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From the Casimir Limit to Phononic Crystals: 20 Years of Phonon Transport Studies Using Silicon-on-Insulator Technology

Silicon-on-insulator (SOI) technology has sparked advances in semiconductor and MEMs manufacturing and revolutionized our ability to study phonon transport phenomena by providing single-crystal silicon layers with thickness down to a few tens of nanometers. These nearly perfect crystalline silicon layers are an ideal platform for studying ballistic phonon transport and the coupling of boundary scattering with other mechanisms, including impurities and periodic pores. Early studies showed clear evidence of the size effect on thermal conduction due to phonon boundary scattering in films down to 20 nm thick and provided the first compelling room temperature evidence for the Casimir limit at room temperature. More recent studies on ultrathin films and periodically porous thin films are exploring the possibility of phonon dispersion modifications in confined geometries and porous films. [DOI: 10.1115/1.4023577]

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1 Introduction

A major research and manufacturing achievement over the last decades of the 20th century was the development and implementation of silicon-on-insulator (SOI) technology, which offers nearly perfect single crystal silicon layers of submicrometer thickness attached to a silicon dioxide passive layer on a bulk silicon substrate. The resulting SOI wafers have become the starting point for a broad variety of innovative devices, including high-performance microprocessors, microfabricated sensors and actuators, and photonic crystals [1–3]. The impact has been particularly profound for the MEMS community, for which a large fraction of the most important device technologies are based on SOI wafers fabricated using either bond and etch back methods or implantation. The silicon dioxide layer between the silicon overlayer and the bulk substrate serves as an etch stop for fabrication processes—enabling freestanding silicon films in some cases—and as a mechanism for controlling the electric field distribution in nanotransistors. This “buried oxide” also dramatically alters the shape and magnitude of heat flux lines leaving active regions of the devices in which it remains, e.g., within SOI nanotransistors for advanced microprocessors [4].

For the community of researchers interested in micro- and nanoscale solid-state heat conduction, the availability of SOI overlayers proved to be a watershed event for fundamental phonon transport research. Prior to the use of SOI substrates in thermal transport studies, there was considerable debate over the specific physics responsible for the reduced conductivity in thin dielectric films. The debate was spurred by several reports of very low thermal conductivity values for non-SOI samples, which were relatively defective compared to bulk samples. The silicon overlayer provided a nearly defect-free silicon layer for suspension and characterization, which provides a unique opportunity for performing fundamental phonon transport research without the complications of process-dependent imperfection scattering. Silicon-on-insulator films have, therefore, become a pivotal platform for

probing phonon-boundary scattering through measurements, many of which determine the effective in-plane thermal conductivity of the silicon layer. Silicon thin films and nanowires of varying dimensions have been studied in depth over the past 20 years [5,6]. In the thinnest films that have been examined experimentally (20 nm [7]), boundary scattering reduces the thermal conductivity to as little as ~15% of the value for bulk silicon. This classical size effect occurs when the dimensions of the sample are smaller than the intrinsic mean free path of the material. The extreme situation when boundary scattering dominates over intrinsic scattering is often called the “Casimir limit” owing to his early work on cylindrical rods [8].

More recently thermal conductivity studies of silicon films patterned with periodic arrays of holes provide insight into the impact of more complex geometries on phonon scattering and potential modifications the phonon band structure, including the possibility of phononic crystal effects (which can induce phonon band gaps). Nanofabricated thermal sensors and actuators such as radiation detectors (bolometers) [9,10] that rely on thermal insulation of particular components to increase the sensitivity, responsiveness, and accuracy could benefit from the low thermal conductivity of these porous films. These films may also prove useful for thermoelectric conversion involving the controlled modification of phonon and electron transport capabilities.

This article reviews experimental measurements of thermal conduction in thin silicon films, nanowires, and porous films fabricated from SOI wafers. An overview of SOI-based thermal conductivity measurement structures is presented in Sec. 2. Section 3 introduces the thermal conductivity integral model, whose application at the microscale was first confirmed using measurements on SOI samples. Sections 4, 5, and 6 discuss the thermal conductivity of thin silicon films, nanobeams, and porous films, respectively.

2 Thermal Conductivity Measurements

Several strategies taking advantage of the SOI structure have been developed to measure the thermal conductivity of the single crystal device layer. Tables 1 and 2 summarize measurements of SOI-based thin films and nanowires, respectively.

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Table 1 Films (solid and periodically porous) thermal conductivity measurements

Article	Year	Measurement configuration	Doping	Temp. range	Si thickness (nm)	Pore diameter (nm)	Pore spacing (nm)
Ju [16]	2005	On-substrate (steady-state joule heating (1); varying heater width)	p-type	Room temp.	20 to 50	—	—
Liu and Asheghi [7]	2004	Suspended heater bridge (steady-state)	Undoped	20 K to 300 K	20 and 100	—	—
Yu et al. [30]	2010	Suspended heater-thermometer	Boron-doping ($2 \times 10^{19} \text{ cm}^{-3}$)	80 K to 320 K	20 to 25	11, 16, or 270	34 or 385
Liu and Asheghi [25]	2005	Suspended heater bridge (steady-state)	Undoped, $2.3 \times 10^{20} \text{ P}$, $1.6 \times 10^{21} \text{ B}$, or $2.3 \times 10^{20} \text{ As}$	300 K to 450 K	30	—	—
Liu et al. [26]	2006	Suspended heater bridge (steady-state)	Undoped	300 K to 450 K	50	—	—
Hao et al. [18]	2006	Suspended (steady-state joule heating (1))	p-type ($1 \times 10^{15} \text{ cm}^{-3}$)	Room temp.	50 to 80	—	—
Ju and Goodson [17]	1999	On-substrate (3- ω technique)	p-type	Room temp.	74 to 240	—	—
Aubain and Bandaru [15]	2010	Scanning thermoreflectance with electrical heating	p-type	Room temp.	68 to 258	—	—
Aubain and Bandaru [13]	2011	Scanning thermoreflectance with electrical heating	p-type (1–10 $\Omega \text{ cm}$)	Room temp.	68, 151, 235, and 258	—	—
Tang et al. [31]	2010	Suspended heater-thermometer	Intrinsic, ($3 \times 10^{14} \text{ cm}^{-3} \text{ P}$), or boron-doped ($5 \times 10^{19} \text{ cm}^{-3} \text{ B}$)	25 K to 300 K	100	32, 81, or 198	55, 140, or 350
Aubain and Bandaru [14]	2010	Scanning thermoreflectance with electrical heating	p-type (14–22 $\Omega \text{ cm}$)	Room temp.	260	—	—
Asheghi et al. [12]	1998	On-substrate (steady-state joule heating (3))	$< 10^{15}$ boron doping	15 K to 300 K	420, 720, and 1420	—	—
Asheghi et al. [11]	1997	On-substrate (steady-state joule heating (3))	n-silicon	20 K to 350 K	420, 830, and 1600	—	—
Kim et al. [20]	2012	Suspended (steady-state joule heating (2))	p-type (boron, 10^{16} cm^{-3})	Room temp.	500	~200 to ~500	500 to 900
Asheghi et al. [19]	2002	Suspended film (steady-state joule heating (3))	Boron or phosphorous (1×10^{17} – $3 \times 10^{19} \text{ cm}^{-3}$)	15 K to 300 K	3000	—	—
Song and Chen [21]	2004	Suspended film (steady-state joule heating (2))	n-type (5×10^{14} – $5 \times 10^{15} \text{ cm}^{-3}$)	50 K to 300 K	4670	2300 or 10,900	4000 or 20,000
Sverdrup et al. [22]	2001	Suspended film (steady-state joule heating (4))	—	100 K to 200 K	5000	—	—
Hopkins et al. [42]	2010	Thermoreflectance (out-of-plane)	(37.5–62.5 $\Omega \text{ cm}$)	Room temp.	500	300 or 400	500, 600, 700, or 800

