A Reexamination of Phonon Transport Through a Nanoscale Point Contact in Vacuum

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Using a silicon nitride cantilever with an integral silicon tip and a microfabricated platinum–carbon resistance thermometer located close to the tip, a method is developed to concurrently measure both the heat transfer through and adhesion energy of a nanoscale point contact formed between the sharp silicon tip and a silicon substrate in an ultrahigh vacuum atomic force microscope at near room temperature. Several models are used to evaluate the contact area critical for interpreting the interfacial resistance. Near field-thermal radiation conductance was found to be negligible compared to the measured interface thermal conductance determined based on the possible contact area range. If the largest possible contact area is assumed, the obtained thermal interface contact resistance can be explained by a nanoconstriction model that allows the transmission of phonons from the whole Brillouin zone of bulk Si with an average finite transmissivity larger than 0.125. In addition, an examination of the quantum thermal conductance expression suggests the inaccuracy of such a model for explaining measurement results obtained at above room temperature. [DOI: 10.1115/1.4025643]

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Introduction

Thermal transport at nanometer scale point constrictions and interfaces is a fundamental problem that is important for a number of existing and emerging technologies. The operating temperature of vertical nanowire electronic devices [1] is limited by the thermal resistance at the nanoscale junction between the nanowire and the substrate. The performance of thermal interface materials based on vertical carbon nanotube arrays is limited by the thermal resistance at the junction between the nanotube and the mating surface [2–4]. In addition, the spatial resolution or bit size of scanning thermoelectric microscopy [5] and thermally assisted magnetic recording [6] methods are determined by the temperature distribution at the nanoscale point contact between a sharp tip and a planar surface. As of today, only a few measurement results of thermal resistances at nanoscale constrictions and interfaces are available [7–14]. Moreover, although there have been extensive theoretical studies of contact thermal resistance between two solids, most of the existing analytical models have been developed for macro to microscale contacts [15,16], whereas mechanisms of phonon transmission through nanoscale contacts remain elusive despite a number of recent studies [12,17–25]. For example, in a new model proposed in a recent work [12], nanoscale contacts are treated as an aggregation of independent and spatially separated atomic contacts [17]. The ballistic thermal conductance per phonon polarization of each atomic contact is taken to be the universal quantum thermal conductance, which is the ballistic thermal conductance of one one-dimensional (1D) channel at sufficiently low temperatures. Because of the use of the quantum thermal conductance expression, this model is accurate only when the temperature is sufficiently low and phonon transmission is allowed for only the lowest lying 1D phonon subbands with vanishing transverse wavevector components. In contrast, phonon modes from the entire Brillouin zone of the bulk crystal may pass through a constriction with a finite mode-dependent transmissivity in the nanoconstriction models [15,19–22,24,26].

Here, we report a measurement of the thermal resistance of a nanoscale contact between a silicon tip and a silicon substrate in ultrahigh vacuum (UHV) of $10^{-8}$ Pa. In the experiment, the temperature of and force on a sharp, heated Si tip are measured as a function of height above a Si substrate in a UHV atomic force microscope (AFM), and the adhesion energy is determined from the calibrated force-distance curves. Given the uncertainty in contact area, we show that for the upper limit of contact area the measurement results can be explained by the constriction model [19,27], whereas the quantum thermal conductance expression [12] is inaccurate for describing the measurement results at above room temperature. For the lower limit of contact area neither model can be used to explain the experimental results in this work. In addition, near field thermal radiation is found to be negligible compared to phonon conductance for the nanoscale tip-substrate contact geometry investigated here.

