Cross-Plane Phonon Conduction in Polycrystalline Silicon Films

Silicon films of submicrometer thickness play a central role in many advanced technologies for computation and energy conversion. Numerous thermal conductivity data for silicon films are available in the literature, but they are mainly for the lateral, or in-plane, direction for both polycrystalline and single crystalline films. Here, we use time-domain thermoreflectance (TDTR), transmission electron microscopy, and semiclassical phonon transport theory to investigate thermal conduction normal to polycrystalline silicon (polysilicon) films of thickness 79, 176, and 630 nm on a diamond substrate. The data agree with theoretical predictions accounting for the coupled effects of phonon scattering on film boundaries and defects related to grain boundaries. Using the data and the phonon transport model, we extract the normal, or cross-plane thermal conductivity of the polysilicon (11.3 ± 3.5, 14.2 ± 3.5, and 25.6 ± 5.8 W m⁻¹ K⁻¹ for the 79, 176, and 630 nm films, respectively), as well as the thermal boundary resistance between polysilicon and diamond (6.5–8 m² K GW⁻¹) at room temperature. The nonuniformity in the extracted thermal conductivities is due to spatially varying distributions of imperfections in the direction normal to the film associated with nucleation and coalescence of grains and their subsequent columnar growth. [DOI: 10.1115/1.4029820]

Keywords: heat transfer, thermal conductivity, thermal boundary resistance, phonon transport, time-domain thermoreflectance, silicon, polycrystalline films

1 Introduction
While there has been much recent interest in low-dimensional nanostructures based on a variety of novel materials, silicon films remain critical for a large fraction of devices proposed or used for information and energy conversion technologies. Many of these are based on silicon-on-insulator technology, which provides single crystalline silicon films of submicrometer thickness (on top of a buried oxide layer on a bulk silicon substrate) for a large number of applications. These applications include high-performance microprocessors, microfabricated sensors and actuators, and other emerging applications such as phononic crystals [1–3]. Polycrystalline silicon (polysilicon) films have also been used for many applications, including microelectromechanical systems and integrated circuits [4]. Of particular recent interest are polysilicon films on a diamond substrate for heat sink applications in high power electronic devices [5].

Because of the wide use of silicon films in a variety of micro- and nanoscale devices, there have been numerous experimental studies on thermal conduction in both single crystalline and polycrystalline silicon films [2–4,6–13]. Many experimental observations [2,4,6–13] have indicated a large reduction in the thermal conductivities of single crystalline silicon films down to 9 nm thickness [13] due to the strong impact of phonon boundary scattering (for a comprehensive review of the data, see Refs. [2,4]). Other experimental studies of polysilicon films have shown that phonon scattering on grain boundaries significantly decreases the thermal conductivity values compared to those of single crystalline silicon films [14,15]. The thermal conductivity can also be strongly reduced by interactions of phonons with dopants and material defects [14–16,18]. However, the largest quantity of data available in the literature is for lateral, or in-plane, conduction in both single crystalline and polycrystalline films [2,4,6–16]. One study [17] attempted to extract the normal, or cross-plane, thermal conductivity of a 2.6-µm-thick, phosphorus doped polysilicon cantilever; another study [3] extracted this conductivity for 500-nm-thick, suspended, single crystalline silicon films (patterned films with periodic arrays of holes as well as an unpatterned one).

This work investigates thermal conduction normal to polysilicon films with three different thicknesses (79, 176, and 630 nm) on a diamond substrate. We use TDTR and the semiclassical phonon transport theory—which uses an approximate solution to the Boltzmann transport equation (BTE)—to examine effects of phonon scattering by film boundaries and defects related to grain boundaries. Our BTE model considers the nonhomogeneity of the phonon scattering rate internal to the polysilicon film due to the varying grain dimension, and thus to varying distributions of imperfections in the direction normal to the film. By combining the data and the phonon transport model, we extract the cross-plane thermal conductivity of the polysilicon films (11.3 ± 3.5, 14.2 ± 3.5, and 25.6 ± 5.8 W m⁻¹ K⁻¹ for the 79, 176, and 630 nm films, respectively) and the polysilicon–diamond thermal boundary resistance (6.5–8 m² K GW⁻¹) at room temperature.

