Thermal conduction normal to diamond-silicon boundaries

K. E. Goodson,[a] O. W. Käding, M. Rösner, and R. Zachai
Daimler-Benz AG, Materials Research, Postfach 2360, 890134 Ulm, Germany

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Passive diamond layers fabricated using chemical vapor deposition can improve thermal conduction in electronic microstructures. The benefit of using diamond depends strongly on the thermal boundary resistance between active semiconducting regions, where heat is generated, and the diamond. Two independent experimental methods measure the total thermal resistance for conduction normal to 0.2, 0.5, and 2.6 μm thick diamond layers deposited on silicon, providing an upper bound for the effective silicon-diamond boundary resistance. The data agree with predictions that couple the local phonon scattering rate in the diamond to the grain size. © *1995 American Institute of Physics.*

Diamond is an excellent thermal conductor and an electrical insulator at room temperature, making it ideal for passive applications in electronic systems. Much research aims to improve the conduction cooling of high-power semiconductor devices by replacing conventional dielectric mounts, often made of aluminum oxide, with diamond plates fabricated using conventional chemical vapor deposition (CVD).[1–4] This approach suffers from the need to attach the diamond plates to devices using interfacial layers, which can strongly impede the flow of heat.[5] Promising alternatives deposit diamond directly on silicon, for which nucleation can be achieved using a bias voltage between the silicon and a microwave-frequency plasma.[6–8] This approach is most beneficial if a low thermal resistance is achieved for conduction normal to the diamond-silicon boundary.

While thermal conduction in diamond layers has been the subject of much research,[9] conduction through the boundaries of diamond with other materials has received little attention. Phonon scattering on imperfections near the boundary of diamond deposited on silicon is expected to yield an effective boundary resistance of the order of 5×10^{-8} $\mathrm{m^2\,K\,W^{-1}}$, which diminishes the improvement due to the use of diamond in novel high-power electronic microstructures.[5] Previous research measured thermal conductivities and diffusivities in the direction *along* diamond layers as thin as 0.3 μm[10–13] but these data provide little information about the effective boundary resistance, which must be investigated using heat flow in the direction normal to the interface. Data for the effective boundary resistance are needed.

Several methods available for this measurement use joule heating and electrical-resistance thermometry in patterned metal microbridges.[14] These techniques have the advantage that they induce quantitatively known heat fluxes that resemble those in electronic microstructures. The steady-state parallel-microbridge method[15] was adapted to measure thermal resistances as small as 5×10^{-8} $\mathrm{m^2\,K^{-1}\,W^{-1}}$ for conduction normal to thin dielectric layers at room temperature.[16,17] Smaller resistances can be measured using transient methods, which diminish the heated volume and therefore the uncertainty due to unnecessary temperature rise in the substrate. Laser heating and laser reflectance thermometry measured thermal resistances using time scales as short as a few hundred nanoseconds.[18] This letter reports on measurements of the thermal resistance for conduction normal to thin diamond layers using two independent, transient methods. One uses joule heating in microbridges and the other uses laser heating.

The experimental methods are described in detail in an accompanying publication.[19] The joule-heating method monitors the temperature rise during a current-induced heating pulse in a patterned metal microbridge for ~100 μs. The current is also used to measure the transient electrical resistance of the microbridge, from which its temperature is calculated using calibration data. The thermal resistance for conduction normal to the diamond is extracted by analyzing transient, three-dimensional thermal conduction in the structure. The laser-heating method uses laser-reflectance thermometry to monitor the transient temperature at the metal surface for about 1 μs after a very brief laser-heating pulse, an approach used previously to investigate conduction in thin silicon-dioxide layers.[18] The thermal resistance for conduction normal to the diamond is extracted using the shape of the measured response and a solution to the transient thermal-conduction equation in the structure.

