

Experimental investigation of thermal conduction normal to diamond-silicon boundaries

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Passive chemical-vapor-deposited diamond layers have the potential to improve thermal conduction in electronic microstructures because of their high thermal conductivities. The thermal resistances for conduction normal to the boundaries of diamond layers, which must be small in order to realize this potential, have not been measured. This research develops two independent experimental methods that measure the total thermal resistance for conduction normal to diamond layers thinner than 5 μm on silicon substrates, yielding an upper bound for the thermal resistance of the diamond-silicon boundary. The data for layers as thin as 0.2 μm agree with predictions that account for phonon scattering on layer boundaries and couple the local scattering rate in the diamond to the grain size. The agreement lends support to the conclusion that the effective diamond-silicon boundary resistance is dominated by a highly localized volume resistance in the diamond near the interface. © 1995 American Institute of Physics.

I. INTRODUCTION

At room temperature, chemical-vapor-deposited (CVD) diamond is an excellent conductor of heat and is an electrical insulator. This makes it an ideal material for passive use in electronic systems containing silicon semiconductor devices. Many applications attach diamond plates thicker than about 100 μm to semiconducting substrates.¹⁻⁵ These methods suffer from the thermal resistance of the attachment, which can strongly impede conduction cooling.⁶ Promising alternatives take advantage of diamond deposition directly on silicon using, for example, a bias voltage to enhance nucleation.⁷⁻⁹ This approach is most effective if a low thermal resistance is achieved at boundaries between active silicon regions, where heat is generated, and the high-thermal-conductivity diamond. While much research investigated the thermal conductivities of diamond layers,¹⁰ the resistances at the boundaries of CVD diamond layers have received very little attention. Near the interface of diamond deposited on silicon, the volume resistance of the highly imperfect diamond is expected⁶ to yield an effective boundary resistance of the order of $5 \times 10^{-8} \text{ m}^2 \text{ K W}^{-1}$, which would diminish the improvement due to the use of diamond in electronic microstructures containing direct diamond-silicon interfaces. There is a need for data on the effective thermal boundary resistance.

Much previous research measured thermal resistances for conduction normal to thin layers and interfaces.¹¹ Steady-state Joule heating in patterned metal layers on dielectric substrates determined metal-dielectric boundary resistances, primarily at cryogenic temperatures.^{12,13} The accuracy of the data was facilitated by the small temperature rise in the dielectric substrates, which have high thermal conductivities at low temperatures. Recent research^{14,15} tailored this approach to measure the room-temperature thermal resistance for conduction normal to metallized silicon-dioxide layers on silicon. The resulting data provide information about the bound-

ary and volume resistances of the silicon dioxide. The uncertainty resulting from the steady-state temperature rise in the silicon substrate rendered this method suitable only for measuring resistances greater than about $5 \times 10^{-8} \text{ m}^2 \text{ K}^{-1} \text{ W}^{-1}$. Pulsed laser heating and laser-reflectance thermometry were used to measure smaller resistances by diminishing the unnecessary temperature rise in the substrate.¹⁶ While laser-heating methods have the disadvantage that it is very difficult to determine the absolute magnitude of the power absorbed by the sample, this problem is compensated by the ability to precisely measure the shape of the response for time scales as small as a few nanoseconds. Joule-heating methods, which cannot easily be applied at such small time scales due to voltage reflections, have the advantage that they induce precisely measurable heat fluxes that resemble those occurring in electronic microstructures.

This research develops independent Joule- and laser-heating measurement techniques to investigate conduction normal to metallized diamond layers on silicon substrates. Data for layers of thickness between 0.2 and 2.6 μm fabricated using the same deposition conditions are interpreted using an approximation to the solution of the Peierls-Boltzmann transport equation, yielding conclusions about the possible cause of an effective silicon-diamond boundary resistance. This research develops measurement technology for investigating relatively small thermal resistances for conduction normal to thin layers and interfaces. The data are needed to assess the benefit of using diamond in specific electronic microstructures.

II. EXPERIMENTS

A. Sample preparation

Three diamond layers are fabricated on (100) silicon substrates using CVD assisted by a microwave-frequency plasma. The substrate temperature is 1100 K and the deposition pressure is 2600 Pa. A voltage bias between the substrate and the plasma source induces nucleation, as described previously.⁹ The three layers, designated A, B, and C, are

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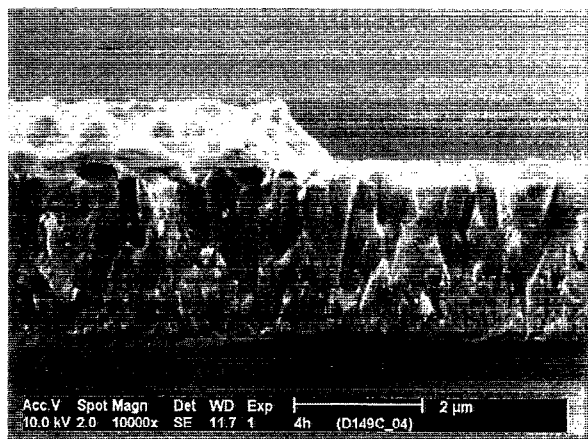


