

The transistor counts on the high-end micro-processor is rushing toward the 400-million mark and the feature dimensions are shrinking toward the nanometer scale. As a result, the thermal properties of semiconductor nanostructures are beginning to attract significant attention. Several major factors explain the recent interest to investigate thermal conductivity in quantum confined structures. The most important one is a continuous scaling down of the feature sizes in electronic devices and circuits. This leads to an increase in power dissipation per unit area despite the reduction of the power supply voltage. In addition, a variety of size effects that manifest themselves at the nanoscale are very interesting from the physics point of view.

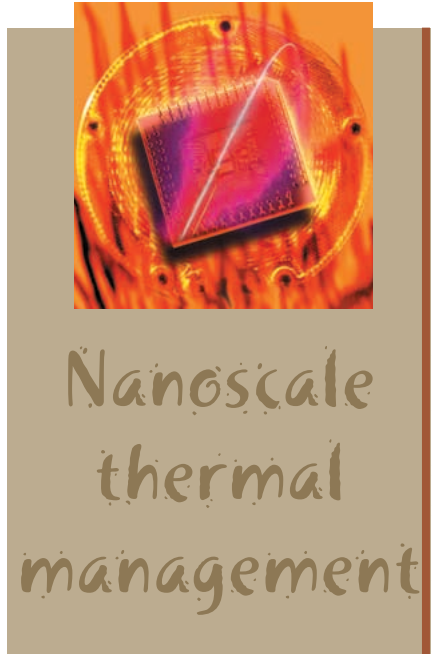
To achieve increased computer chip performance and reduce cost, for the past three decades the semiconductor industry has pursued a strategy of decreasing the feature size of devices with each new product generation or technology node. The technology node is defined by the smallest device or circuit feature size. Conventionally, this feature element is the half-pitch of the first level interconnect lines in the dynamic random access memory (DRAM) or the transistor gate length.

Following the projections of the International Technology Roadmap for Semiconductors, the industry will reach the 70-nanometer technology node by the year 2008. The 70-nanometer technology node corresponds to the feature size of 70 nanometers or 7×10^{-8} meters. For comparison, the feature size of state-of-the-art devices is 0.18 micrometers. Thus, rather soon, the electronic industry will completely enter the realm of nanoscale and face many new challenges.

Scaling transistors to the nanometer scale is plagued with challenges. Some examples are quantum mechanical gate tunneling, electron mobility degradation, and reliability problems due to statistical fluctuations in the positioning of dopant atoms.

A specific problem is related to interconnects. Making interconnects smaller, unlike transistors, does not enhance their performance. For example, it is predicted that the intrinsic delay-time of the 1-mm-long interconnect at the 35 nm technology node will

overwhelm the transistor's delay-time by two orders of magnitude: 250 ps vs 2.5 ps. With more interconnects and smaller transistor feature size, the thermal resistance of the integrated circuit



(IC) increases as well as the difficulties of heat removal associated with it.

Despite reducing the power supply voltage, the total power consumption in future ultra-large scale integration (ULSI) circuits will increase. Figure 1 illustrates the expected change in the power-supply voltage (a), and in the maximum total power dissipated in high-performance chips with an external heat sink (b). The shown data corresponds to the projections of the International Technology Roadmap for Semiconductors. Higher operating frequency and the higher overall capacitance and resistance of larger chips with more on-chip functions primarily drive the predicted increase.

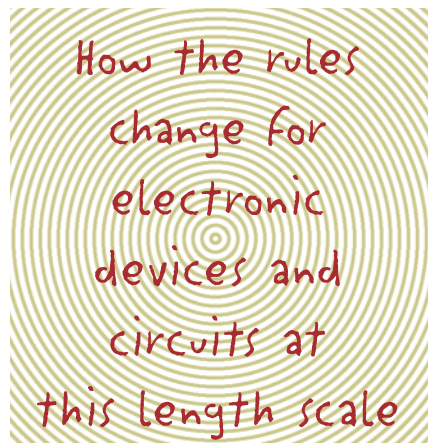
Besides its practical importance, the investigation of heat transport in nanostructures offer other rewards. For instance, the related physical phenomena that emerge at this length scale. These size-related phenomena are expected to affect the thermal conductivity of materials used to fabricate the devices. Better understanding of these phenomena may help future engineers not only to reduce the adverse nanoscale effects but also use them to advantage. This will ultimately lead to better design of devices and ICs.