Table 2 Nanobeam thermal conductivity measurements

Article	Year	Measurement configuration	Temp. range	Si thickness (nm)	Beam width (nm)
Yu et al. [30]	2010	Suspended heater-thermometer	90 K to 310 K	20	28
Bourgeois et al. [27]	2007	Suspended heater bridge (3- ω)	$< 2 \text{ K}$	130	200
Heron et al. [28]	2009	Suspended heater bridge (3- ω)	0.3 K to 6 K	100	200
Heron et al. [29]	2010	Suspended heater bridge (3- ω)	$< 5 \text{ K}$	100	200 (straight and serpentine)
Hippalgaonkar et al. [32]	2010	Suspended heater-thermometer (array of nanowires)	20 K to 300 K	20 to 100	40 to 150
Boukai et al. [33]	2008	Suspended heater-thermometer (array of nanowires)	100 K to 300 K	20, 35	10 and 20, 520
Marconnet et al. [50]	2012	Suspended heater bridge (steady-state)	300 K	196	550

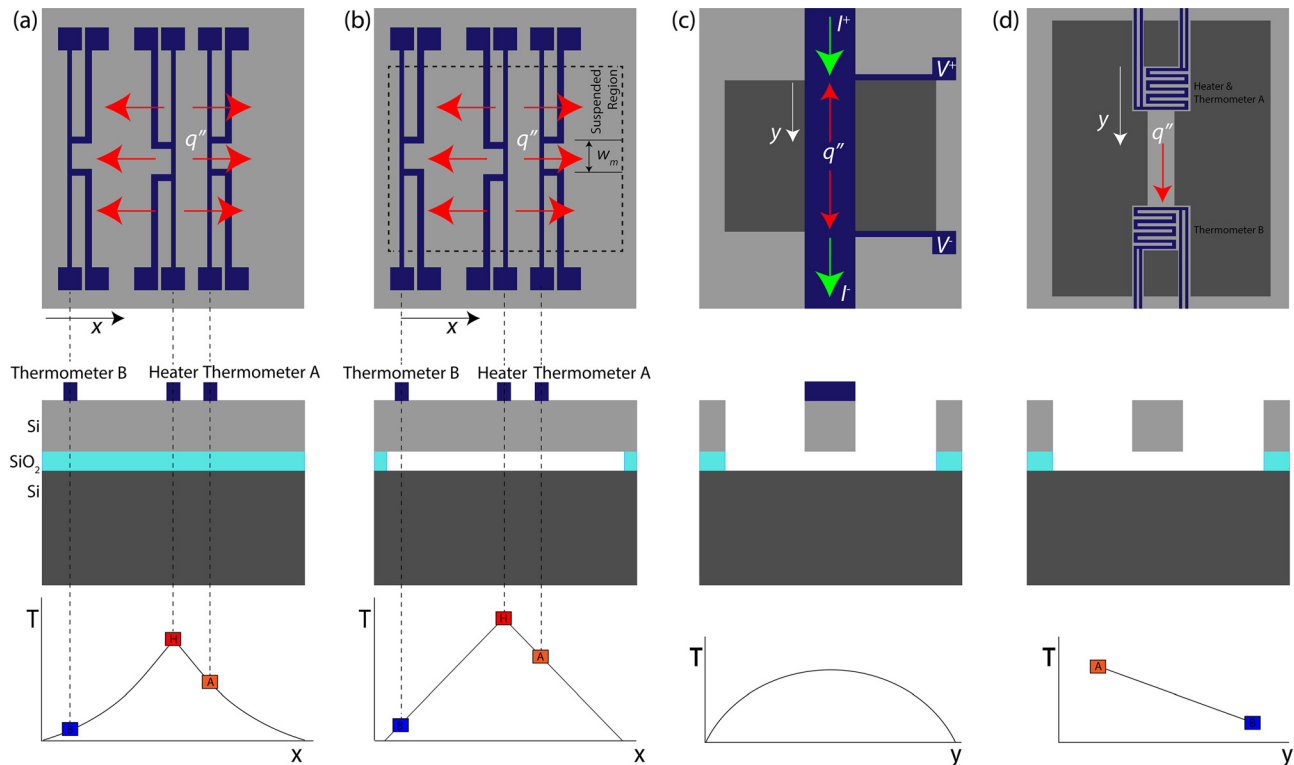


Fig. 1 SOI thermal measurement structures. (a) On-substrate steady-state joule heating structure. (b) Suspended steady-state joule heating structure. (c) Suspended heater bridge structure. (d) Suspended heater-thermometer structure.