2 Experimental Details

2.1 Sample Preparation. Three polysilicon films with thicknesses of 79, 176, and 630 nm are grown on a diamond substrate...
by thermal chemical vapor deposition (CVD) at 600 °C. The diamond is a polycrystalline wafer with thermal conductivity on the order of 1500 W m⁻¹ K⁻¹. The three polysilicon films are not doped. Figure 1 shows cross-sectional transmission electron micrographs (TEMs) of the three samples, which provide qualitative information about the grain size and orientation in the polysilicon film. With increasing film thickness, the columnar grain structure is clearly visible, with the long axes of the grains oriented in the film-normal direction. This is in agreement with past studies [14,15], which showed that polysilicon films grown by CVD at temperatures between 600 and 650 °C have columnar grain structure. For a film with columnar grains, the lateral grain size increases with increasing distance from the deposition interface of the film [14,15]. An atomic force microscopy (AFM) measurement characterizes the average lateral grain size of a 700-nm-thick polysilicon film that is grown separately but under the same growth conditions as the other three samples. We use the line-intercept method [19] to obtain the average lateral grain size of the 700 nm film from the plan-view AFM image, which yields 360 ± 80 nm. The higher magnification TEM of the 630 nm film near the polysilicon–diamond interface shows that the minimum grain dimension of the film at its growth interface (with the diamond) is approximately of the order of a few tens of nanometers. Overall, the micrographs indicate that the grain structure of the polysilicon film becomes columnar with increasing film thickness, and the columnar gains are aligned with respect to the film-normal direction. Approximately 45-nm-thick, evaporated Al films on top of these samples serve as the transducer for thermoreflectance measurements.

2.2 TDTR. Cross-plane thermal conduction from the polysilicon to the diamond substrate is investigated by TDTR, an ultrafast optical measurement technique using a pump–probe arrangement. This technique is well-established for measuring cross-plane thermal conductivity and thermal boundary resistance in multilayer thin-film structures [20–27]. In our setup, a mode-locked Nd:YVO₄ laser emits 9.2 ps optical pulses at a wavelength of 1064 nm and a repetition rate of 82 MHz, which are divided into a pump (as a heater) and probe (as a thermometer) component. Pump pulses are modulated at a frequency of 2 MHz using an electro-optic modulator for lock-in detection and are frequency-doubled to 532 nm using a periodically poled LiNbO₃ crystal for the spectral separation of the pump and probe pulses. The modulated pump pulses rapidly heat the metal transducer and create a transient temperature field within the material stack. The probe pulses are temporally delayed (from 0 to 3.5 ns) with respect to the pump optical heating by using a mechanical delay stage, and they measure the transient surface temperature decay of the metal.
film via the temperature-induced changes in the metal reflectivity. The changes in the reflected intensity of the probe pulses are detected by an RF lock-in amplifier at the modulation frequency of the pump pulses as a function of the delay time \( t \) between the pump and probe pulses. The \( 1/e^2 \) diameters of the focused pump and probe beams are \( \sim 10 \) and \( \sim 6 \mu m \), respectively, in our experiments.

We monitor the amplitude \( \sqrt{V_{in}^2 + V_{out}^2} \) of the in-phase \( V_{in}(t) \) and out-of-phase \( V_{out}(t) \) voltage signals of the RF lock-in amplifier over 3.5 ns of delay time between pump and probe. We use a single-mode fiber after the delay stage to address the problems created by (i) changes in the probe spot size and (ii) variations in the alignment and overlap of the pump and probe beams as the delay time is varied [20,25,26]. The pump beam amplitude and the delay-time-dependent amplitude of the probe beam are monitored independently from the thermoreflectance amplitude signal to correct for intensity fluctuations and for the intensity dependence on the stage position [25,26]. The corrected thermoreflectance amplitude data are fitted to the solution of the three-dimensional radial-symmetric heat diffusion equation for the multilayer stack taking into account surface heating by a modulated periodic pulse train to extract the relevant thermal properties beneath the metal transducer [21]. We validate system accuracy by extracting a room-temperature thermal conductivity of \( 1.33 \pm 0.1 \text{ W m}^{-1} \text{ K}^{-1} \) and \( 145 \pm 15 \text{ W m}^{-1} \text{ K}^{-1} \) for a SiO\(_2\) calibration sample and an intrinsic single crystalline Si calibration sample, respectively, each of which is within 2% of reference literature values for thermally grown SiO\(_2\) and bulk single crystalline silicon [28,29]. Further details of our TDTR setup are described in Refs. [25,26].