Power dissipation and power supply voltage

One obvious way to deal with power dissipation in nanoscale devices and circuits is to reduce the supply voltage V_{DD} . A supply voltage of 3.3 V currently prevails in conventional CMOS-based very-large scale integration (VLSI) circuits. CMOS stands for complementary metal oxide semiconductor and denotes the most common integrated circuit technology that dominates the electronics market.

Although some reduction of V_{DD} is projected, it cannot go too far because of the limitations imposed by thermal fluctuations and noise margins. Integrated circuits that are not actively cooled typically operate at a temperature of 100 °C ($T = 373$ K) and give off heat at room temperature. At this temperature, thermal fluctuations have the energy of $k_B T \sim 5 \times 10^{-21}$ Joules (k_B is the Boltzmann's constant).

Let's consider the digital design. In binary operations, for a bit to be stable against thermal fluctuations, the energy needed to flip a bit must be about 10 times more. Thus, the energy dissipated per operation is about 5×10^{-20} Joules. We cannot engineer a conventional circuit that dissipates less heat per operation than the amount indicated. This statement is true unless we consider some of the revolutionary new ideas of quantum computing or reversible com-



puting, but that is an entirely different story. For the time being, we will restrict ourselves to good old binary logic implemented on CMOS ICs.

The power per square centimeter dissipated by IC is approximately given by the device density multiplied by the energy dissipated and the number of operations per second per device. The amount of energy that can be transported away from a given device and a cir-

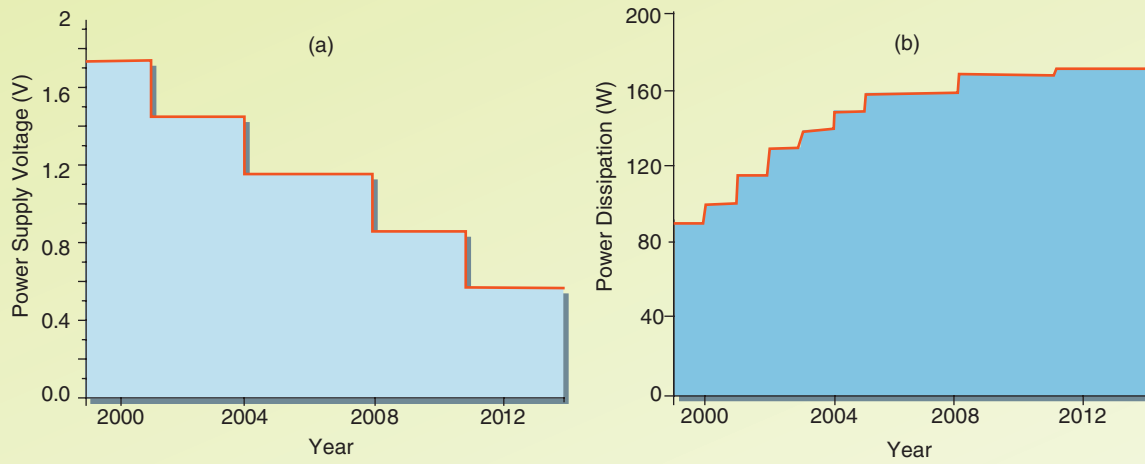


Fig. 1 Predicted change in the power-supply voltage and maximum total power dissipated in high-performance chips.

circuit is limited by the thermal conductivity of the circuit material and the environment.

The typical amount of power that can be removed from the circuit is about 25 W/cm². The minimum power supply voltage calculated from the limit imposed by the thermal fluctuation is about $4 k_B T / e \sim 0.1$ V. More conservative estimates that rigorously take into account noise margins predict that the V_{DD} should be limited to range from 1.2 V to 2.5 V. Thus, since the supply voltage cannot be reduced indefinitely, one has to maintain relatively large thermal conductivity in the device structure to remove generated heat in future ULSIs.

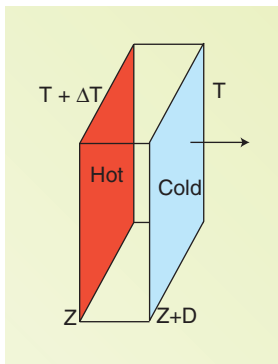


Fig. 2 Illustration of Fourier's law of heat conduction.