FIG. 1. Cross section of diamond layer C, of thickness $2.6 \mu\text{m}$, deposited on a (100) silicon substrate. Also visible is the patterned gold-titanium metallization.

grown for 0.5, 1, and 4 h, respectively. The molar concentration of methane diluted in hydrogen during nucleation and deposition is 2%. The thicknesses of the three layers, measured using electron micrographs, are 0.2, 0.5, and $2.6 \mu\text{m}$, respectively. The thinner two diamond layers are metallized with 10 nm of titanium and 300 nm of gold. In order to ensure closure on layer C, which had a relatively large surface roughness, the gold thickness is $1 \mu\text{m}$. The metallization is patterned using standard lithographic techniques.

The samples are studied using electron microscopy, revealing that the grain size and the layer surface roughness vary significantly. Top-view micrographs of layers A and B show that they consist of grains with dimensions considerably less than 100 nm . The thickest layer, C, consists of grains of dimension up to $0.5 \mu\text{m}$. When viewed from the side, layers A and B had roughness features with dimensions considerably less than 50 nm . Layer C had roughness features of dimension as large as $0.2 \mu\text{m}$. Figure 1 is a cross-sectional micrograph of layer C. Since the three samples are prepared using identical deposition and nucleation parameters, the approximate internal microstructures of layers A and B can be deduced from that of layer C shown in Fig. 1.

B. Joule-heating method

Current in a microbridge is used to simultaneously induce heat flow normal to the diamond layer and measure the electrical resistance along the microbridge, which depends on temperature. Figure 2 is a schematic of the microbridge structure, which is on the top surface of the thin diamond layer, and the Wheatstone-bridge circuit. The experimental structure is on a silicon wafer, which is mounted on a temperature-controlled chuck. The input voltage V_{in} is provided by a pulse generator. The Wheatstone-bridge circuit facilitates measurement of changes of the electrical resistance along the microbridge. The floating output voltage of the Wheatstone-bridge circuit V_{out} is referenced to ground using a differential amplifier and monitored using a digital oscilloscope.

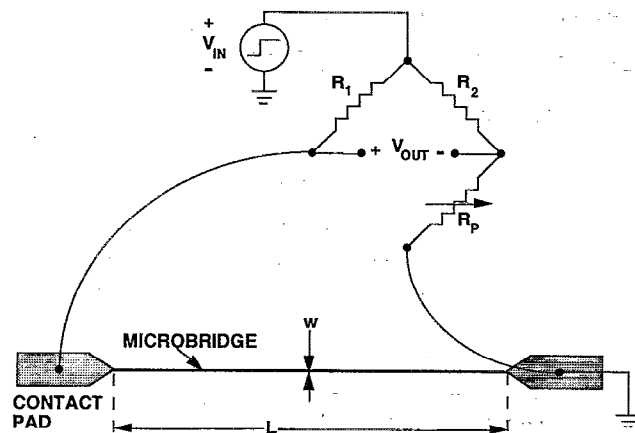


FIG. 2. Schematic of the patterned microbridge and the Wheatstone-bridge circuit used for the Joule-heating method. The dimensions are $L=5.5 \text{ mm}$ and $w=20 \mu\text{m}$. The electrical resistances of the microbridge structures are of the order of magnitude of 50Ω .

Calibration pulses V_{in} of amplitude less than 5 V are sustained along the microbridge, such that Joule heating and the microbridge temperature rise during the pulse are negligible. Under this condition, the Wheatstone bridge is balanced at room temperature using the potentiometer. The structure and the bridge are then calibrated by measuring the dependence of the ratio $V_{\text{out}}/V_{\text{in}}$ on the steady-state wafer temperature, which is controlled using an isothermal chuck and measured using an independent thermocouple attached to the wafer.

During the experiment, measurement pulses of amplitude as large as 75 V induce Joule heating in the microbridge and heat flow normal to the diamond. The calibration data are used to convert the transient ratio $V_{\text{out}}/V_{\text{in}}$ during the high-voltage pulses into the transient microbridge temperature rise $\Delta T_{\text{B}}(t)$. The voltage and current induced in the microbridge, V_{B} and I_{B} , are measured independently. The heat flux induced normal to the diamond layer during the pulse is $q = I_{\text{B}} V_{\text{B}} / (wL)$.