We fit the TDTR data with three adjustable parameters in the analytical heat diffusion model: (i) the thermal boundary resistance at the Al–polysilicon interface \( R_{b,Al-Si} \), (ii) the cross-plane thermal conductivity of the polysilicon film \( k_{Si} \), and (iii) the thermal boundary resistance at the polysilicon–diamond interface \( R_{b, Si-Diam} \). The validity of this approach is addressed through a discussion of sensitivity in Sec. 2.3. All the other parameters in the multilayer thermal model are taken from the literature or experiments.

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2.3 Sensitivity Analysis. The TDTR sensitivity coefficient is defined as the logarithmic derivative of the thermoreflectance signal \( R \) with respect to the thermal parameter of interest \( \beta \) [23,24,26,27]

\[
S_{\beta} = \frac{\partial \ln(R)}{\partial \ln(\beta)} \tag{1}
\]

For the TDTR measurements in the present study, \( R \) is the amplitude signal \( \sqrt{V_{in}^2 + V_{out}^2} \) (We discuss in more detail the TDTR signal approach later in this section.) Figure 2 shows the sensitivity of the amplitude signal to the three unknown parameters (i.e., \( R_{b,Al-Si}, k_{Si}, \) and \( R_{b, Si-Diam} \)) and to the thermal conductivity of the diamond substrate \( k_{Diam} \) as a function of the delay time for the three polysilicon samples at room temperature. The values of the sensitivity coefficients are evaluated at the 2MHz pump modulation frequency and assuming best-fit values for each of the fitted variables. For all three samples, the sensitivity of the amplitude signal to \( R_{b,Al-Si} \) is different from that to \( k_{Si} \) and \( R_{b, Si-Diam} \) in terms of the curvature. Since the sensitivity to \( R_{b,Al-Si} \) is highly
dependent on the earliest part of the thermoreflectance traces (at delay times below approximately 1 ns), its values increase with increasing delay time up to ~1 ns, whereas at longer delay times (\( t > 1 \) ns) they remain relatively constant (see Fig. 2(a)) or decrease with delay time (see Figs. 2(b) and 2(c)). On the other hand, the absolute values of the sensitivity to \( k_{Si} \) and \( R_{Si-Diam} \) monotonically increase with increasing delay time. These different curvatures of the sensitivities allow us to separate the Al–polysilicon boundary resistance from the other two components (\( k_{Si} \) and \( R_{Si-Diam} \)). The latter two are not possible to uniquely separate since their sensitivity curves are similar in shape over the entire range of delay time. They are rather lumped into an effective polysilicon thermal resistance \( R_{Si eff} \) which combines the volumetric polysilicon resistance \( d_{Si}/k_{Si} \) (where \( d_{Si} \) is the thickness of the polysilicon film) and the polysilicon–diamond boundary resistance [27,35–37], which can be expressed as

\[
R_{Si eff} = \frac{d_{Si}}{k_{Si}} + R_{b, Si-Diam}
\]

The measurement is insensitive to the in-plane heat conduction along the polysilicon films because the sensitivity to the in-plane polysilicon thermal conductivity is essentially zero for all three samples (as illustrated in Fig. 2). The sensitivity to \( k_{Diam} \) is also extremely low for all three samples. The absolute sensitivity values are \(-0.03\) and \(-0.01\) for the thinnest and thickest polysilicon samples, respectively. Therefore, variations in the diamond thermal conductivity will not significantly impact the fitted variables—e.g., a 30% error in the diamond thermal conductivity propagates to a 2% error in the effective polysilicon thermal resistance for the thinnest sample and a 1% error for the thickest sample.