Heat conduction in solid materials

Let's review some basics of thermal conduction in bulk solid materials. A French mathematician, J.B.J. Fourier (1768-1830) in his *Theory Analytique De La Chaleur* formulated the commonly used law of heat conduction in 1822. From phenomenological considerations he showed that the rate of heat transfer Q in solids is proportional to the temperature difference $T_1 - T_2$ between the hot

and cold ends of the slab of material, or more accurately, the temperature gradient. This law is conventionally written as

$$Q/A = -K \nabla T$$

where K is the coefficient of thermal conductivity which is a property of the particular material, A is the cross-sectional area that the heat is flowing through. The quantity Q/A has a special name, which is the heat flux. It represents the flow of heat energy across a unit area per unit time (or Joules/second-square meters).

The coefficient K may vary with temperature T . Although in simple calculations, it is often assumed to be constant for temperatures that are not too low. The coefficient of thermal conductivity is always a positive constant. This can be easily understood from the molecular concept of temperature. The heat, which is essentially kinetic energy of atoms and molecules, tends to flow from regions of high internal energy to regions of low internal energy. The latter is consistent with the aforementioned formula that states that the heat flow is in the opposite direction of the temperature gradient, e.g., from the hot end of the sample to the cold end of the sample. Illustration of the heat flux across a slab of thickness D is given in Fig. 2.

A slightly modified form of this equation, written for the steady state heat flow, resembles the well-known Ohm's law for an electrical current flow I through a resistor R . These two equations are given by the following expressions

$$Q = \frac{1}{R_T} (T_1 - T_2) \Leftrightarrow I = \frac{1}{R} (V_1 - V_2).$$

Here the rate of heat transfer Q is analo-

gous to the electrical current I in Ohm's law, the temperature difference $T_1 - T_2$ is similar to the voltage difference $V_1 - V_2$. Note that the electrical current I is nothing but a flow of conduction electrons or holes in semiconductor material.

A definition of the thermal resistance $R_T = L / (K \times A)$ is also equivalent to the electrical resistance. The analogy with electrical currents and fields can be taken even further. In particular, if there are no heat sources present, one can write for temperature distribution Laplace's equation $\nabla^2 T = 0$, which is similar to $\nabla^2 V = 0$ for the electric potential.

Fourier's law is based on the continuum assumption of the material. It does not distinguish among different microscopic mechanisms of heat transfer. We have to consider the mechanisms of heat transfer and identify the heat carriers. In metals, for example, heat is carried by free electrons. Since electrons are also current carriers, there is a strict correlation between thermal conductivity K and electrical conductivity σ . These two quantities are related through Wiedemann-Franz law that states that the ratio K/σ is constant independent of material and is equal to $(\pi^2/3)(k_B/e)^2 T$, where e is the charge of an electron.

Heat in intrinsic, or moderately doped, semiconductors is mostly carried by lattice waves. The lattice waves or crystal lattice vibrations are conveniently described by some imaginary, e.g. quasi, particles called phonons. Since electric current is still carried by electrons or holes, thermal conductance is not as strongly correlated with electrical conductance in this case. Knowing electrical conductivity does not provide an answer to the question of what is the thermal conductivity of a given semiconductor

material. To calculate the coefficient of thermal conductivity, one needs to develop a formalism that describes propagation of lattice waves that carry heat.

The coefficient of thermal conductivity K of semiconductor and dielectric solids is usually inversely proportional to the absolute temperature T in the range of temperatures from liquid air temperature up to higher-than-the room temperature. Physicist Peter Debye (1884-1966) explained this dependence in the following way. The lattice vibrations can be resolved into travelling waves that carry heat. These waves have a finite attenuation length Λ due to the anharmonicities and imperfections in the crystal, which leads to the waves being scattered. The thermal conductivity is expressed as

$$K \propto C v \Lambda$$

where C is the specific heat per unit volume; and, v is the velocity of sound in the given material which is related to the velocity of the traveling waves of vibration. Debye further showed that the attenuation length, and thus the thermal conductivity, varies as $1/T$ when the temperature is not too low and C can be assumed constant.

