.

While Fourier's Law is the basis for analysis of thermal conduction, it does not provide a means for predicting the thermal conductivity itself. Progress in this direction began with modeling of thermal transport in gases. The application of elementary kinetic theory to a dilute gas leads to:

$$\kappa = 1/3 \, C_v \, \nu \, \lambda \quad (2)$$

where C_v is the heat capacity at constant volume, ν is the mean velocity of particles in the gas, and λ is the mean free path. Thus, the thermal conductivity is the product of the amount of energy that can be carried by a particle, the speed at which it moves, and the average distance it travels before scattering.

Debye first suggested that eq 2 could be applied to dielectric solids. In this approach, the gas is a gas of phonons – vibrational excitations of the system – and the mean free path is the average distance traveled by a phonon before scattering from another phonon or a structural defect. Although, in reality, the phonon gas is not dilute (except at low temperatures), this interpretation has led to models that fit experimental data well. The kinetic theory equation can also be applied to metals, with electrons as the dominant carriers, and to liquids.

Since the specific heat and speed of sound can be considered as materials parameters that are largely independent of the structure, the key mechanistic variable in describing conduction is the mean free path, which, in a solid, can range from nanometers (disordered materials) to microns (perfect crystals). For a crystalline solid at room temperature, the mean free path is at most a few microns, i.e. much less than the grain size in conventional materials. Thus, for the

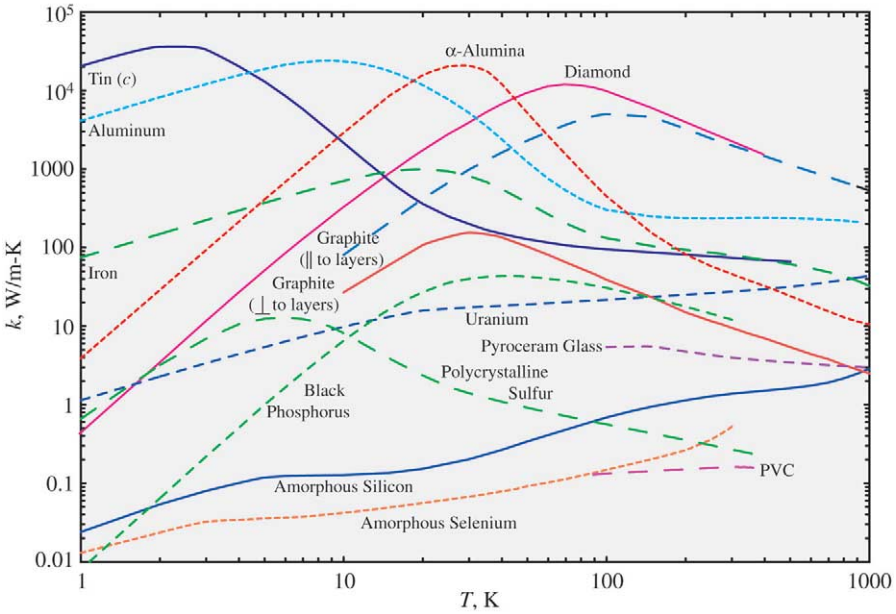

Fig. 1 Experimental thermal conductivities of crystalline and amorphous solids[1]. The materials presented cover the spectrum of electron-dominated to phonon-dominated thermal transport.

macroscopic structures that we are most familiar with, phonon-phonon scattering (via so-called Normal and Umklapp processes) dominates the thermal transport. However, the situation is different for materials and structures with nanoscale dimensions. In particular, when the mean free path is larger than the dimensions of the structure (e.g. grain size, layer thickness), phonon-phonon interactions become negligible and scattering from surfaces, dislocations, interfaces, and other structural imperfections can dominate. In these cases, the thermal conductivity is no longer strictly a material property.

In this ballistic transport regime, Fourier's Law cannot be directly applied and more sophisticated approaches are required. The Boltzmann transport equation (BTE) models the phonons themselves and their interactions; it can thus account for both diffusive and ballistic transport. A yet more detailed view of thermal conductivity comes from molecular-dynamics simulations in which the trajectories of the atoms that make up a system are predicted, allowing the phonons and their scattering processes to be modeled directly.

Surface convection

Under most conditions, the heat transfer between a solid and a fluid is dominated by convective effects (i.e. a result of the motion of the fluid particles). Surface convection may result from a forced flow or from a flow induced by thermobuoyant effects. For a fluid flowing over a solid surface (an external flow), the convective heat flux at a distance x from the leading edge is given by:

$$J_Q = \mathrm{Nu}_x \, \kappa \, \Delta T / x \qquad (3)$$

where Nu_x is the local Nusselt number. This parameter is a dimensionless surface convection conductance and is related to the system geometry, fluid properties, and flow characteristics. The temperature difference ΔT is taken as that between the solid surface and the bulk fluid. In the case of internal flows, the specification of the characteristic length and temperature difference are slightly modified[2]. For some laminar flows, the form of the Nusselt number may be theoretically predicted, but in most cases experimental data are used to develop empirical expressions. The thermal conductivity plays a key role, both directly in the expression for the heat flux and in the Nusselt number.

Fluid flow in nanochannels is characterized by large drag forces. As such, surface convection at the nanoscale is not an efficient means of managing thermal energy. Current interest lies more in the molecular structure of fluids and, specifically, in how additives (e.g. nanoparticles) can enhance the thermal conductivity, as has been observed experimentally. Behavior at these small length scales can have a profound effect on macroscopic behavior, and yet there is still little understanding of the underlying mechanisms.

Conclusions

The qualitative change of the conduction mechanism at the nanoscale is at the heart of the revival of interest in thermal transport in solids. These efforts are driven by both basic scientific interest and the pervasiveness of nanostructures in modern technologies. Much of the current work is focused on understanding how atomic structure and thermal transport are linked, and this equally applies to the development, study, and modeling of nanofluids. Goals include identifying limits of performance, both theoretical and practical, and designing new materials with desired behaviors.

The Review Features in this issue of *Materials Today* explore three frontiers in thermal transport research. Although they address rather different materials systems, the challenge in each case is to overcome the limitations of the narrow range of available thermal-transport properties. For microelectronic and heat-transfer fluid applications, the challenge is to maximize the heat flow, while for thermal barrier coatings the objective is to minimize it. A second commonality is that in each area a judicious combination of intuitive arguments, simulation, and experiment is driving current developments. Finally, all three articles demonstrate that there is a long way to go in both materials development and conceptual understanding before we can manage heat to anything like the degree that we currently manage electricity. MT

REFERENCES

1. Touloukian, Y., *Thermophysical Properties of Matter*, Volumes 2 and 3, Plenum Press, New York, (1970)
2. Kaviany, M., *Principles of Heat Transfer*, Wiley, New York, (2002)
3. Tien, C.-L., *et al.*, (eds.), *Microscale Energy Transport*, Taylor and Francis, Washington, (1998)
4. Cahill, D. G., *et al.*, *J. Appl. Phys.* (2003) **93**, 793
5. Chen, G., *Nanoscale Energy Transfer and Conversion*, Oxford University Press, Oxford, (2005)