It is helpful to consider the temperature rise that would occur in the absence of the diamond layer and any thermal boundary resistance between the metal and silicon $\Delta T_{\text{B0}}(t)$. If the diamond has a thermal conductivity higher than that of silicon and the thermal resistances at the diamond-metal and diamond-silicon boundaries are negligible, then the measured temperature rise in the gold must be smaller than $\Delta T_{\text{B0}}(t)$ at all times. In contrast, if the diamond layer has a conductivity smaller than that of the silicon or if either of the boundary resistances is sufficiently large, then the measured temperature rise can be considerably larger than $\Delta T_{\text{B0}}(t)$. Thermal conduction through the diamond layer and its boundaries is described by the total thermal resistance R_{T} . Since the layers are much thinner than the microbridge width, R_{T} nearly satisfies

$$qR_{\text{T}} = \Delta T_{\text{B}}(t) - \Delta T_{\text{B0}}(t). \quad (1)$$

But, lateral conduction in the diamond causes Eq. (1) to

slightly underpredict the one-dimensional thermal resistance normal to the layer and its boundaries, particularly for layer C. This problem is addressed using an approximation. The diamond is assumed to have a homogeneous, isotropic conductivity and to have a volume resistance that is much larger than the metal-diamond and diamond-silicon boundary resistances. The transient, three-dimensional thermal-conduction equation is solved in the diamond and silicon for this ideal-

ized situation. The heat generation from the metal is modeled as a uniform heat flux into the diamond upper boundary within a rectangle of dimensions $w \times L$. For simplicity, the bottom boundary of the silicon is modelled as adiabatic; but, the short measurement time scale renders this boundary condition unimportant.

The spatially averaged temperature rise of the gold microbridge due to a periodic heat flux $q \exp(i\omega_h t)$ is

$$\Delta T_B(\omega_h, t) = q \exp(i\omega_h t) \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \frac{S_n S_m [\tanh(Q_1 d_1) + (Q_1 k_1 / Q_2 k_2) \coth(Q_2 d_2)]}{Q_1 k_1 + Q_2 k_2 \coth(Q_2 d_2) \tanh(Q_1 d_1)}, \quad (2)$$

where k_1 and d_1 are the conductivity and thickness of the silicon substrate and k_2 and d_2 are the conductivity and thickness of the diamond layer and the other parameters satisfy

$$S_n = \begin{cases} \frac{L}{2L_X}, & n=0, \\ \frac{4}{(n\pi)^2} \frac{L_X}{L} \sin^2\left(\frac{n\pi L}{2L_X}\right), & n \geq 1, \end{cases} \quad (3)$$

$$S_m = \begin{cases} \frac{w}{2L_Y}, & m=0, \\ \frac{4}{(m\pi)^2} \frac{L_Y}{L} \sin^2\left(\frac{m\pi w}{2L_Y}\right), & m \geq 1, \end{cases}$$

$$Q_1 = \left[\left(\frac{n\pi}{L_X} \right)^2 + \left(\frac{m\pi}{L_Y} \right)^2 + \frac{i\omega_h}{\kappa_1} \right]^{1/2}, \quad (4)$$

$$Q_2 = \left[\left(\frac{n\pi}{L_X} \right)^2 + \left(\frac{m\pi}{L_Y} \right)^2 + \frac{i\omega_h}{\kappa_2} \right]^{1/2}.$$

The thermal diffusivities of the silicon and diamond are κ_1 and κ_2 , respectively, L_Y is an arbitrary length much larger than the thermal-diffusion length in silicon during the measurement, $\sim 400 \mu\text{m}$, and L_X is much larger than L . The real temperature rise due to a single pulse in the time domain is obtained using a Fourier integral,

$$\Delta T_B(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1 - \exp(-i\omega_h t_p)}{i\omega_h} \Delta T_B(\omega_h, t) d\omega_h, \quad (5)$$

where t_p is the pulse duration. The silicon conductivity and diffusivity used to interpret the present room-temperature measurements are $k_1 = 144 \text{ W m}^{-1} \text{ K}^{-1}$ and $\kappa_1 = 8.8 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$.

The diamond conductivity k_2 in Eqs. (2)–(5) is fitted such that the predicted temperature rise $\Delta T_B(t)$ agrees with the measured temperature rise. The thermal resistance for conduction normal to the layer is calculated using $R_T = d_2/k_2$. For the thinner two layers A and B, the thermal resistance R_T calculated in this manner differs by less than a few percent from the much simpler expression, Eq. (1). For the thickest layer C, Eqs. (2)–(5) yield a significantly more

accurate value for R_T than Eq. (1) because they account for the lateral spreading of isotherms in the diamond.

Figure 3 compares the reduced temperature rise, $\Delta T_B(t)/P$, for layer B with that of sample D, which is an identical gold-titanium-silicon structure without the diamond layer. For times shorter than about $5 \mu\text{s}$ after the pulse start, voltage-signal reflections in the circuit yield spurious data. The data in Fig. 3 are only presented for $t > 25 \mu\text{s}$, when the voltage-signal reflections are small. Figure 3 also shows temperature rises predicted using Eqs. (2)–(5). The relative uncertainty of the temperature-rise data is estimated to be 3.5% due to the uncertainty of the temperature change on the wafer surface during calibration. This results in an uncertainty in the values of R_T extracted for the diamond layers of about $0.5 \times 10^{-8} \text{ m}^2 \text{ K W}^{-1}$, which is a significant improvement compared to the uncertainty yielded by previous methods using Joule heating.^{14,15} The relative uncertainty in the temperature rise is much smaller than that of the diamond thermal resistance measured using this method.