Early measurements of SOI wafers utilized on-substrate steady-state electrothermal measurement configurations [11,12]. These measurements utilized three resistive elements as sketched in Fig. 1(a). Heat generated at the center element through joule heating is conducted laterally through the silicon layer yielding a non-linear temperature profile symmetric about the center heater line. The thermal healing length, i.e., the characteristic length scale of lateral diffusion within the silicon layer, can be estimated from [11,12]

$$L_H = \sqrt{d_s d_o k_s / k_o} \quad (1)$$

where d_o and d_s are the oxide and silicon thicknesses, k_o is the vertical thermal conductivity of the oxide layer, and k_s is the in plane thermal conductivity of the silicon film. This approximation requires that the lateral thermal conduction in the oxide layer is small compared to the lateral conduction in the silicon layer ($d_o k_o \ll d_s k_s$), the vertical thermal resistance through the silicon layer is much smaller than that through the oxide layer ($(d_s / k_s) \ll (d_o / k_o)$), and the silicon substrate below the oxide layer is nearly isothermal. The two remaining resistive elements were used as resistive temperature sensors, which allow measurement of the in-plane silicon thermal conductivity [11,12]. More recently, Aubain and Bandaru [13–15] combined a similar on-substrate joule heating with scanning thermoreflectance in order to measure the in-plane thermal conductivity. An electrical heater line patterned on the SOI wafers was heated using a sinusoidal current. The amplitude of the temperature rise in the lateral direction was characterized using scanning thermal reflectance and the thermal conductivity extracted using a time-dependent COMSOL finite element model [13–15].

Additional on-substrate measurement techniques have been developed using varying heater widths and taking advantage of lateral spreading within the silicon layer to probe the in-plane conductivity using both steady-state joule heating [16] and harmonic (3ω) [17] methods. When the heater width is comparable with or smaller than the thermal healing length, the temperature rise in the heater is dependent on the in-plane silicon thermal conductivity, while meas-

urements with larger heater widths allow extraction of the contribution of the buried oxide layer.

Suspended structures provide a convenient platform for measuring the in-plane conductivity as the heat flow is confined to the lateral direction. Although the required fabrication is more complex than for on-substrate measurements, the buried oxide layer provides a suitable etch stop and/or sacrificial layer for suspending the silicon device layer. Several suspended measurement structures have been developed to measure the thermal conductivity and are illustrated in Figs. 1(b)–1(d).

Several groups have used a suspended measurement structure with several electrical resistive elements to generate and characterize the temperature profile in the suspended thin film (see Fig. 1(b)). The resistive element at the center of the suspended film generates a heat flux that is conducted through the thin film. The temperature profile along the length of the film is linear and symmetric about the heater line (as sketched in the bottom panel of the figure). The thermal conductivity is estimated from the measured lateral temperature gradient in the film, the applied heating power, and the geometry. To allow for the assumption of one-dimensional heat conduction from the heater line, the voltage probes are often spaced near the center of the heater element as indicated in Fig. 1(b). Note that if the oxide layer is not removed during fabrication (e.g., the film is suspended through a back-side etch), the impact of thermal conduction through the oxide layer must be accounted for in the calculation of the thin silicon film conductivity. Although estimates of the thermal conductivity are possible from a single heater (e.g., Ref. [18]), more accurate measurements utilize one to three additional temperature sensors to characterize the temperature profile within the thin film [11,12,19–22]. It is important to note that the measured temperature rise at the heater line may be impacted by ballistic phonon emission [23] if the heater size is on the order of the dominant phonon mean free path. For example, Sverdrup et al. [22] observed evidence of these ballistic effects with $0.3 \mu\text{m} \times 3 \mu\text{m}$ heaters at 100 K to 200 K, where the dominant phonon mean free path in bulk silicon ranges from $2 \mu\text{m}$ to $10 \mu\text{m}$, and found that the measured temperature rise at the heater line exceeded that expected from diffusive transport by up to 60%.

Suspended heater bridge measurement structures (Fig. 1(c)) allow determination of the in-plane conductivity for thin films [7,24–26] and nanowires [27–29]. Specifically the suspended silicon is coated with a thin metal film that serves as a heater and thermometer during the measurements. The temperature profile along the length of the suspended film depends on the thermal conductivity of the silicon layer and can be calculated from the heat diffusion equation. The electrical resistance of the metal film depends on the temperature profile, and thus, the thermal conductivity of the silicon layer can be extracted from measurements of the electrical resistance as a function of applied current. However, care must be taken to account for thermal conduction through the metal film as well. Both steady-state and harmonic (3ω) measurements are possible with this measurement structure.

Suspended heater-thermometer structures (Fig. 1(d)) have proven useful for characterizing a variety of nanostructures, including silicon-based films [30,31] and nanowires [32,33]. The thin films or nanowires are suspended between two pads with lithographically patterned resistive heater-thermometer elements. Heat generated at one resistive element conducts through the nanostructure to the second resistive element. The thermal conductivity of the nanostructure is measured using the applied power and the measured temperature difference between the two resistive elements. Care must be taken in the design to ensure that heat generated is primarily conducted through the nanostructure and not lost through the support structure. Thermal resistance between the resistive elements and the nanostructure may impact the thermal conductivity measurements. However, when the resistive element pads are continuous with the fabricated nanostructure (i.e., both are patterned from the device layer), the impact of boundary resistance should be small. However, when the nanostructure is placed upon the resistive elements (e.g., Ref. [31]), the thermal boundary resistance leads to a larger temperature difference between the resistive elements than would be due to the thermal conductivity of the nanostructure, and thus, the thermal conductance of the nanostructure can be underestimated.

3 Modeling the Thermal Conductivity of Silicon

Much progress has been made in recent years in subcontinuum simulations of thermal conduction in silicon, including solutions to the Boltzmann transport equation, lattice dynamics methods, and atomistic calculations accounting for size effects and other physical phenomena (e.g., Refs. [34–38]). While experimental progress has accelerated in parallel with this work, much of the existing data (including those obtained using SOI) can be predicted from the semiclassical approach [11,39–41]. This section introduces enough theory to help with the discussion of experimental data in subsequent sections. Starting from kinetic theory, a simple model of the thermal conductivity of silicon considers the heat capacity C , the average acoustic phonon velocity v_{avg} , and the phonon mean free path Λ , or phonon relaxation time τ :

$$k = \frac{1}{3} C v_{avg} \Lambda = \frac{1}{3} C v_{avg}^2 \tau \quad (2)$$

For thin films or nanostructures, boundary scattering reduces the thermal conductivity compared to bulk silicon and a reduced phonon mean free path and relaxation time can be calculated.