To further support the validity of our data fitting approach, we plot the TDTR data along with the optimal analytical fit for the 176 nm polysilicon sample in Fig. 3(a), and we also illustrate degenerate solutions by varying \( R_{Si-Diam} \) from its optimal value (\( \pm 10\% \)) and then reoptimizing the remaining two free parameters (\( R_{b, Al-Si} \) and \( k_{Si} \)). The reoptimized polysilicon thermal conductivity varies by \(-4.1\%\) from its original optimal value due to the \(-10\%\) perturbation in \( R_{Si-Diam} \) (see dashed–dotted line in Fig. 3(a)); this variation in the polysilicon thermal conductivity is +4.5% for the \(+10\%\) perturbation in \( R_{Si-Diam} \) (see dotted line in Fig. 3(a)). The variations in \( R_{b, Al-Si} \) due to the \( \pm 10\% \) perturbation in \( R_{b, Si-Diam} \) are negligible. Since these three analytical fits, with different combinations of \( k_{Si} \) and \( R_{Si-Diam} \), are not distinguishable from each other and replicate the data well, this indicates that the TDTR measurement is not able to uniquely separate \( k_{Si} \) and \( R_{Si-Diam} \). Instead, the measurement is sensitive to the sum of the polysilicon volume resistance and the polysilicon–diamond boundary resistance (i.e., sensitive to the effective polysilicon thermal resistance \( R_{Si eff} \), as suggested above). Figure 3(b) presents the TDTR data and the optimal analytical fit for the thinnest sample (79 nm) and also illustrates the sensitivity of the TDTR measurement to \( k_{Diam} \) for this sample—where the diamond thermal conductivity is expected to play the largest role. This analysis clearly shows that variations in the diamond thermal conductivity (e.g., \( \pm 30\% \)) have a negligible impact on the thermal trace of the samples.

In typical TDTR experiments, both the amplitude \( \sqrt{V_{in}^2 + V_{out}^2} \) and the ratio \(-V_{in}/V_{out}\) of the in-phase and out-of-phase voltage signals of the RF lock-in amplifier versus delay time can be analyzed to extract the relevant thermal properties (e.g., the sample thermal conductivity). We have found that both the amplitude and ratio approaches offer sufficient sensitivity to extract the thermal conductivity of samples having low to intermediate conductivity values—from that of thermally grown SiO\(_2\) (\(~1.4\) W m\(^{-1}\) K\(^{-1}\)\) to that of bulk single crystalline silicon (\(~150\) W m\(^{-1}\) K\(^{-1}\)\) [26,27,38]. However, if the sample thermal conductivity is higher than this range of values, the ratio approach provides higher sensitivity to extract the sample conductivity than the amplitude approach [27,38].

The cross-plane thermal conductivity values of our three polysilicon films range from approximately 11 to 26 W m\(^{-1}\) K\(^{-1}\) (we present these results in more detail in Sec. 3), and they hence are approximately an order of magnitude lower than that of bulk single crystalline silicon. This means that both the amplitude and ratio approaches can be used for our polysilicon samples. We choose to analyze the amplitude signal in this study because the amplitude approach has some advantages over the ratio approach for this specific set of samples:

1. The error propagated by the uncertainty in the thermal conductivity of the diamond substrate \( k_{Diam} \) is smaller in the

![Fig. 3](http://samples.asmedigitalcollection.asme.org/)