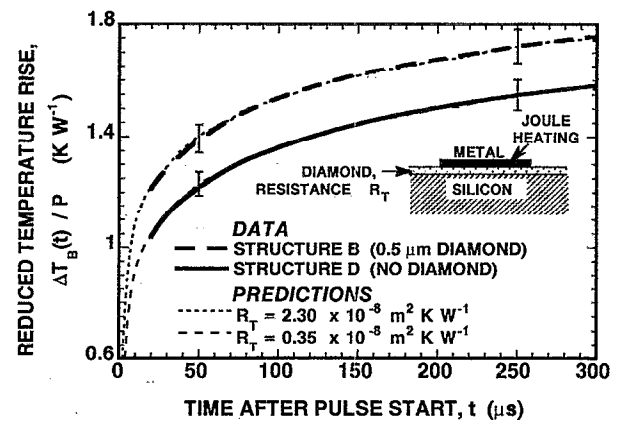


FIG. 3. Reduced absolute temperature rises measured using the Joule-heating method in the metal-diamond-silicon structure B and in a similar metal-silicon structure without diamond, D. Also shown are predictions of the three-dimensional conduction analysis that yield best-fit values of R_T , the thermal resistance for conduction from the metal to the silicon.

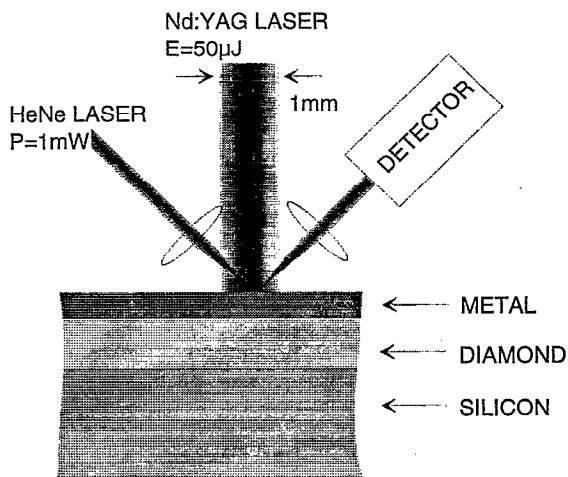


FIG. 4. Schematic of the laser-heating method. The shape of the temperature rise is measured using laser-reflectance thermometry.

C. Laser-heating method

The laser-heating method is similar to a method developed recently to measure the thermal resistance for conduction normal to a thin silicon-dioxide layer bounded by gold and silicon.¹⁶ Heat flux normal to the layered structure is generated by absorption at the gold surface of light from a frequency-doubled neodymium-doped yttrium-aluminum garnet laser, as shown in Fig. 4. The laser power is pulsed with a duration of 6 ns and repetition period of 0.15 s. The gold-surface temperature is probed using laser-reflectance thermometry. Temperature-induced changes in the reflectivity of the gold-layer surface are monitored by detection of the reflected light from a continuous-wave helium-neon laser.

A disadvantage of laser-reflectance thermometry is the extreme difficulty of calibration of the derivative of the gold-layer reflectance with respect to temperature. This problem is overcome through the use of much shorter time scales for the measurement, which cause the shape of the temperature response to be strongly influenced by thermal conduction in the diamond. In contrast to the Joule-heating method, which monitors the temperature rise during a heating pulse for about 100 μ s, the laser-heating method monitors the temperature relaxation after a very brief heating pulse for about 1 μ s. The response shape is sensitive to the conductivity and boundary resistances of the diamond layer because it is observed with a temporal resolution comparable to the time required for thermal diffusion through the metal and diamond, ~ 20 ns.

The measured temperature response shape is interpreted by analyzing transient, one-dimensional conduction normal to the layered structure. The geometry is one dimensional because the lateral extent of the heating laser light is several orders of magnitude larger than the penetration depth of thermal energy into the silicon, ~ 10 μ m, during the measurement. Because of the short time scale, it is necessary to account for the impact of the metal on the transient temperature

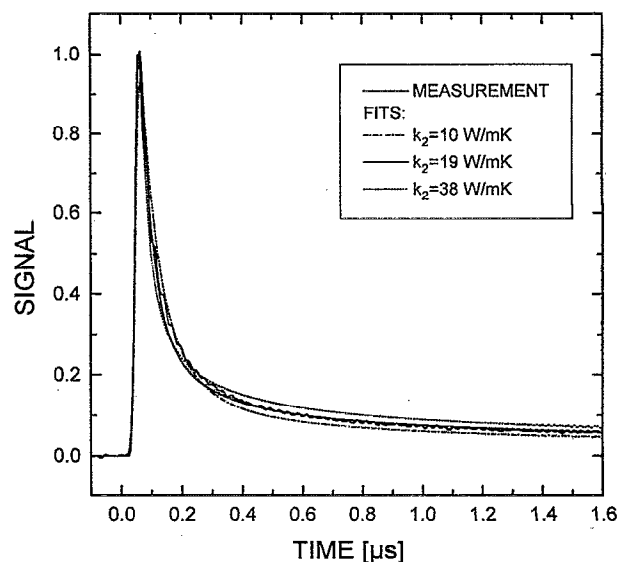


FIG. 5. Normalized temperature rise at the surface of the metal-diamond-silicon structure B induced by the laser-heating method. The shape of the measured temperature rise is fitted using the thermal conductivity of the diamond as a free parameter. The figure contrasts the best fit with two fits that use other values of the conductivity.