While this simple model in Eq. (2) lumps together the contribution of all phonons, the thermal conductivity integral includes the impact of the phonon dispersion relations, as well as mode- and wavevector-dependent phonon relaxation times. These thermal conductivity integral models have been used for decades to model using the thermal conductivity of silicon, including work on nanoscale thin films [24]. Specifically, the thermal conductivity in the direction given by the unit vector $\hat{i}$ can be computed from the thermal conductivity integral model [41]:

$$k_i = \frac{1}{(2\pi)^3} \sum_j \int C_j(\mathbf{q}, T) (\mathbf{v}_j(\mathbf{q}) \cdot \hat{i})^2 \tau_j(\mathbf{q}, T) d\mathbf{q} \quad (3)$$

where $C_j(\mathbf{q}, T)$, $\mathbf{v}_j(\mathbf{q})$, and $\tau_j(\mathbf{q}, T)$ are the specific heat per phonon mode, velocity, and relaxation time of the phonons in branch j with wavevector $\mathbf{q}$ at temperature T .

The spectral-dependent scattering times (mean free paths) for bulk silicon are well documented in literature (e.g., Holland [41]). Typical models for scattering times bulk silicon consider the impact of Umklapp, impurity, and boundary scattering using Matthiessen's rule. Even for models of bulk silicon, the impact of boundary scattering must be included at low temperatures where the mean free path (due to Umklapp and impurity scattering) is quite long. Neglecting boundary scattering would lead to increasing thermal conductivity with decreasing temperature at low temperature (< 100 K) where decreasing thermal conductivity with decreasing temperature is experimentally observed for bulk and nanostructured silicon. As the sample dimensions shrink, boundary scattering becomes increasingly important at higher temperatures. For example, at room temperature, molecular dynamics models predict that 35% of the thermal conductivity is attributed to phonons with mean free paths longer than $1 \mu\text{m}$ [35]. Methods for accounting for phonon-boundary scattering are discussed in Sec. 4 (thin films), 5 (nanobeams), and 6 (porous films).

4 Thin Film Thermal Conductivity

4.1 Impact of Film Thickness. SOI-based metrology techniques have allowed the measurement of the thermal conductivity of single-crystal silicon layers from 20 nm to $5 \mu\text{m}$ thick. Figure 2 shows the measured room temperature in-plane and out-of-plane thermal conductivity of thin films from the sources listed in Table 1.¹ For the thickest films, the in-plane conductivity nears that of bulk silicon and the thermal conductivity decreases appreciably from the bulk value as the film thickness decreases below $\sim 5 \mu\text{m}$. Significant variations in the measured results between samples are evident and suggest that other factors, including surface roughness, doping concentration, and film quality, impact the results.

To predict the thermal conductivity reduction due to phonon-boundary scattering, the phonon-boundary scattering relaxation time $\tau_{j,\text{boundary}}$ is estimated from the film thickness and phonon velocity:

$$\tau_{j,\text{boundary}}^{-1} = \frac{v_j(q)}{\Gamma d_s} \quad (4)$$

where Γ is a correction factor, which must be included to account for geometrical factors and the specularly of the surface (e.g., Ref. [41]). This parameter is typically determined from fitting the models to experimental results. Matthiessen's rule is then used to calculate the total relaxation time ($\tau_j^{-1} = \tau_{j,\text{bulk}}^{-1} + \tau_{j,\text{boundary}}^{-1}$).

However, boundary scattering is a surface phenomenon, not an intrinsic scattering process, so accounting for boundary scattering using the above method is not rigorous. Sondheimer [43] derived from the Boltzmann transport equation an analytical expression for calculating the reduction in electrical conductivity due to boundary scattering. This method has been adapted to calculating the reduced thermal conductivity within thin films and wires. In the simplest iteration, neglecting spectral variations in the phonon mean free path and velocity, the reduced thermal conductivity of a thin film can be estimated from the conductivity reduction function F :

$$\frac{k_{\text{film}}}{k_{\text{bulk}}} \approx F(\delta, p) = 1 - \frac{3(1-p)}{2\delta} \int_1^\infty \left(\frac{1}{\xi^3} - \frac{1}{\xi^5} \right) \frac{1 - \exp(-\delta\xi)}{1 - p \exp(-\delta\xi)} d\xi \quad (5)$$

where $\delta = d_s/\Lambda$ is the reduced layer thickness and Λ is the mean free path within the film, p is the fraction of phonons specularly reflected by the boundaries, and ξ is a variable of integration. The results of this model are shown in comparison to the data in Fig. 2 for two cases: $\Lambda = 100 \text{ nm}$ and $\Lambda = 300 \text{ nm}$. Although simple

¹References cited in Table 1 are [7,11–22,25,26,30,31,42].

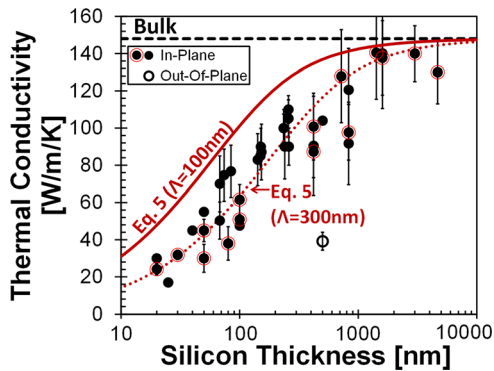


Fig. 2 Thickness dependence of the thermal conductivity of silicon thin films [7,11–22,25,26,30,31,42]. For the reported in-plane thermal conductivity data; red rings around the solid circular data markers indicate nearly pure samples (intrinsic, nearly pure, or $<10^{15} \text{ cm}^{-3}$ dopant atoms). The Sondheimer model (Eq. (5)) for the reduced thermal conductivity as a function of film thickness is shown for a mean free path of 100 nm and 300 nm, assuming purely diffuse scattering ($p=0$) at the film boundaries.

estimates of the phonon mean free path from the kinetic theory (Eq. (2)) suggest a mean free path on the order of 40 nm, several studies have shown that phonons with longer mean free path contribute significantly to the thermal conductivity. In fact, the Sondheimer model assuming a longer mean free path (300 nm) provides a better estimate of experimental data (as shown in Fig. 2).

