Experimental Investigation of Metal-Diamond Thermal Interface Conductance With Different Diamond Surface Terminations

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ABSTRACT

Synthetic diamond has potential as a heat spreading material due to its uniquely high thermal conductivity. In small-scale devices, interfaces can dominate the resistance to heat transport, and thus play an important role in determining device performance. Here we use transient thermoreflectance techniques to measure the thermal interface conductance at metal-diamond interfaces. We study single crystal diamond samples with various surface terminations. We measure thermal interface conductance values over a range of temperatures from 88 K to 300 K, and find roughly 60 percent higher thermal interface conductance between Al and oxygenated diamond samples as compared to hydrogen terminated samples. The results reported here will be useful for device design and for advancing models of interfacial heat transport.

BACKGROUND

As the power density of integrated circuits continues to increase, thermal management has emerged as a limiting factor to further increases in device performance. Diamond has an exceptionally high thermal conductivity, around 2000 W/m-K at room temperature, and thus is attractive as a possible heat spreader if it can be formed into a metal matrix composite with an appropriate coefficient of thermal expansion [1-3]. Diamond also has favorable electrical properties that make it attractive as a possible transistor material [4].

In small scale devices, interfaces play an important role in determining performance. Numerous studies of the electrical properties, and in particular the surface conductivity, of diamond interfaces have been reported [5-11]. It was found that the surface termination of diamond has a significant impact on the surface electrical properties and the interfacial electronic properties with various metals [8-11]. There have also been studies of metal-diamond adhesion that indicate diamond surface termination influences adhesion strength [12-15].

Very few studies of thermal interface properties between metal and diamond have been reported. Measurements have been reported for the interface conductance between isotopically enriched diamond and Al, Au, Pb and Ti [16], as well as for the interface conductance between H-terminated diamond and Bi and Pb [17]. These measurements were performed using picosecond optical techniques similar to the technique employed in this study. To our knowledge no previously reported study of thermal interface conductance exists that considers different surface terminations.

In addition to practical importance, experimental study on thermal interface conductance has value for understanding heat transfer across interfaces. The origin of Kapitza resistance [18] has been studied extensively [19-22], but theory continues to weakly correlate to experimental measurements. The prevailing models in the literature are the diffuse mismatch model (DMM) proposed by Swartz and Pohl, and the acoustic mismatch model (AMM) [19]. Modifications to the DMM to include electron-phonon coupling [21] and the possible effects of inelastic phonon scattering at the interface [22] have been considered. An experimental study of the effects of surface chemistry on the thermal interface conductance will complement further theoretical studies.

Here we report measurements of the thermal interface conductance between Al and two samples of single crystal diamond with varying surface terminations: an H-
terminated sample and a sample with some amount of O-termination.

EXPERIMENT

Single crystal diamond samples with different surface terminations were prepared by Apollo Diamond Inc. The samples were grown homo-epitaxially on diamond wafers and then removed from the wafers. All samples are of IIA purity, with 1 ppm nitrogen content as the primary impurity. The samples were scaife polished to have a RMS surface roughness of approximately 20 nm. The crystal orientation of the polished side is (1 0 0). After polishing, one sample was oxidized by heating in air at 500 C [23]. Another sample was hydrogen terminated by exposure to a hydrogen plasma at 700 C [24].

The hydrophobicities of the as-received samples were tested by observing the contact angle of a water droplet with the surface. Oxygen terminated diamond is more hydrophilic than hydrogen terminated diamond [25]. The results, shown in Figure 1, clearly show that the oxygen-baked sample is more hydrophilic, suggesting the presence of oxygen groups on the surface. Following a drop test, the as-received samples were cleaned with isopropanol and coated with a 100 nm layer of Al. The Al was sputter deposited at 1 A/s at pressure of 3 mTorr.

![Figure 1: Water drop test results on (a) H-terminated and (b) oxygenated diamond samples.](image)

Measurements of the thermal boundary conductance were carried out using pump and probe transient thermoreflectance (TTR), a method widely used for such studies [16,17]. A pulsed laser heats (pumps) the metal surface, and a subsequent beam measures (probes) the change in surface reflectance due to the heating. Figure 2a shows a simplified schematic. One example of the measured reflectance signal is shown in Figure 2b, where the horizontal axis corresponds to the time after pulsed heating of the surface. The inset in Figure 2b shows the initial 200 ps of signal in which acoustic echoes across the metal film are apparent. Due to the large acoustic mismatch between diamond and Al, many echoes are present.

![Figure 2: (a) Experimental schematic. (b) Measured signal.](image)

Our TTR setup uses a Ti-Sapphire laser that emits a train of 800 nm pulses at 80 MHz with a pulse width of 150 fs. We heat the sample using a frequency doubled, 400 nm, pump beam with a diameter of 60 μm, and measure the surface reflectance using an 800 nm probe beam with a diameter of 10 μm. Measurements were performed over a temperature range from 88 K to 300 K. Further details about our system can be found elsewhere [26, 27].

RESULTS

Figure 3 shows the measured thermal interface conductance values, along with other reported literature values [20]. For comparison, we have also plotted the prediction of the DMM [19].

![Figure 3: Results for the thermal interface conductance between Al and diamond.](image)
The results of this study are in line with previously reported results [20], and in the range predicted by the DMM. A clear difference exists in the thermal interface conductance of oxygenated and H-terminated diamond. Oxygenated diamond shows an increase in thermal interface conductance of approximately 60 percent over H-terminated diamond.

SUMMARY

We report measurements of the thermal interface conductance between Al and single crystal diamond samples with different surface terminations. Oxygenated diamond has approximately 60 percent higher thermal interface conductance than H-terminated diamond. These results demonstrate the importance of surface chemistry to thermal interface conductance and have implications for device design and future theory work.

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