When we invoke a concept of phonons to explain the same phenomenon, instead of attenuation length we use the term phonon mean free path (MFP). More accurately defined MFP is the average distance Λ that phonons travel until they are scattered by some crystal imperfection or other phonons.

In this formulation, Debye's model is similar to the free gas models used to describe molecules in gases. The phonons play a role of the localized particles. The MFP in this case can be expressed $\Lambda = v \times \tau$, where τ is the phonon lifetime or time that the phonon travels until it is scattered by defects, boundaries or other phonons. Inverse of this quantity, $1/\tau$, gives the phonon scattering rate.

Despite its simplicity and very approximate nature of the assumptions, Debye's model of thermal conductivity proved to be very useful and sufficient for many practical applications. As long as the feature sizes of electronic or optoelectronic devices L are larger than the phonon mean free path L , the engineer who calculates thermal balance for given devices can use tabulated bulk values of the coefficient of thermal conductivity and disregard any size effects. The situation starts to change when the device feature shrinks below MFP. It undergoes drastic change when the device feature

approaches the wavelength of the phonons that carry heat.

Acoustic and optical phonons

There are some fundamental concepts required for understanding size effects on heat transport in nanoscale devices. As stated, most of the heat in technologically important semiconductors is carried by crystal lattice waves or phonons. A phonon is a quasi particle representing a quantum of the crystal lattice vibrations.

There are two possible modes of vibrations of atoms in the crystal: longitudinal and transverse. For longitudinal phonons, the displacement of atoms from their equilibrium position coincides with the direction of propagation of the wave, whereas for transverse phonons, atoms move perpendicular to the wave propagation direction.

For semiconductor crystals with one atom per unit cell, the phonon dispersion, which is phonon energy dependence on the phonon wave-vector q , is represented by one, acoustic, branch only. However, if the crystal has more than one atom in the unit cell, optical branches will appear in the dispersion (see Fig. 3).

The difference between acoustical and optical branches arises because there are more options for vibration displacements of atoms in the unit cell. Figure 4 shows transverse optical and transverse acoustic phonon modes in a diatomic linear crystal lattice illustrated by the atom displacement for the two modes at the same wavelength. Arrows in Fig. 4 indicate the direction of propagation of the waves. Since in technologically important semiconductors (Si, GaAs, Ge, etc.) optical phonons do not contribute much to thermal conduction, we will concentrate on acoustic phonons.

The expression that describes acoustic phonon branch depicted in Fig. 3 can be obtained from a very simple classical treatment. Let's consider a linear chain of identical atoms of mass M positioned at a distance a , the lattice constant, connected by some imaginary springs that imitate interaction between atoms. These springs obey Hooke's law which states that the restoring force is proportional to the displacement of the atoms from their equilibrium positions.

For simplicity, we will consider longitudinal deformations. That is, displacements of atoms are parallel to the chain. We introduce the following notation: U_j is the displacement of atom n from its

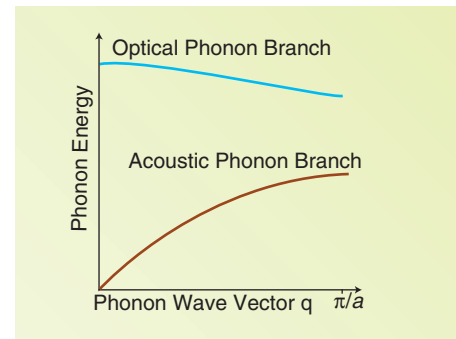


Fig. 3 Phonon dispersion in bulk semiconductor crystal.

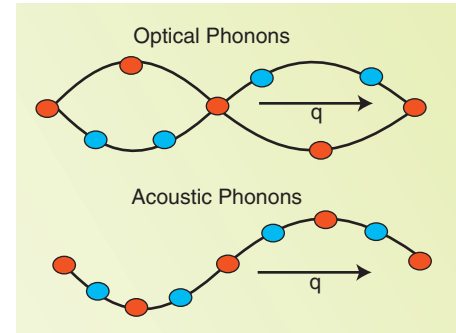


Fig. 4 Transverse optical and transverse acoustic phonon modes.