response, which is not necessary for the Joule-heating method. Similar to the approximation used to obtain Eqs. (2)–(5) above, the analysis here assumes that the thermal conductivities of the gold, diamond, and silicon are homogeneous and that the resistances at the diamond-silicon and diamond-metal boundaries are negligible. These approximations are more important for the laser-heating method, since the short time scale causes the response to be much more sensitive to nonhomogeneities in the diamond and to boundary resistances. The silicon is modeled as an infinite medium, which is justified by the small ratio of the thermal diffusion depth in the silicon to the silicon thickness. The heating at the gold surface is modeled using a heat-flux boundary condition.

The expected response is calculated from the exact solution to the thermal-conduction equation considering the transfer function of the detection electronics and the temporal shape of the laser pulse. The silicon thermal conductivity and diffusivity are those used for the Joule-heating method above. The response is found to depend on the thickness and heat capacity per unit volume of the gold layer rather than on its thermal conductivity. The gold-layer thickness is measured for each layer from cross-sectional electron micrographs, such as that shown in Fig. 1, and the heat capacity per unit volume of the gold layer is assumed to be that of bulk gold at room temperature, 2.5×10^6 J K⁻¹ m⁻³.

Figure 5 compares the normalized response measured for layer B with fits that use three values of the diamond thermal conductivity, obtained using a sum-of-squares technique. The best fit, which uses $k_2 = 19$ W m⁻¹ K⁻¹, shows good agreement with the measured shape. The disagreement at times near about 200 ns may be due to resistances at the boundaries of the diamond layer or to nonhomogeneities of

the thermal conductivities of the gold or diamond layers, which are not considered by the thermal-conduction analysis. The thermal resistance for conduction normal to the diamond is calculated using $R_T = d_2/k_2$, where d_2 is the diamond layer thickness. The uncertainty of the conductivity k_2 is estimated from the impact of variation of this and other parameters on the quality of the analytical fits. The laser-heating method has the potential to investigate nonhomogeneities in the diamond thermal conductivity, information that cannot be observed using the Joule-heating method due to its longer time scale, but this potential is not investigated here.

III. PREDICTION

The data obtained using the two methods are interpreted using an analysis of transport due to phonons, the carriers of heat in diamond. The predictions consider the nonhomogeneity of the phonon scattering rate internal to the layer and the impact of phonon scattering on the layer boundaries.¹⁷ It is helpful to model total internal phonon scattering rate $1/\tau$ as the sum of three independent scattering rates,

$$[\tau(z, \omega, T)]^{-1} = [\tau_U(\omega, T)]^{-1} + [\tau_{HD}(z, \omega)]^{-1} + [\tau_{GB}(z, \omega)]^{-1}. \quad (6)$$

Terms in Eq. (6) depend on the phonon angular frequency ω , the temperature T , and the position in the diamond with respect to the diamond-silicon interface z . The first term on the right-hand side is due to phonon-phonon Umklapp scattering. The second term on the right-hand side is the sum of phonon scattering rates on defects of type j whose concentrations $c_{HD,j}$ are homogeneously distributed within a given plane located at z ,

$$[\tau_{HD}(z, \omega)]^{-1} = v \sum_{j=1}^J \sigma_j(\omega) c_j(z), \quad (7)$$

where v is the phonon velocity and σ_j is the scattering cross section of the imperfection of type j . The third term on the right-hand-side of Eq. (6) is the phonon scattering rate due to grain boundaries, which depends on the local grain size. The grain size is described here using the characteristic grain dimension $d_G(z)$, which is the average distance between intersections of grain boundaries with a reference line placed on a top-view electron micrograph of a layer of thickness z . Although d_G for almost all CVD diamond layers increases with increasing z , the precise relationship depends strongly on the deposition conditions. For the layers in the present study, which were all fabricated using the same parameters, the following linear dependence of the grain dimension on z is estimated using previously published⁶ top-view electron micrographs of these layers,

$$d_G(z) = d_{G0} + 0.2z. \quad (8)$$

The grain dimension at the interface with silicon d_{G0} is estimated to be of the order of 50 nm.