While simple models consider only a single mean free path for all phonons, the mean free path varies significantly across the phonon spectrum. The Sondheimer approach can be combined with the thermal conductivity integral model (Eq. (3)) in order to consider the spectral dependence of phonon-boundary scattering [11,12,19]. In this case, the bulk scattering time for each mode $\tau_{j,\text{bulk}}(q, T)$ is reduced by the conductivity reduction function $F(\delta, p)$:

$$\tau_j(q, T) = F(\delta, p) \tau_{j,\text{bulk}}(q, T) = F\left(\frac{d_s}{\Lambda_{j,\text{bulk}}(q, T)}, p\right) \tau_{j,\text{bulk}}(q, T) \quad (6)$$

Note that the reduction function F is that of Eq. (5) (for thin films), where the reduced thickness δ is mode dependent. A mode-dependent specularly parameter can also be determined from the surface roughness and the wavelength of each phonon mode [44] or a single value of specularly can be assumed for all modes (e.g., $p=0$ for purely diffuse scattering).

4.2 Impact of Temperature. Figure 3 shows the temperature dependence of the thermal conductivity of silicon thin films ($d_s=20 \text{ nm}$, 420 nm , and $1.42 \mu\text{m}$ [7,12]) in comparison to the measured value for bulk silicon [45]. The results of a thermal conductivity integral model considering the spectral-dependent diffuse boundary scattering (Eqs. (3), (5), and (6)) shows good agreement with the measured values.

At low temperatures, the phonon mean free path is limited by boundary scattering and the thermal conductivity follows the dependence of the heat capacity. At these temperatures, much lower than the Debye temperature, the phonon heat capacity follows a T^3 dependence as the phonon population increases with increasing temperature. The impact of boundary scattering is more pronounced at low temperatures than at room temperature because the intrinsic mean free path is much longer.

As the temperature increases, the phonon population continues to increase, but phonon scattering rate also increases. A peak in the thermal conductivity is observed as the increased scattering begins to

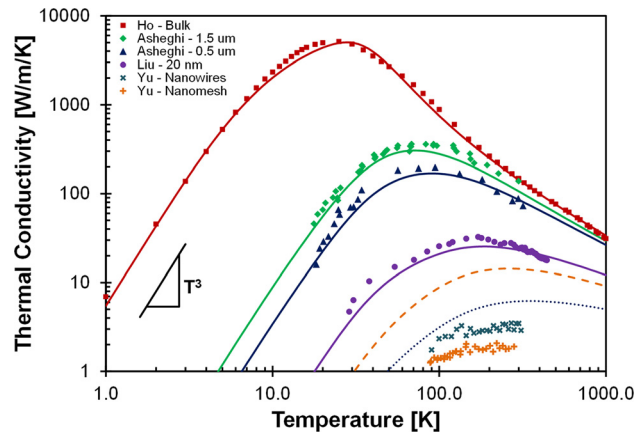


Fig. 3 Temperature-dependent thermal conductivity of several different SOI-based silicon structures: thin films (Asheghi and colleagues [7,12]), $20 \text{ nm} \times 28 \text{ nm}$ rectangular nanobeams (Yu et al. [30]), and 22 nm thick nanoporous films (results shown for both 11 and 16 nm diameter holes spaced by 34 nm from Yu et al. [30]). The thermal conductivity of bulk silicon (Ho et al. [45]) is shown for comparison. While the modeling results agree fairly well for the thin film data, the nanobeam and nanomesh results fall below the predicted thermal conductivities.

outweigh the impact of increasing heat capacity. The peak thermal conductivity shifts to higher temperatures with decreasing film thickness. At high temperatures, the thermal conductivity decreases with increasing temperature as the phonon mean free path decreases.

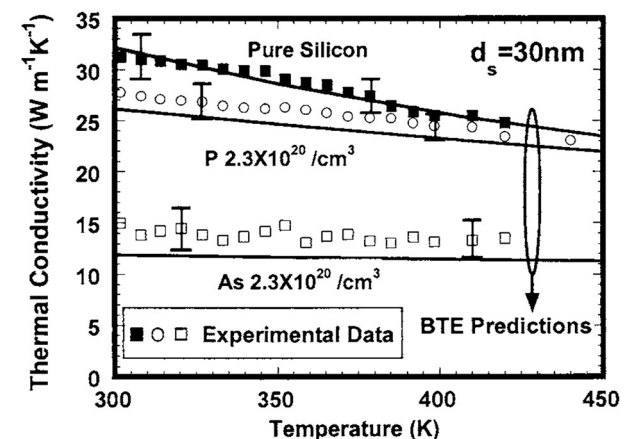
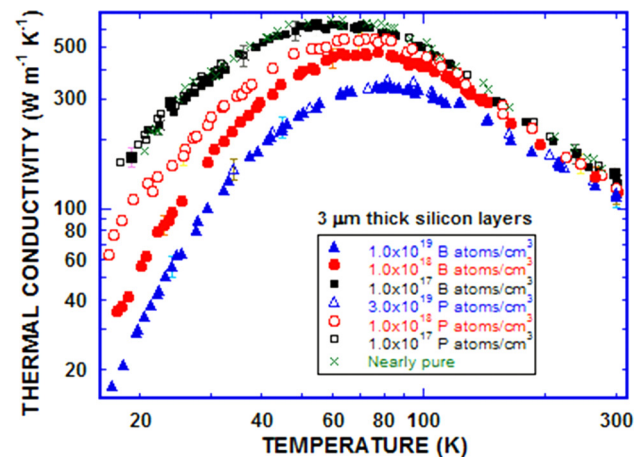


Fig. 4 Impact of doping on the thermal conductivity of (a) $3 \mu\text{m}$ and (b) 30 nm thick silicon films. Figures reprinted with permission from (a) Asheghi et al. [19] and (b) Asheghi and Liu [25].