Diamond layers with thicknesses 0.2, 0.5, and 2.6 μm, referred to here as A, B, and C, respectively, are deposited on (100) silicon using microwave-plasma assisted CVD, as described previously.[8] A voltage bias between the substrate and the plasma source induces nucleation, which eliminates the need for conventional procedures such as scratching the substrate. The layers are metallized with 10 nm of titanium and 300 nm or more of gold. Figure 1 is a cross-sectional micrograph of the thickest layer C, from which the approximate internal microstructures of the thinner layers A and B can be deduced. The micrograph shows the increase of the grain size with increasing height above the substrate.

The data for the total thermal resistance R_T, for conduction normal to diamond layers A, B, and C are presented in Table I and plotted as a function of layer thickness d in Fig. 2. The Table also includes the measured thermal resistance for sample D, which has no diamond, as a reference. The data obtained using the Joule heating and laser-heating meth-

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[a] Present address: Stanford University, Mechanical Engineering Department, Stanford, CA 94305-3030.

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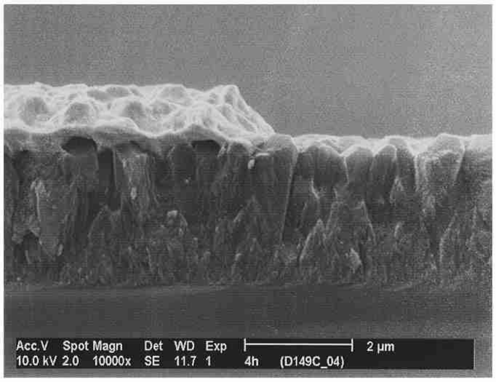

FIG. 1. Cross section of diamond layer C, of thickness 2.6 μm, deposited on a (100) silicon substrate. Also visible is the patterned gold-titanium metallization.

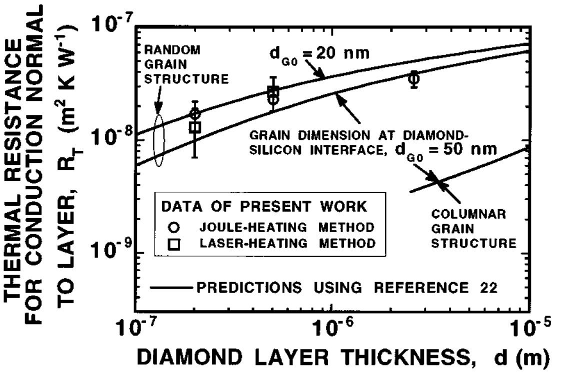

FIG. 2. Thermal resistance for conduction normal to thin metallized diamond layers on silicon. The predictions assume a grain dimension within the layers given by $d_G = d_{G0} + 0.2z$, where z is the separation from the deposition interface. This relationship is consistent with top-view electron micrographs of the layers in the present study.

ods are consistent. The uncertainty of the thermal resistance for the Joule-heating method is $\sim 0.5\times 10^{-8}$ $m^2\,K\,W^{-1}$, which only allowed the measurement of an upper bound for sample D. The sensitivity of the shape of the response for the laser-heating method to the total thermal resistance R_T diminishes with increasing layer thickness, making possible the measurement only of a lower bound resistance for sample C.

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 3.5×10^{-8} $m^2\,K\,W^{-1}$. This supports the hypothesis that thermal resistances at the silicon-diamond and metal-diamond boundaries yield a thickness-indendent component to the total measured thermal resistance. Another possibility is that a highly imperfect region near the silicon-diamond interface, such as the $\sim$100 Å thick amorphous silicon/carbon region observed in electron micrographs,[20] yields a large local volume resistance. This resistance can be estimated to be roughly 10^{-8} $m^2\,K\,W^{-1}$,[16] 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, $\sim 1.5\times 10^{-8}$ $m^2\,K\,W^{-1}$, 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 $k_{n,\mathrm{eff}} = d/R_T$, where d is the layer thickness. Because R_T may be significantly increased by resistances at the layer boundaries, the effective conductivity $k_{n,\mathrm{eff}}$ 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 W m^{-1} 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[11–13,21] 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 measured[13] along free-standing layers of thicknesses near0.35 and 5.5 μm, for example, correspond to lateral conductivities of $\sim$75 and 150 W m^{-1} 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 sili-

TABLE I. 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 $k_{n,\mathrm{eff}} = d/R_T$, where d is the diamond layer thickness. The range of possible conductivities considering the uncertainty in the thermal resistance are indicated in small print. Also given are thermal resistance data for sample D, which have no diamond layers.