There is strong evidence that at temperatures above a few K, phonon scattering on localized imperfections concentrated near grain boundaries is more important than scatter-

ing on grain boundaries.^{10,18} The scattering rate due to imperfection concentrations near grain boundaries that are randomly oriented was derived to be¹⁷

$$[\tau_{GB}(z, \omega)]^{-1} = \frac{2v \eta(z, \omega)}{d_G(z)}, \quad (9)$$

where v is the average phonon velocity and the dimensionless grain-boundary scattering strength is

$$\eta(z, \omega) = \sum_{j=1}^J \sigma_j(\omega) n_{GB,j}(z). \quad (10)$$

The number density of imperfections of type j per unit grain-boundary area is $n_{GB,j}$. The parameter η is expected to vary much less strongly within a given layer than τ_{GB} . For simplicity the variation of η within the layer is neglected here. This assumption yielded reasonable agreement between data for the effective conductivity along diamond layers and predictions of the lateral conductivity in layers of thickness between 0.3 and 300 μm .⁶

The scattering rate in Eq. (9) can be made arbitrarily large by increasing the scattering strength at grain boundaries η . But, for the case of conduction normal to layers with ideal columnar grains, i.e., grains with boundaries normal to the silicon-diamond interface, defects at grain boundaries can at most increase the phonon scattering rate to a value comparable to d_G/v . An expression appropriate for conduction normal to layers with an entirely columnar grain structure is¹⁷

$$[\tau_{GB}(z, \omega)]^{-1} = \frac{2v}{\pi d_G(z)} \left(1 + \frac{1}{\exp\left[\left(\frac{\pi}{2}\right)^2 \eta(z, \omega)\right] - 1} \right)^{-1}. \quad (11)$$

If the grain size is sufficiently small, e.g., in the very thin layers in the present work, the scattering on the imperfections very near grain boundaries may dominate over scattering on imperfections within grains. This hypothesis is made more plausible by electron micrographs of diamond grains,¹⁹ which show a much higher concentration of imperfections near grain boundaries than within grains. This approximation is used for the very thin, small-grained layers in the present work, allowing the second term on the right-hand side of Eq. (6) to be neglected.

The first term on the right-hand side of Eq. (1) is modeled using¹⁰

$$[\tau_U(x_\omega, T)]^{-1} = A_U(x_\omega)^2 T^3 \exp\left(\frac{-B_U}{T}\right), \quad (12)$$

where $A_U = 640 \text{ s}^{-1} \text{ K}^{-3}$ and $B_U = 470 \text{ K}$. The dimensionless phonon frequency is $x_\omega = \hbar \omega / (k_B T)$, where $\hbar$ is Planck's constant divided by 2π and k_B is the Boltzmann constant. Imperfections are considered using¹⁰

$$\sigma_1(x_\omega, T) = \frac{V_0^2 x_\omega^4 T^4}{4 \pi v^4} \left(\frac{k_B}{\hbar} \right)^4 \quad (13)$$

for point defects, where $V_0 = 5.68 \times 10^{-30} \text{ m}^3$, and¹⁰

TABLE I. Phonon transport and scattering parameters for CVD diamond.

θ (K)	v (m s ⁻¹)	A_U (s ⁻¹ K ⁻³)	B_U (K)
2030	1.32×10^4	640	470
$n_{GB,1}$ (m ⁻²)	$n_{GB,2}$ (m ⁻²)	D_{RC} (m)	
2.2×10^{20}	1.5×10^{18}	1.4×10^{-9}	

$$\sigma_2(x_\omega, T) = \begin{cases} \frac{\pi D_{RC}^6}{4v^4} \left(\frac{k_B}{\hbar_P}\right)^4 x_\omega^4 T^4 & \text{for } x_\omega < \frac{\hbar_P v}{k_B T D_{RC}}, \\ \frac{\pi (D_{RC})^2}{4} & \text{for } x_\omega \geq \frac{\hbar_P v}{k_B T D_{RC}}, \end{cases} \quad (14)$$

for extended defects, e.g., groups of point defects or small regions with amorphous microstructure. The diameter of extended defects D_{RC} , and the number densities of defects per unit grain-boundary area, $n_{GB,1}$ and $n_{GB,2}$, were calculated previously⁶ from data for thick layers and are given in Table I along with the other phonon scattering and transport parameters in diamond.

Equation (6) describes the phonon scattering rate internal to diamond layers. For layers that are sufficiently thin, phonon scattering on layer boundaries can also be important. To accurately calculate rates of heat transport in thin diamond layers, it is necessary to solve the phonon transport equation of Peierls²⁰ based on the Boltzmann equation, whose boundary conditions describe the interaction of phonons with the interfaces of a layer. To accommodate the internal scattering rate in Eq. (6) the collision integral must be modified using the relaxation-time approximation. A useful approximate approach for solving a transport equation of this type is to enforce energy conservation within each energy level,^{21,22} which in this case is distinguished by the phonon angular frequency ω . While this approach is not strictly correct and may lead to inaccurate predictions of phonon distribution functions, it is expected to yield good predictions of the total phonon heat flux. For this case, the solution to the Peierls-Boltzmann transport equation for conduction normal to a layer is equivalent to that found in

textbooks for photon transport normal to a gray medium with gray, diffuse boundaries.^{21,23} The solution is well approximated by

$$\frac{1}{R_T} = \frac{k_{n,\text{eff}}}{d_2} = \frac{v}{3} \int_0^{\theta/T} \frac{C_V(x_\omega, T) dx_\omega}{d_E(x_\omega, T) + \frac{4}{3} \left(\frac{1}{\alpha_0} + \frac{1}{\alpha_1} - 1 \right)}. \quad (15)$$