(a) 176 nm Polysilicon

(b) 79 nm Polysilicon

Fig. 3  (a) TDTR data for the 176 nm polysilicon sample (solid line) along with the best analytical fit (dashed line) yielding the optimal parameter set \( R_{b, Al-Si} = 6.7 \) m\(^2\) K GW\(^{-1}\), \( k_{Si} = 14.7 \) W m\(^{-1}\) K\(^{-1}\), and \( R_{Si-Diam} = 7.7 \) m\(^2\) K GW\(^{-1}\). The dashed–dotted and dotted curves represent the analytical fits obtained by varying the best-fit \( R_{b, Si-Diam} \) by \(-10\%\) and \(+10\%\), respectively, and then by reoptimizing \( R_{b, Al-Si} \) and \( k_{Si} \). The re-optimized polysilicon thermal conductivity varies by \(-4.1\%\) (dashed–dotted line) and \(+4.5\%\) (dotted line) from its original optimal value of \( 14.7 \) W m\(^{-1}\) K\(^{-1}\). The variations in \( R_{b, Al-Si} \) are negligible. (b) TDTR data for the 79 nm polysilicon sample (solid line) along with the best analytical fit (dashed line) yielding the optimal parameter set \( R_{b, Al-Si} = 7.5 \) m\(^2\) K GW\(^{-1}\), \( k_{Si} = 12.0 \) W m\(^{-1}\) K\(^{-1}\), and \( R_{Si-Diam} = 6.8 \) m\(^2\) K GW\(^{-1}\). The best-fit curve assumes \( k_{Diam} = 1600 \) W m\(^{-1}\) K\(^{-1}\) (from manufacturer’s specification). The dashed–dotted and dotted curves represent the analytical fits obtained by varying this diamond thermal conductivity by \(-30\%\) and \(+30\%\), respectively, and by assuming best-fit values for each of the fitted variables.

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amplitude approach than in the ratio approach because the latter is more sensitive to the diamond substrate thermal conductivity than the former [26]. The propagation of uncertainty from $k_{Diam}$ into the uncertainties of the measured properties ($k_{Al}$ and $R_{Si-Si-Diam}$) is proportional to the ratio of the sensitivities to these properties, i.e., $\delta k_{Diam}/\delta k_{Al}$ and $\delta k_{Diam}/\delta R_{Si-Si-Diam}$. (The error propagation is this ratio—multiplied by the uncertainty in $k_{Diam}$.) The absolute values of these two ratios for the thinnest sample (79 nm) are $|\delta k_{Diam}/\delta k_{Al}| < 0.2$ and $|\delta k_{Diam}/\delta R_{Si-Si-Diam}| < 0.6$ for the amplitude approach and $|\delta k_{Diam}/\delta k_{Al}| > 2$ and $|\delta k_{Diam}/\delta R_{Si-Si-Diam}| > 1.3$ for the ratio approach—all at delay times from 100 ps to 3.5 ns. For the thickest sample (630 nm), $|\delta k_{Diam}/\delta k_{Al}| < 0.05$ and $|\delta k_{Diam}/\delta R_{Si-Si-Diam}| < 0.23$ for the amplitude approach and $|\delta k_{Diam}/\delta k_{Al}| > 0.16$ and $|\delta k_{Diam}/\delta R_{Si-Si-Diam}| > 0.38$ for the ratio approach—all at delay times from 100 ps to 3.5 ns.

(2) The amplitude approach is free of propagation associated with the uncertainty in setting the correct reference phase of the RFllock-in amplifier, whereas in the ratio approach this uncertainty is one of the major sources of the total uncertainty, especially for a low-frequency measurement [24]. Since we use a relatively low pump modulation frequency of 2MHz to probe the buried film–substrate interface, the amplitude approach is beneficial for extracting the thermal resistance of this buried interface with lower uncertainty [26].

The thermal penetration depths of the modulated pump beam at 2 MHz correspond to approximately 1–1.6 μm polysilicon (depending on the polysilicon thermal conductivity), which are larger than the three polysilicon thicknesses. The 2 MHz data are thus sensitive to both the polysilicon conductivity and the polysilicon–diamond boundary resistance, as illustrated in Fig. 2. The thermal penetration depths at higher modulation frequencies are smaller than those at 2 MHz; e.g., the thermal penetration depth at 5 MHz and 8 MHz correspond to approximately 1–1.6 μm and 0.7–1 μm polysilicon, respectively. TDTR measurements are also performed on each sample at 5 MHz, at which the thermal penetration depths are still larger than the film thicknesses. No modulation frequency dependence is observed between the 2 MHz and 5 MHz data; variations in the extracted parameters are less than 3%.