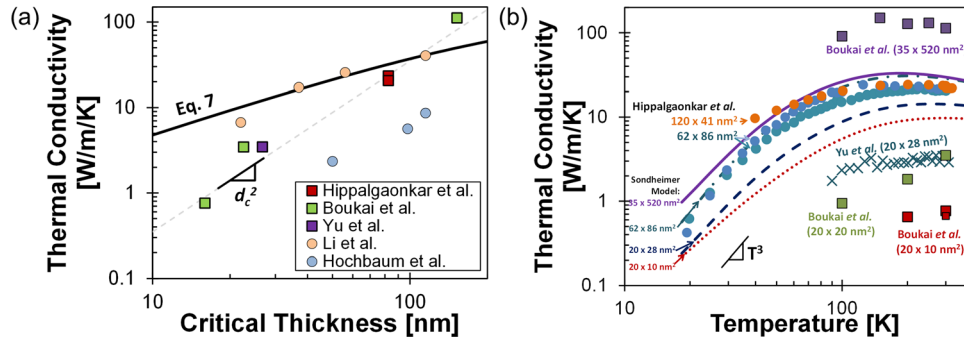


Fig. 5 Thermal conductivity of silicon nanobeams [30,32,33] as a function of (a) critical thickness and (b) temperature. The thermal conductivity of rough [52] and smooth [53] cylindrical nanowires are shown in panel (a) for comparison to the nanobeam data. The results of the simple model for nanowire thermal conductivity from Eq. (7) are shown with the solid line in panel (a), while the data for the rectangular nanobeams appear to follow an approximate trend of $k \sim d_c^2$. In panel (b), the temperature-dependent thermal conductivity results from a thermal conductivity integral model with the Sondheimer-type reduction function to account for the boundary scattering in rectangular nanobeams are shown for in comparison to the experimental data. The large nanowires from Boukai et al. [33] fall significantly higher than the model for nanobeams (and also the prediction for 35 nm thick films), while the smaller nanowires from Boukai et al. [33] and Yu et al. [30] fall below the predictions.

4.3 Impact of Doping. Doping of single-crystal silicon films is required for many applications, including semiconductor devices. Both intentional and unintentional impurities cause increased phonon scattering and reduce the thermal conductivity. Thus, comparing measured thermal conductivities from different authors is complicated by the range of doping levels and dopant atoms considered (see Table 1). A few authors have studied the impact of doping by measuring samples with different doping species and concentrations. Figure 4 illustrates the impact of doping for 3 μm thick films doped with various concentrations (1×10^{17} to $3 \times 10^{19} \text{ cm}^{-3}$) of boron or phosphorous [19] and 30 nm films doped with boron ($1.6 \times 10^{21} \text{ cm}^{-3}$), arsenic ($2.3 \times 10^{20} \text{ cm}^{-3}$), or phosphorous ($2.3 \times 10^{20} \text{ cm}^{-3}$) from 300 K to 450 K [25].

4.4 Beyond the Classical Size Effect. Recent work on ultra-thin films has shown that the dispersion relations can be modified by the confined geometry. Raman scattering spectra for suspended silicon membranes (24 nm to 32 nm thick) have shown evidence of confined phonon modes [46]. Additionally, in silicon membranes (8 nm to 32 nm thick), angle-resolved Brillouin scattering spectroscopy measurements show a strong reduction in the phonon velocities for the fundamental flexural mode compared to bulk silicon [47]. In addition to the boundary scattering effects on the phonon mean free paths, these types of modifications to the dispersion relation can impact the thermal conductivity of nano-scale thin film and other confined nanostructures.

Ballistic effects are also important to consider when the dimensions of the heat source are comparable to the phonon mean free paths. In SOI-based measurements, nondiffusive thermal transport in silicon films has been observed using electrothermal [22] and thermal grating [48,49] techniques and for bulk silicon using thermoreflectance measurements [49]. These measurements provide insight into the distribution of mean free paths and their contribution to thermal conductivity. Both these experimental measurements and models (e.g., Ref. [35]) have shown that phonons with very long mean free paths ($\Lambda > 1 \mu\text{m}$) contribute significantly to the thermal conductivity.

5 Nanobeam Thermal Conductivities

Rectangular cross-section nanobeams can be etched from the silicon device layers and directly integrated into the suspended heater-thermometer measurement structures or the suspended heater bridge configuration, both of which are described in Sec. 2. In the heater-thermometer configuration, SOI-based manufactur-

ing (with the nanowire directly integrated with the heating/sensing pads during fabrication) provides an advantage over measurements of other nanowires that must be placed onto the resistive elements. In the latter case, thermal boundary resistance between the nanowire and the resistive element can lead to errors in extracting the thermal conductivity and this effect is minimized in the SOI-based structure. Table 2 summarizes experimental measurements of silicon nanobeams.²

The phonon mean free path due to boundary scattering in the Casimir limit [8] is the nanowire diameter D_w for circular nanowires and $1.12W$ for square nanowires with a side width W . The combined impact of boundary scattering and intrinsic scattering can be evaluated using Matthiessen's rule and the relative reduction to the thermal conductivity can be approximated as [51]

$$\frac{k_{\text{nanowire}}}{k_{\text{bulk}}} \approx \left(1 + \frac{\Lambda}{D_w}\right)^{-1} \quad (7)$$

for circular nanowires. For rectangular nanobeams of width W and thickness d_s , a critical thickness (or effective diameter) can be defined [32] as $d_c = 2\sqrt{d_s W}/\sqrt{\pi}$ (which reduces to $d_c \approx 1.12W$ for square nanobeams). This dimension can replace the nanowire diameter in Eq. (7) to estimate the reduced thermal conductivity of noncircular nanobeams. However, as shown in Fig. 5(a), the experimentally measured room temperature thermal conductivity of several rectangular nanowires does not appear to follow the trend of Eq. (7). Although there are few experimental data points, the thermal conductivity appears to scale with d_c^2 , which means that the thermal conductivity scales proportional to the nanowire cross-sectional area. For comparison, the thermal conductivity of rough [52] and smooth [53] cylindrical nanowires are also shown in Fig. 5(a). The reduced thermal conductivity of the rough nanowires demonstrates the impact of surface quality on the thermal conduction in nanostructures.