To account for nonhomogeneous phonon scattering rate in the layer, the dimensionless layer thickness is¹⁷

$$d_E = \int_0^{d_2} \frac{dz}{v \tau(z, x_\omega, T)}. \quad (16)$$

The transmission coefficients for phonons traveling from within the diamond into the silicon and the titanium are α_0 and α_1 , respectively, and are calculated using the diffuse mismatch theory.¹³ The phonon specific-heat function is

$$C_V(x_\omega, T) = \frac{3k_B}{2\pi^2 v^3} \left(\frac{k_B T}{\hbar_P}\right)^3 \frac{x_\omega^4 \exp(x_\omega)}{[\exp(x_\omega) - 1]^2}. \quad (17)$$

Predictions of R_T in the present work use Eqs. (6), (8)–(10), and (12)–(17). A prediction for the idealized case of a random grain structure is also provided using Eq. (11) rather than Eq. (10).

IV. RESULTS AND DISCUSSION

Table II summarizes the data obtained using the two independent methods. The results are compared with the values of R_T measured for structure D, which has no diamond layer. The data for a given layer are in very good agreement considering the differences in the techniques. An important distinction between the two methods is that the laser-heating method lateral spatial resolution is comparable with the square of the diameter of the probe laser beam, about $4 \mu\text{m}^2$. The Joule-heating method yields a property averaged over the dimensions of the metal microbridge, whose area is several orders of magnitude larger. This distinction is important for layer C, for which the data obtained using the laser-heating method depend strongly on the location of the probe laser-beam focus. A lower bound for the measured conduc-

TABLE II. Thermal resistance data for conduction normal to thin metallized diamond layers on silicon, samples A, B, and C. The data account for the volume and boundary resistances of the diamond. Effective conductivities for conduction normal to the layers are calculated using $k_{n,\text{eff}} = d_2/R_T$, where d_2 is the diamond layer thickness. The indicated range of possible conductivities considers the uncertainty in the thermal resistance data. Also given are thermal resistance data for sample D, which has no diamond layer.

Sample	Diamond thickness d_2 (μm)	Joule-heating method		Laser-heating method	
		Resistance R_T ($10^{-8} \text{ m}^2 \text{ K W}^{-1}$)	Effective conductivity $k_{n,\text{eff}}$ ($\text{W m}^{-1} \text{ K}^{-1}$)	Resistance R_T ($10^{-8} \text{ m}^2 \text{ K W}^{-1}$)	Effective conductivity $k_{n,\text{eff}}$ ($\text{W m}^{-1} \text{ K}^{-1}$)
A	0.2	1.7 ± 0.5	12_{-3}^{+4}	1.3 ± 0.6	15_{-4}^{+13}
B	0.5	2.3 ± 0.5	22_{-4}^{+6}	2.7 ± 0.9	19_{-5}^{+10}
C	2.6	3.5 ± 0.5	74_{-9}^{+13}	less than 5	greater than 50
D	no diamond	less than 0.8	...	0.4 ± 0.1	...

tivity is provided in the table. The upper bound lies within the uncertainty of the data and therefore is not given here.

The resistance R_T increases with increasing layer thickness due to the addition of volume resistance within the diamond layer. The rate of increase with respect to the layer thickness diminishes rapidly, such that increasing the layer thickness by more than an order of magnitude, from 0.2 to 2.6 μm , increases the thermal resistance by little more than a factor of 2, from about 1.5 to $3.5 \times 10^{-8} \text{ m}^2 \text{ K W}^{-1}$. This supports the hypothesis that thermal resistances at the silicon-diamond and metal-diamond boundaries yield a thickness-independent component to the total measured thermal resistance. Another possibility is that a highly imperfect layer near the silicon-diamond interface, such as the ~ 100 -Å-thick amorphous silicon/carbon region observed in electron micrographs,²⁴ yields a large local volume resistance. This resistance can be estimated to be roughly $10^{-8} \text{ m}^2 \text{ K W}^{-1}$,¹⁴ which is consistent with the data reported here. In practice, a highly localized volume resistance near a boundary is indistinguishable from the boundary resistance, such that it is appropriate to define the sum of these as an effective boundary resistance. The total resistance for the thinnest layer, $\sim 1.5 \times 10^{-8} \text{ m}^2 \text{ K W}^{-1}$ is an upper bound for the effective silicon-diamond boundary resistance.