		Joule-heating method		Laser-heating method	
Sample	Diamond thickness, d, μm	Resistance, R_T, 10^{-8} $m^2\,K\,W^{-1}$	Effective conductivity, $k_{n,\mathrm{eff}}$, W m^{-1} K^{-1}	Resistance, R_T, 10^{-8} $m^2\,K\,W^{-1}$	Effective conductivity, $k_{n,\mathrm{eff}}$, W m^{-1} K^{-1}
A	0.2	1.7+/−0.5	12^{+4}_{-3}	1.3+/−0.6	1215^{+13}_{-4}
B	0.5	2.3+/−0.5	22^{+6}_{-4}	2.7+/−0.9	19^{+10}_{-5}
C	2.6	3.5+/−0.5	74^{+13}_{-9}	<5	>50
D	no diamond	<0.8	⋯	0.4+/−0.1	⋯

con, 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,[9] for which the lateral conductivity is less than the vertical conductivity.

In order to help interpret the new data, they are compared with predictions[22] that couple the local internal phonon scattering rate to the nonhomogeneous characteristic grain dimension, which is the average separation between grain boundaries that intersect a line placed on a top-view electron micrograph. For simplicity, scattering on imperfections very near grain boundaries was assumed to dominate over scattering on imperfections within grains, a hypothesis that finds some support from transmission electron micrographs.[23] The *grain-boundary scattering strength*, a dimensionless functioni of the scattering cross sections and the number densities per unit grain-boundary area of imperfections, was assumed not to vary within a given layer. In contrast, the characteristic grain dimension increased with increasing spatial coordinate z, the height above the deposition interface. Using top-view electron micrographs, the relationship, for the layers in the present study is estimated to be $d_G = d_{G0} + 0.2z$, where d_{G0} is $\sim$50 nm. The impact of phonon scattering on layer boundaries was determined using an approximation to the solution of the Peierls–Boltzmann phonon transport equation for conduction normal to layers with a nonhomogeneous internal scattering rate.[22]

The predictions are compared with the data in Fig. 2. The data agree well with predictions that assume a random grain structure and values of d_{G0} between 20 and 50 nm. This is consistent with top-view electron micrographs of the thinnest layers in this study, presented elsewhere,[5] which show randomly oriented grains with dimension of the order of 50 nm. The minimum grain dimensions used here indicate grain densities per unit area of the diamond-silicon interface that are comparable with the nucleation densities of diamond on silicon as observed previously.[20] The resistance measured for the thickest 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. To estimate the impact of this transition, predictions were also developed that account for conduction normal to layers with ideal columnar grains.[22] The unobstructed path of phonons between the upper and lower layer boundaries results in a much lower thermal resistance, as shown in Fig. 2.

The data reported here are important for the thermal engineering of electronic microstructures containing CVD diamond. Previous research[5] showed that a resistance of $3.3 \times 10^{-8}\ \mathrm{m^2\,K\,W^{-1}}$ at the silicon-diamond boundary, whcih is comparable to the values measured here, can increase the temperature rise due to pulsed heating in a lateral field-effect transistor by 60% compared with the temperature rise for the case of an ideal diamond-silicon boundary. The effective thermal boundary resistance is expected to depend on the details of the CVD process. Figure 2 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.

The thermal resistances reported here for the direct silicon-diamond interface are less by more than an order of magnitude than those estimated for diamond-silicon attachments based on metallic alloys,[5] such as that developed for laser systems.[24] This shows that direct diamond deposition on semiconducting substrates is a promising alternative to the attachment of diamond plates.

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