equilibrium position, U_{j-1} is the displacement of atom $j-1$ from its equilibrium position, U_{j+1} is the displacement of atom $j+1$ from its equilibrium position. The force on atom j will be given by its displacement and the displacement of its nearest neighbors via the expression

$$F_j = \beta(U_{j+1} - 2U_j + U_{j-1})$$

Here β is the spring constant. The equation of motion is then written as follows

$$M \frac{\partial^2 U_j}{\partial t^2} = \beta(U_{j+1} - 2U_j + U_{j-1})$$

The general solution of this equation is known to have a form of travelling plane waves

$$U_j = U_{j_0} \exp\{i(jqa \pm \omega t)\}.$$

Substitution of this general solution into the equation of motion give us the phonon dispersion relation for the linear monoatomic chain of atoms

$$\omega = \pm \sqrt{\frac{4\beta}{M}} \sin\left\{\frac{qa}{2}\right\}.$$

In this solution, we tacitly used the assumption of the infinitely large crystal lattice and its periodicity. The lattice periodicity (period is the unit cell length a) is reflected in the dispersion which has a repeat period of $2\pi/a$. Therefore all useful information is contained in the waves with wave vectors lying between the limits $-2\pi/a < q \leq \pi/a$. This range of wave vectors is called the first Brillouin

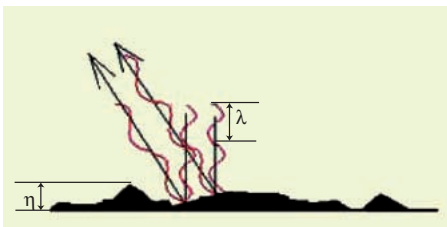


Fig. 5 Illustration of boundary scattering of acoustic phonons.

zone. At the Brillouin zone boundaries, the atoms nearest to the chain vibrate in the opposite directions and the wave becomes a standing wave. As q approaches zero, which corresponds to the long-wavelength limit, the above dispersion reduces to

$$\omega = v_o q$$

where v_o is the phonon phase velocity, which is equivalent to the velocity of a sound in the crystal. Phonons with frequencies that approach zero in the limit of small q are known as acoustical phonons. Acoustic phonons are the ones that carry heat in semiconductors since they have larger group velocity. This is determined by the slope of the dispersion branches. They are more heavily populated than the optical phonons (since they have lower energy).

The important point to emphasize here is that this derivation is valid for very large, e.g., bulk semiconductor samples where $L \gg \lambda$. When the size of the semiconductor structure approaches nanoscale, one has to introduce new boundary conditions, which will result in changed phonon dispersion.

Effects of boundary scattering on phonon heat conduction

Phonon heat conduction at nanoscale differs from that at the macro- or microscale for several fundamental reasons. Firstly, the increased surface to volume ratio results in increased phonon scattering from device structure boundaries and interfaces between different materials. Provided that the structure boundaries are always characterized by certain roughness p , it leads to an increase

in the thermal boundary resistance.

Secondly, as the size of electronic devices decreases below the phonon MFP and starts to approach the wavelength of the dominant thermal phonon λ , the acoustic phonon spectra undergoes a drastic change. This modification leads

this case, the phonon can fly all the way from one boundary to another without being scattered by defects. But since consumer electronic devices normally operate at temperatures higher than room temperature, engineers are not that concerned by boundary scattering. This attitude started to change when the device feature size became smaller than the phonon MFP at room temperature.

Experiments have shown that the effective MFP of the dominant phonons at room temperature in silicon thin films is close to 300 nms. It is much longer than believed earlier. The theoretical values for the effective phonon MFP in silicon extracted from the Debye model is about 41 nms and about 260 nms calculated from more precise theory that takes into account non-linearity of phonon dispersion.

Since the state-of-the-art devices have feature size L of about 180 nms (and are expected to be much smaller soon), we may have a condition $L \leq \lambda$ even at room temperature. Now the phonon mean free path is limited by scattering from the boundaries, which prevent phonons from propagation. Thus, the thermal conductivity coefficient decreases. Indeed, now we can write for the thermal conductivity

$$K \propto Cv/L$$

which gives us smaller value for $L < \lambda$. Note that unlike mean free path, L in the equation is independent of phonon frequency and polarization and is completely determined by the geometry of the structure.

Here we assume that the boundaries have some roughness so that phonons can scatter at any direction after being reflected by the boundary (see Fig. 5). This type of scattering, commonly called diffusive, contributes to thermal resistance. These simple semi-quantitative considerations lead us to correct results.