Similar to the thin films described above, for purely diffuse scattering in a nanowire with an arbitrary cross section A_c , the conductivity reduction function can be calculated [43]:

$$F(\Lambda, p=0) = 1 - \frac{3}{4\pi A_c} \int_{A_c} \int_0^{2\pi} \int_0^\pi \sin \theta \cos^2 \theta \exp\left(\frac{-L_{OP}}{\Lambda}\right) d\theta d\phi dA_c \quad (8)$$

²References cited in Table 2 are [27–30,32,33,50].

where L_{OP} is the distance from a point O on the cross section of the nanowire to a point P on the surface of the nanowire along the direction given by the azimuthal angle θ and radial angle ϕ . Conductivity reduction functions have been derived from Eq. (8) for circular [43] and rectangular nanowires [40,54]. For circular nanowires, the approximate solution from the Casimir limit and Matthiessen's rule (Eq. (7)) agrees well with the conductivity reduction function (Eq. (8)) [55]. The spectral dependence of the conductivity can be taken into account using the thermal conductivity integral approach (Eqs. (3) and (6)).

The temperature-dependent thermal conductivities of several rectangular nanowires are shown in Fig. 5(b). The results of a thermal conductivity integral model (using a Sondheimer-type reduction function) are shown in comparison to the experimental data for four nanobeam cross sections. Thermal conductivity integral models reducing the bulk mean free path with Matthiessen's rule and the critical thickness do not vary significantly in magnitude or trend from these results. While the model agrees well with the magnitude and trend of the data from Hippalgaonkar et al. [32], the remaining data fall far from the predicted values. The thermal conductivities of the larger nanowire from Boukai et al. [33] are underpredicted by the models, and the experimental data are actually larger than those of thin films of the same thickness [7]. In contrast, the measured thermal conductivities of the smaller nanowires [30,33] are overpredicted by the models.

Adding serpentine kinks to nanobeam geometry has been shown to reduce the thermal conductance by up to 40% at very low temperatures ($T < 5$ K) [28,29]. A spectral-dependent model for the thermal conductance suggests that the origin of this reduction is that the serpentine structures block a small fraction of the phonons that would have had very long mean free paths in the straight nanowires [29].

6 Aligned Porous Thin Film Thermal Conductivity

Silicon films with controlled, periodic arrays of cylindrical holes can be fabricated by patterning the SOI device layer. These controlled, porous films have proven useful for nanophotonic devices [56–59] and are promising for a number of other emerging technologies [60], including high ZT thermoelectric materials [30,31,61]. Measurements of the aligned porous thin films are summarized in Table 1. The introduction of the pore structure can significantly reduce the thermal conductivity of the silicon layer compared to solid films of the same thickness (see Fig. 6). The temperature dependence of the thermal conductivity for a nanoporous film from Yu et al. [30] is included in Fig. 3.

A key challenge in measuring the thermal conductivity of the porous silicon arises from the highly nonuniform cross-sectional area for heat transfer. Many measurements actually measure the

thermal conductance across the nanoporous film. Several correction methods for estimating the solid thermal conductivity from the measured value (typically conductance) have been developed, including using the Eucken factor [62], corrections based on finite element analyses [20], normalizing the data by the porosity [31], or determining an upper bound on thermal conductivity by considering only the minimum cross section for thermal conduction ($A_{\min} = (S - D)d_s$) [30]. The variety of correction methods used makes comparing data sets from different authors challenging. In this work, the solid thermal conductivities as reported by the authors are plotted.

Two-dimensional periodically porous films have been studied across a range of dimensions (film thickness d_s , hole diameter D , and hole spacing S). Early samples fabricated with conventional photolithography techniques yielded samples with $\sim 2 \mu\text{m}$ to $10 \mu\text{m}$ diameter holes in $\sim 5 \mu\text{m}$ thick silicon [21]. In more recent measurements, hole diameters as small as 11 nm have been achieved through a superlattice nanowire pattern transfer (SNAP) technique [30]. Despite advances in fabrication techniques over the last decade, the largest achievable aspect ratio for the holes appears to be limited to $d_s/D < 3$.

In two-dimensional porous films, key dimensions include the film thickness, hole diameter, and hole spacing. The introduction of nano- or microscale pore structures leads to a large increase in the density of interfaces within the structure and increased phonon scattering. As with the nanowires, the impact of geometry on phonon transport can either be included by reducing the mean free path with Matthiessen's rule or through a conductivity reduction function. For microporous and nanoporous solids, Hopkins et al. [62,63] utilize a phonon-pore boundary scattering term based on the limiting dimension in the systems ($\tau_{\text{pores}} = L_d/v_j(q)$), where L_d is the limiting dimension. For thermal transport, the intrapore distance (pore edge-to-pore-edge distance, or "neck width") is often considered the limiting dimension $L_d = S - D$ in the system as it represents the minimum cross section for heat transport. Figure 7(a) shows the thermal conductivity as a function of limiting dimension for several porous films. Also shown is the recent measurement [50] of periodically porous nanobeams, which are a 1D analog to the 2D films. Because of the additional side wall boundaries for nanobeams, the limiting dimension is the minimum of the intrapore distance and the distance from the pore edge to the edge of the nanobeam. A clear decrease in the thermal conductivity is observed as the limiting dimension is reduced. The results of a thermal conductivity integral model considering the limiting dimension using Matthiessen's rule is shown in Fig. 7(a). As the limiting dimension depends only on the pore geometry, the results of this model are independent of film thickness. As the small limiting dimension samples were generally fabricated from thinner films, the overestimation of the thermal conductivity at small limiting dimensions could be associated with increased scattering due to the film boundaries. Furthermore, the limiting dimension model does not take into account the varying cross section for heat transport and other details of the geometry. However, this highly spatially nonuniform geometry does not easily lend itself to calculations of a Sondheimer-type thermal conductivity reduction function analogous to Eq. (5) for solid thin films. Monte Carlo-type methods for estimating the reduced phonon mean free path are proving useful to calculating the reduced thermal conductivity in nanostructures and have been applied to porous nanobeams [50].