### 3 Results and Discussion

A nonlinear least-squares curve-fitting algorithm finds the Al–polysilicon thermal boundary resistance and the effective polysilicon thermal resistance that optimize the model fit to the measured TDTR data. We normalize the TDTR data at 100 ps to the first tens of picoseconds after the pump heating) on our data and set all of the measured TDTR data. We normalize the TDTR data at 100 ps to the first tens of picoseconds after the pump heating on our data and set all of the measured TDTR data. We normalize the TDTR data at 100 ps to the first tens of picoseconds after the pump heating on our data and set all of the measured TDTR data. We normalize the TDTR data at 100 ps to the first tens of picoseconds after the pump heating on our data and set all of the measured TDTR data.

where the subscript $j$ refers to the longitudinal phonon (L) and the low and high frequency transverse phonon (TO and T) modes, $v_j$ is the appropriate phonon group velocity for the different modes, $k_B$ is the averaged phonon group velocity, $\theta$ is the Debye temperature, and $\alpha_d = h/\omega_0T$ is the dimensionless phonon frequency. The phonon specific-heat function $C_V(x_d, T)$ can be found in Ref. [14]. The diffuse mismatch model (DMM) [50,51] is employed to predict the rates of phonon transmission from within the polysilicon into the Al and the diamond, which are $\alpha_d$ and $\alpha_{Diam}$, respectively (see Table 1). This form of the BTE model has yielded predictions that were consistent with experimental data when a crystalline dielectric or semiconductor layer—with thickness comparable to mean free paths of phonons—is sandwiched between two media [26,48,52–54].

To consider the nonhomogeneity of the internal phonon scattering rate in the polysilicon film due to the varying grain

### Table 1 BTE model parameters. (The normal and Umklapp scattering parameters as well as the detailed phonon properties of Si (such as the phonon group velocities and the Debye temperatures) are taken directly from Ref. [49].)

<table>
<thead>
<tr>
<th>$\omega_0$</th>
<th>$\alpha_{Diam}$</th>
<th>$\alpha_d$</th>
<th>$\Gamma$</th>
<th>$n_{Si, p}$ ($\times 10^{19}$ m$^{-2}$)</th>
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<td>0.74</td>
<td>0.16</td>
<td>50</td>
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*The transmission coefficients determined by the DMM [50] for the phonon transmission from the polysilicon into the Al ($\alpha_d$) and the diamond ($\alpha_{Diam}$).*
dimensions, we define the dimensionless layer thickness as \[ d_{eq}(x_n, T) = \int_{0}^{z_n} \frac{dz}{v_i \tau_i(z, x_n, T)} \] where \( z \) is the coordinate normal to the polysilicon film, measured from the polysilicon–diamond interface. The total internal phonon scattering rate \( \tau_i(z) \) of each of the phonon modes (i.e., longitudinal and low/high frequency transverse modes) is the sum of the phonon–phonon (normal or Umklapp) and the grain boundary scattering rates (according to Matthiessen’s rule). The normal and Umklapp scattering parameters as well as the detailed phonon properties of Si (such as the phonon group velocities and the Debye temperatures) are taken directly from Ref. [49]. We use the grain boundary scattering term \( \kappa_{GB}(z, x_n) \) that was developed in prior studies [46,48] for polycrystalline diamond thin films with columnar grains. These past studies revealed that for the polycrystalline films phonon scattering on localized defects concentrated near grain boundaries may be more important than scattering on grain boundaries and on defects homogeneously distributed within grains. Even if defects homogeneously distributed within grains are important, Eqs. (3) and (4) can be used together with this hypothesis to study the impact of spatial variations of imperfections under the assumption that their concentrations correlate inversely with the grain size.

The BTE model (Eq (3)) considers two grain structures of polycrystalline films: (i) randomly oriented grains and (ii) entirely columnar grains. These past studies revealed that for the polycrystalline films phonon scattering on localized defects concentrated near grain boundaries may be more important than scattering on grain boundaries and on defects homogeneously distributed within grains. Even if defects homogeneously distributed within grains are important, Eqs. (3) and (4) can be used together with this hypothesis to study the impact of spatial variations of imperfections under the assumption that their concentrations correlate inversely with the grain size.