For comparison with previous data, it is helpful to calculate an effective conductivity using $k_{n,\text{eff}} = d/R_T$, where d is the layer thickness. Because R_T may be significantly increased by resistances at the layer boundaries, the effective conductivity $k_{n,\text{eff}}$ is a lower bound for the conductivity internal to the layer. The effective conductivity increases rapidly with increasing layer thickness, from about 14 to 75 $\text{W m}^{-1} \text{ K}^{-1}$ for the 0.2- and 2.6- μm -thick layers, respectively. A similar trend was observed for lateral thermal diffusivities and conductivities in diamond within microns of the deposition interface;²⁵⁻²⁸ but, the magnitude of the effective vertical conductivities measured here for a given layer thickness, which include boundary and volume resistances, are smaller than the lateral conductivities reported elsewhere for comparable layer thicknesses. Thermal diffusivities measured²⁷ along free-standing layers of thicknesses near 0.35 and 5.5 μm , for example, correspond to lateral conductivities of 75 and 150 $\text{W m}^{-1} \text{ K}^{-1}$, respectively. The lower vertical conductivities reported here support the conclusion that an effective silicon-diamond boundary resistance, which would have little or no effect on the lateral conductivity, is important. For conduction normal to thin diamond layers on silicon, this shows that the use of lateral conductivity data can lead to heat-flux predictions that are much too large. This is in stark contrast to the situation for conduction internal to relatively thick layers,¹⁰ for which the lateral conductivity is less than the vertical conductivity.

This trend is governed by the higher concentration of imperfections near the deposition interface, which is the subject of the analysis described in Sec. III. Figure 6 compares the data in Table II with the predictions. The agreement is good for randomly oriented grains with dimensions at the silicon interface between 20 and 50 nm, values that are both consistent with a top-view electron micrograph of thinnest diamond layer used here.⁶ These grain dimensions result in

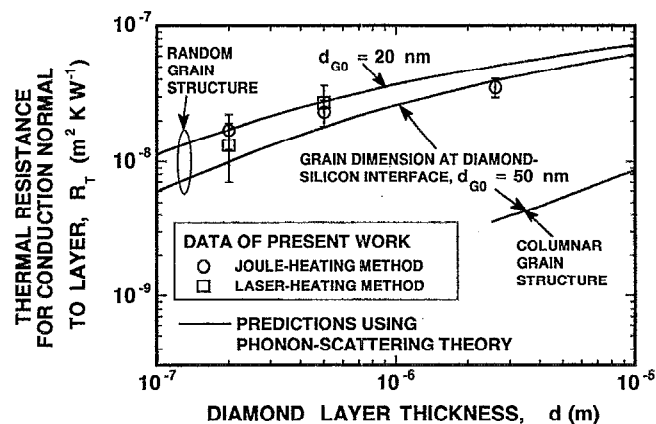


FIG. 6. Thermal resistance for conduction normal to thin metallized diamond layers on silicon. The predictions assume a grain dimension within the layers given by $d_G = d_{G0} + 0.2z$, where z is the separation from the deposition interface. This relationship is consistent with top-view electron micrographs of the layers in the present study.

grain densities per unit area of the diamond-silicon interface that are comparable with the nucleation densities of diamond on silicon observed previously.²⁴ The measurement for layer C is slightly overpredicted by the analysis for randomly oriented grains. This may be due to the transition of the grain structure from random to columnar with increasing layer thickness, which can be observed in the micrograph in Fig. 1. Columnar grains result in a much longer phonon mean free path in the direction normal to layers than randomly oriented grains, which yields a lower thermal resistance for conduction in this direction.

V. CONCLUSIONS

The experimental techniques developed here measure with reasonable certainty the thermal resistances for conduction normal to thin diamond layers. The measured thermal resistance is the sum of the volume resistance within the diamond and the silicon-diamond and metal-diamond boundary resistances. New methods must be developed to determine any one or two of these properties independently. The use of a doped-diamond bridge in the Joule-heating method, for example, has the potential to eliminate the metal-diamond boundary resistance. The short time scale of the laser-heating method yields the potential to investigate boundary resistances and nonhomogeneities in the diamond layer if these are considered by the thermal analysis.

The agreement of the data and predictions in Fig. 6 lend support to the conclusion that an effective silicon-diamond boundary resistance results from the high rate of phonon scattering within the diamond near the interface. This effective resistance appears to be strongly coupled to the grain dimension at the interface. The effective boundary resistance is very important in high-power electronic circuits, containing diamond. A silicon-diamond boundary resistance of $3.3 \times 10^{-8} \text{ m}^2 \text{ K W}^{-1}$, which is comparable to the values measured here, would increase the temperature rise due to pulsed heating in a lateral field-effect transistor by 60% com-

pared with the temperature rise for the case of an ideal diamond-silicon boundary.⁶ The effective thermal boundary resistance is expected to depend on the details of the CVD process. Figure 6 suggests that parameters influencing the nucleation density, which affects the grain dimension near the interface, are important. Decreasing the nucleation density can yield larger grains near the interface, which diminish the phonon scattering rate, but can also result in voids, which impede thermal conduction.

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