Recently several groups reported reductions of phonon thermal conductivity in semiconductor thin films and superlattices. They attributed these reductions by the most part to increased acoustic phonon-boundary scattering. The observed reductions were from moderate 20%-50% to huge, two orders of magnitude drop in some cases.

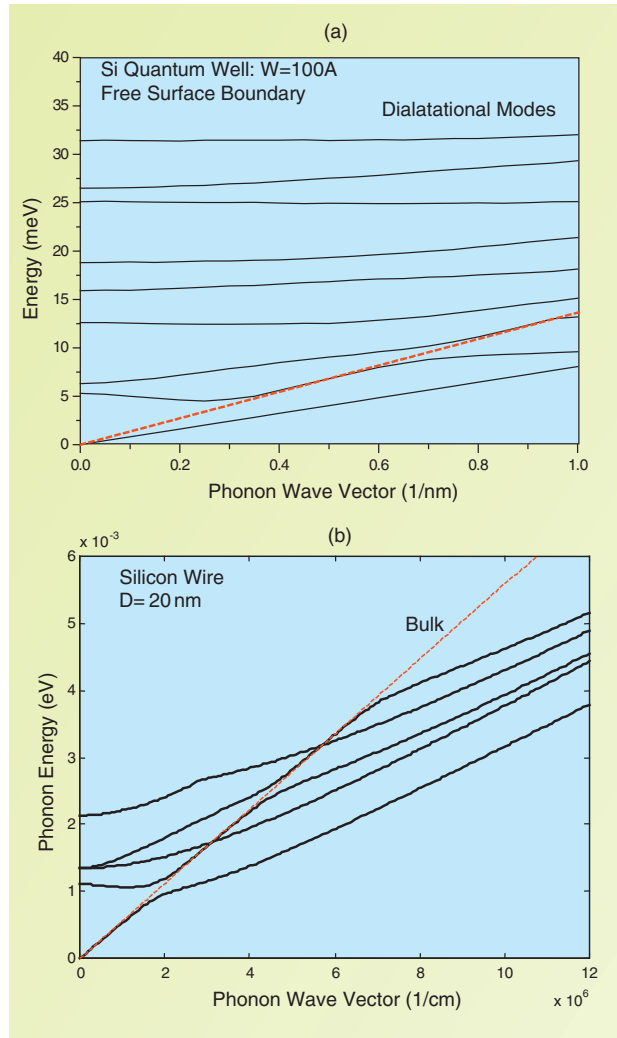


Fig. 6 First few confined acoustic phonon dispersion branches in a silicon thin film and cylindrical nanowire.

to the change in the average phonon group velocity and, correspondingly, the ability of phonons to carry heat. In silicon thin films and nanowires with lateral dimensions on the order of 10 nms, such modification of the phonon dispersion results in significant decrease of the phonon thermal conductivity.

First, we will discuss the effects associated with increased acoustic phonon-boundary scattering. When the device size is rather large, say a micrometer, the contributions of boundaries to thermal resistance can only be felt at low temperatures when phonon MFP is also close to a micrometer. In

Phonon dispersion modification

Another phenomenon that produces change in the thermal conductivity coefficient is related to modifying the acoustic phonon dispersion in nanoscale structures. As we stated, the phonon dispersion shown in Fig. 3 is obtained under assumption of “very” large crystals. Thus, we do not care about vibrations of the boundary atoms and use generic *periodic* boundary conditions. When the feature size of the device structure L is much smaller than the phonon mean free path l and starts to approach characteristic acoustic phonon wavelength l , this assumption cannot be used. For structures a few nanometer thick (or a few tens of nanometers), one has to calculate the phonon dispersion for specific boundary conditions.

Several of the lowest branches of the acoustic phonon dispersion for a silicon thin film and a cylindrical nanowire of the same feature dimension (thickness or diameter) $L=20$ nanometers are shown in Fig. 6 (a-b), respectively. One can see that spatial confinement in these nanostructures leads to many dispersion branches, their flattening and corresponding decrease of the phonon group velocity. For comparison, dashed lines show the corresponding bulk dispersion branches. The very first confined branch in both nanostructures is of the “true” acoustic type. This means that the energy goes to zero as the wave vector q approaches zero. This is exactly the same behavior as in bulk (see Fig. 3).