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two interfaces is approximately $14 \text{ m}^2 \text{ K GW}^{-1}$. Since the measured Al–polysilicon boundary resistance ranges between 6 and $7.5 \text{ m}^2 \text{ K GW}^{-1}$ for the three samples, the polysilicon–diamond boundary resistance is estimated to be $6.5–8 \text{ m}^2 \text{ K GW}^{-1}$.

The cross-plane polysilicon thermal conductivity data are obtained for all three measured samples by subtracting the sum of the two boundary resistances (i.e., $14 \text{ m}^2 \text{ K GW}^{-1}$) from the total thermal resistance. This procedure yields the thermal conductivity of $11.3 \pm 3.5 \text{ W m}^{-1} \text{ K}^{-1}$ for the 79 nm sample, $14.2 \pm 3.5 \text{ W m}^{-1} \text{ K}^{-1}$ for the 176 nm sample, and $25.6 \pm 5.8 \text{ W m}^{-1} \text{ K}^{-1}$ for the 630 nm sample. These conductivity values agree with those determined by assuming the above specified range of values for the polysilicon–diamond boundary resistance (i.e., $6.5–8 \text{ m}^2 \text{ K GW}^{-1}$) and by fitting for the polysilicon thermal conductivity for all three measured samples. It is worth noting that each conductivity value determined here is an average over the entire film thickness, and that spatially varying imperfections along the film-normal direction (and thus the spatially varying phonon scattering rate along this direction) create the nonuniformity in the conductivity values.

Figure 5 shows the room-temperature cross-plane and in-plane thermal conductivity data of silicon films, including our cross-plane polysilicon data and other data available in the literature. Also shown are the predictions of the BTE model for the cross-plane polysilicon thermal conductivity from Eq. (3) (with the boundary resistances removed), which consider both random and columnar grain structures and assume $d_{GB}$ of 50 nm and $n_{GB,P}$ of $1.5 \times 10^{19} \text{ m}^{-2}$ while assuming $d_{GB}$ of 50 nm.

As indicated in Fig. 5, the cross-plane polysilicon thermal conductivity data for the 79 and 176 nm films again agree well with the prediction of the random grain structure model (see a solid line). The data for the thickest film (630 nm) are slightly above the prediction of the random grain structure model, which indicates the transition from random to columnar grain structure with increasing film thickness (as discussed above). Figure 5 also includes the molecular dynamics (MD) calculation for the cross-plane thermal conductivity of a 10-nm-thick polysilicon film [56] (unfilled diamond) is shown for comparison. This MD calculation assumes a random shape of grains and an average grain size of 4 nm. The results of the BTE model for the cross-plane polysilicon thermal conductivity from Eq. (3) (with the boundary resistances removed) are shown with the solid (random grain structure) and dashed (columnar grain structure) lines.
conduction of a 10-nm-thick polysilicon film with a random shape of grains and an average grain size of 4 nm [36]. This MD calculation is consistent with the predictions of our BTE model.

We make a further effort here to extract the local, cross-plane polysilicon thermal conductivity $k_{\text{polysilicon}}^{\text{local}}(z)$—which depends on the distance $z$ from the growth interface—by utilizing three different thickness samples, which share the same microstructure. As a first step, we use the data for the 79 and 176 nm samples and determine the local thermal conductivity corresponding to a region of $79 \text{ nm} < z < 176 \text{ nm}$. Assuming that we know the volume resistance of the polysilicon corresponding to a region of $0 \text{ nm} < z < 79 \text{ nm}$, and the bottom boundary resistance (the sum of the two is the effective resistance of the 79 nm film), as we determined earlier in this section, we create a two-layer model within the 176 nm film: $-45 \text{ nm}$ of Al on a 97-nm-thick layer with unknown local thermal conductivity on a 79-nm-thick layer with known properties on diamond. Using the effective resistance data of the 79 nm film, we fit for this local conductivity and find $k_{\text{polysilicon}}^{\text{local}} = 16 \text{ W m}^{-1} \text{ K}^{-1}$ (for $79 \text{ nm} < z < 176 \text{ nm}$). We repeat this procedure for the 176 nm and 630 nm samples and fit for the local thermal conductivity characteristic of a region of $176 \text{ nm} < z < 630 \text{ nm}$. This fitted local conductivity is approximately $28 \text{ W m}^{-1} \text{ K}^{-1}$. Because of the submicrometer thicknesses of the three films, the local conductivities and the averaged conductivities (over the entire film thickness) do not differ substantially, but the difference is expected to be significant with increasing grain size and film thickness [33].