In classical effective medium theories for porous solids (e.g., Eucken), the thermal conductivity depends only on the porosity of the film. Figure 7(b) shows the thermal conductivity of two-dimensional periodic porous films as a function of porosity. Early work by Song and Chen [21] showed that, contrary to the classical models, as the temperature decreased the ratio of $k_{\text{porous}}/k_{\text{bulk}}$ decreased and hypothesized that the increasing phonon mean free path with decreasing temperature led to the deviation. More recently, Tang et al. [31] showed that for constant porosity (35%), the thermal conductivity decreases with decreasing hole size. Furthermore, comparing the results of Yu et al. [30] with dimension

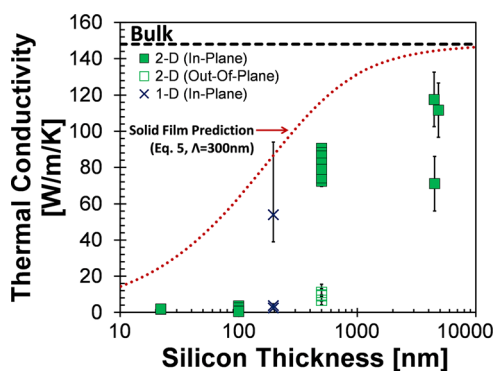


Fig. 6 Room temperature thermal conductivity of 2D periodically porous thin films [20,21,30,31] and 1D periodically porous nanobeams [50] as a function of the film thickness. The porous film data are compared to the predictions from Eq. (5) for in-plane thermal conductivity of solid films.

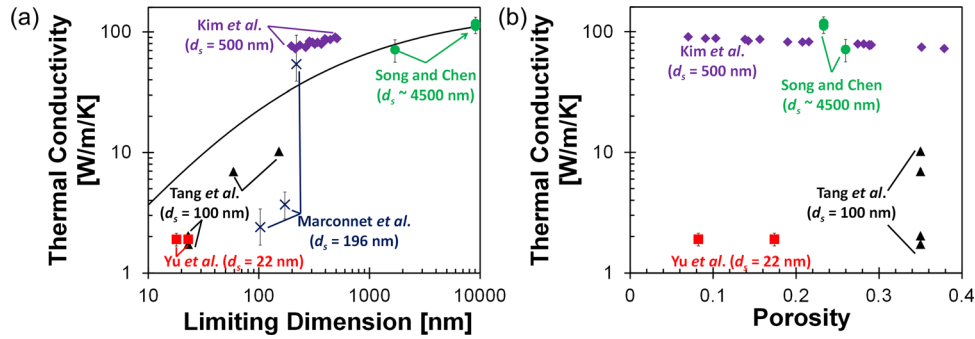


Fig. 7 Room temperature thermal conductivity of 2D periodically porous thin films [20,21,30,31] and 1D periodically porous nanowires [50] as a function of (a) the limiting dimension and (b) the porosity. In panel (a), for the films, the limiting dimension is the intrapore distance ($S-D$). For the 1D porous nanoladders Marconnet et al. [50], the limiting dimension is the smaller of the intrapore distance and the distance from the edge of the nanowire to the pore wall, $(W-D)/2$. Film thicknesses d_s are indicated in the legend. The thermal conductivity data are compared to the results of the thermal conductivity integral model with the mean free path reduced using Matthiessen's rule and the limiting dimension. The results of the thermal conductivity integral model are independent of film thickness.

on the order of 10 nm to that of Kim et al. [20] with dimensions on the order of 100 nm, a clear size effect is evident beyond the impact of porosity. These results highlight the need to use and develop detailed models of thermal conduction in these nanoporous systems that take into account the impact of varying mean free paths and scattering size effects.

Furthermore, several groups [30,42,61,63] have hypothesized that these periodic, porous structures impact the phonon band structure leading to an additional reduction in the thermal conductivity beyond that due to boundary scattering. There have been extensive theoretical studies of the phonon dispersion modifications due to periodic pore structures [60,63–66]. In particular, periodically porous films have been shown to lead to phonon bandgaps (e.g., Ref. [67]) and these structures are sometimes referred to as “phononic crystals.” Even in the absence of phononic bandgaps, the porous structure has been predicted to modify the phonon dispersion leading to reduced phonon group velocity and density of states (e.g., Ref. [68]). However, because of the difficulties in accurately modeling the phonon-pore scattering (even for idealized pores), it has not been proven unequivocally that the coherent effects are responsible for any additional reduction in thermal conductivity of these porous, thin films.

7 Concluding Remarks

Twenty years ago, there was a surging interest in microscale and nanoscale heat conduction physics, including a variety of manuscripts in the *Journal of Heat Transfer* and elsewhere on phonon transport. There was, however, a troubling lack of experimental data or, when data were available, it was challenging to determine whether the governing physics were related to processing details or to basic physics. The use of SOI technology—while being inarguably more important for MEMS development—fundamentally changed this situation by providing nearly defect-free, high quality, thin silicon films. Measurements of SOI-based silicon films spanning three orders of magnitude in thickness have shown clear evidence of the size effect matching well with semiclassical models for thermal conductivity, including phonon-boundary scattering. Over the past two decades, SOI technology, combined with improved lithography techniques, have provided a robust platform for studying the complex phonon transport in geometries including straight and bent nanobeams and periodically porous films.

Nomenclature

A_c = cross-sectional area (m^2)
 C = heat capacity ($\text{J m}^{-3} \text{K}^{-1}$)

C_j = heat capacity per phonon mode ($\text{J m}^{-3} \text{K}^{-1}$)
 D = hole diameter (m)
 D_w = nanowire diameter (m)
 D_H = hydraulic diameter (m)
 d_c = critical thickness (m)
 d_s = silicon device layer thickness (m)
 d_o = buried oxide layer thickness (m)
 F = conductivity reduction function
 $\hat{i}$ = unit vector in the i th direction
 k = thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)
 k_s = silicon thermal conductivity (in-plane for films; axial for nanowires) ($\text{W m}^{-1} \text{K}^{-1}$)
 k_o = oxide thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)
 L_d = limiting dimension (m)
 L_h = thermal healing length (m)
 L_{OP} = distance from point O on cross section of the nanowire to a point P on the nanowire boundary
 p = specularity
 q = phonon wavevector (m^{-1})
 S = hole spacing (m)
 T = temperature (K)
 v_{avg} = average acoustic phonon velocity (m s^{-1})
 W = nanobeam width (m)

Greek Symbols

Γ = correction factor for boundary scattering
 δ = reduced layer thickness, $\delta = d_s/\Lambda$
 θ = azimuthal angle (radians)
 Λ = phonon mean free path (m)
 ξ = integration variable
 τ = phonon relaxation time (s)
 ϕ = radial angle (radians)
 ω = phonon angular frequency (s^{-1})

Subscripts

boundary = due to boundary scattering
bulk = due to bulk/intrinsic processes
film = of the thin film
 i = direction index
 j = phonon branch index
nanowire = of the nanowire
pores = due to phonon-pore boundary scattering
porous = of the porous film

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