For the higher acoustic branches, there exist the cut-off frequencies, e.g. the energy does not go to zero as the wave vector q approaches zero. These branches look more like the optical branch in bulk semiconductors shown in Fig. 3. Since these quasi-optical branches are still relatively low in energy and their group velocity is non-zero, they do contribute to heat transfer.

Calculating the phonon group velocity averaged over all confined dispersion branches we obtain the average velocity value. It is smaller than in the corresponding bulk material. Figure 7 shows the average phonon group velocity as a function of phonon energy for a thin silicon film and a nanowire.

As one can see, the asymptotic values for the average phonon group velocity in the wire and thin film are 5.39×10^5 cm/s and 5.67×10^5 cm/s, respectively. Both values are smaller than the phonon velocity in bulk silicon,

which is 8.47×10^5 cm/s. This decrease in the group velocity results in a corresponding drop of thermal conductivity. Slow phonons are easier to scatter by impurities or defects.

Naturally, the decrease in thermal conductivity will also depend on the surface quality, particularly on how the surface roughness compares with the dominant phonon wavelength (see Fig. 5). The thermal conductivity coefficient calculated as a function of the surface “roughness” parameter p is shown in Fig. 8. Parameter p , which is related to the surface asperity η (defined in Fig. 5), is a fraction of the diffusely reflected acoustic phonons. The value $p=0$ corresponds to a very rough surface while $p=1$ corresponds to a perfect surface. One can see a strong decrease of the thermal conductivity in thin films and nanowires due to the increased boundary scattering and modification of phonon dispersion.

Summary

Here we outlined only a few nanoscale phenomena that adversely affect thermal conductivity and can complicate heat removal from nanoscale electronic devices. Since progress in the electronic industry is largely associated with device down-scaling, it is worth researching the subject more.

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Read more about it

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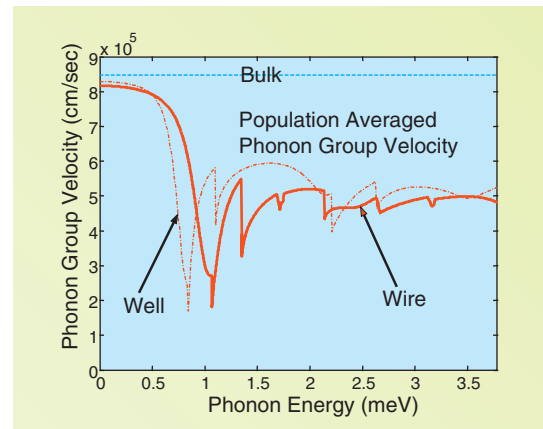


Fig. 7 Average phonon group velocity as a function of phonon energy.

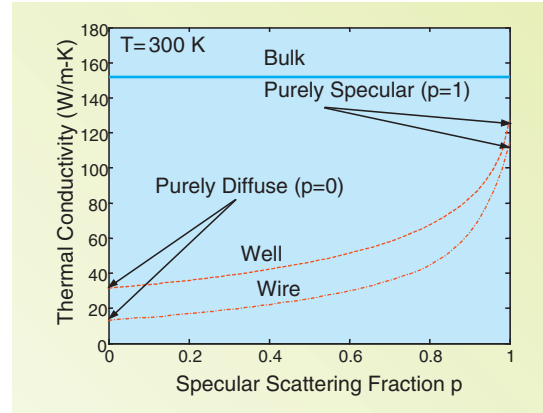


Fig. 8 Phonon thermal conductivity as a function of the surface “roughness” parameter p .

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About the author

Alexander A. Balandin is an associate professor at the Department of Electrical Engineering in the University of California–Riverside (UCR). He received his M.S. degree in Applied Physics from the Moscow Institute of Physics and Technology (MIPT) in 1991 and his Ph.D. degree in Electrical Engineering from the University of Notre Dame in 1997. He has conducted research in solid-state devices; thermal, electrical and optical properties of nanostructures; and low-frequency noise in electronic devices. He has published over 50 refereed journal and conference papers. He belongs to Eta Kappa Nu and IEEE. His group’s research on nanoscale thermal management is supported by NSF. For more info on his research: <http://www.ee.ucr.edu/~alex/b/>.