4 Conclusions

This work investigates the thermal resistance for conduction normal to polysilicon films with three different thicknesses on a diamond substrate using TDTR and semiclassical phonon transport theory. By combining the data and the phonon transport model, we extract the cross-plane thermal conductivity of the polysilicon films (11.3, 14.2, 25.6 $\text{ W m}^{-1} \text{ K}^{-1}$ for the 79, 176, and 630 nm films, respectively), as well as the polysilicon–diamond thermal boundary resistance (6.5–8 $\text{ m}^{2} \text{ KW}^{-1}$). The cross-plane thermal conductivity data for the 79 and 176 nm samples are consistent with simulations assuming a random grain structure with a minimum grain dimension of 50 nm and a point defect density per unit grain boundary area of $1.5 \times 10^{19} \text{ m}^{-2}$. The conductivity data for the thickest sample (630 nm) are slightly overpredicted by the random grain structure model and underpredicted by the columnar grain structure model, which indicates the transition of the grain structure from the former to the latter with increasing film thickness. Nonuniform thermal conductivity values between the samples can be attributed to the impact of spatially varying defect concentrations along the direction normal to the film.

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Nomenclature

- $C_v$: phonon specific heat per unit volume ($\text{J m}^{-3} \text{ K}^{-1}$)
- $d$: layer thickness ($\text{m}$)
- $d_n$: nondimensional layer thickness, defined in Eq. (4)
- $d_G$: characteristic grain dimension ($\text{m}$)
- $d_{GB}$: minimum grain dimension ($\text{m}$)

$\hbar$: Planck’s constant divided by 2$\pi$ ($\text{J s}$)
$k$: thermal conductivity ($\text{W m}^{-1} \text{ K}^{-1}$)
$k_B$: Boltzmann’s constant ($\text{K}^{-1}$)
$n_{GB}$: number of defects of type $i$ per unit grain boundary area ($\text{m}^{-1}$)
$R$: thermal resistance ($\text{m}^{2} \text{ K W}^{-1}$)
$S_{\beta}$: TDTR sensitivity to some parameter $\beta$
$t$: pump–probe delay time ($\text{s}$)
$T$: temperature ($\text{K}$)
$v$: phonon group velocity ($\text{m s}^{-1}$)
$v_\text{g}$: average phonon group velocity ($\text{m s}^{-1}$)
$V_{\text{na}}$: in-phase voltage of RF lock-in amplifier ($\text{V}$)
$V_{\text{off}}$: out-of-phase voltage of RF lock-in amplifier ($\text{V}$)
$x_{\text{in}}$: nondimensional phonon frequency $= h\omega/k_B T$
$z$: coordinate normal to layer ($\text{m}$)

Greek Symbols

- $\alpha$: transmission coefficient
- $\eta$: grain boundary scattering strength, defined by Eq. (7)
- $\theta$: Debye temperature ($\text{K}$)
- $\sigma_i$: phonon scattering cross section of defects of type $i$ ($\text{m}^2$)
- $\tau$: phonon relaxation time ($\text{s}$)
- $\omega$: phonon angular frequency ($\text{s}^{-1}$)

Subscripts

- $b$: boundary
- Diam: diamond
- eff: effective
- GB: grain boundary
- $i$: index denoting defect type
- $j$: phonon branch index
- $L$: longitudinal phonon mode
- $P$: point defect
- $s$: total
- $\text{TO}$: low frequency transverse phonon mode
- $\text{TU}$: high frequency transverse phonon mode

References