Theoretical Background

Although both the constriction model and the quantized point contact model have been discussed extensively in the literature, it can be useful to reexamine the origins of both models, especially the assumptions and conditions that are needed to obtain the simplified quantum thermal conductance expression. For a conductor bridging two thermal reservoirs with a small temperature difference, the Landauer approach can be used to obtain the following expression of the thermal conductance between the two reservoirs [28]

$$G = \sum_p \frac{1}{L} \sum_{k_{\text{max}}} k_{\text{max}} \sum_{-k_{\text{max}}} k_{\text{max}} \sum_0 \alpha g_v \hbar c \frac{dp(\omega, T)}{dt}$$  \hspace{1cm} (1)

where $L$ is the length of the system along the transport direction, which is parallel to the coordinate $x$ and perpendicular to
coordinates \( y \) and \( z \) is the mode-dependent transmission coefficient, \( v_i \) is the phonon group velocity component along \( x \), \( \alpha \) is the phonon angular frequency, \( k \) is the phonon wavevector, \( h \) is the reduced Planck constant, \( \eta = [e^{\omega/T} - 1]^{-1} \) is the Bose-Einstein distribution, \( k_B \) is the Boltzmann constant, and \( T \) is the absolute temperature. The subscript \( p \) is used to denote each of the phonon polarizations, and the limits of summation \( k_{\text{max}} \) are defined by the Brillouin zone boundary.

The summation over \( k \) can be changed into the following integration in the frequency domain over a one-dimensional (1D) energy subband

\[
G = \sum_{k_{\text{max}}} \frac{\hbar k T}{\pi x^2} \int_{\text{max}}^{\text{min}} x e^{x} (e^{x} - 1)^{-2} dx
\]

where \( x = \hbar \omega / k T \), \( x_{\text{max}} = \hbar \omega_{\text{max}} / k T \), \( x_{\text{max}} = \hbar \omega_{\text{max}} / k T \), \( k_{\text{max}} \) for each 1D subband specified by \( n \), \( k \), and \( \omega \). For a 1D subband satisfying the conditions of \( x_{\text{max}} = 0 \), \( x_{\text{max}} = \infty \), and \( x = 1 \), the integration yields a value of \( \pi^2/3 \), so that the thermal conductance contribution of this 1D subband becomes

\[
G_0 = \frac{\pi^2 k_B T}{3h}
\]

which is the universal quantum of thermal conductance [28]. Only the lowest few 1D acoustic phonon subbands with vanishing \( k_z \) and \( k \) satisfy the condition of \( \omega_{\text{max}} = 0 \) and \( x_{\text{max}} = 0 \). Therefore, \( x_{\text{max}} = \infty \), and \( \omega_{\text{max}} \) for each of the three acoustic 1D subbands with \( \omega_{\text{max}} = 0 \) are populated. Thus, the thermal conductance approaches \( 3G_0 \) in the ballistic limit and low temperature limit, where \( N \) is the number of the acoustic 1D subbands with \( \omega_{\text{max}} = 0 \).

For an earlier measurement of phonon transport across nanoscale constrictions patterned in a SiN beam, only the four lowest acoustic 1D subbands with \( \omega_{\text{max}} = 0 \) are excited at temperatures below 600 mK [7]. These four subbands include one dilatational, one torsional, and two flexural degrees of freedom of a 1D wire. At \( T < 600 \text{ mK} \), it is adequate to assume \( x_{\text{max}} \) approaches infinity so that each SiN constriction contributes \( 4G_0 \) to the measured thermal conductance. As temperature increases to the range between 1 K and 6 K, the measured thermal conductance of each constriction exceeds \( 4G_0 \) and exhibits the \( T^2 \) dependence of the low temperature specific heat of bulk crystals because of the excitation of modes with \( k_0 > \pi/L_x \) and \( k_0 > \pi/L_z \).

For the rather high temperature range of the measurements reported in this work and in Ref. [12], \( x_{\text{max}} \) is finite so that the accuracy of the low-temperature quantum thermal conductance expression (Eq. 3) needs to be examined carefully. For the longitudinal acoustic (LA) branch along the \( \Gamma-X \) high symmetry direction of bulk Si, \( x_{\text{max}} \) is still only 1.36 at 433 K, the measurement temperature of Ref. [12]. Consequently, the \( 3G_0 \) value is a factor of 4.3 larger than the calculated ballistic thermal conductance contribution from the one LA and two transverse acoustic 1D subbands propagating along the \( \Gamma-X \) direction of bulk Si, i.e., \( k_z = k_L = 0 \), and a factor of 3.4 larger than the calculated ballistic thermal conductance of these three acoustic 1D subbands and three additional optical 1D subbands with \( k_z = k_L = 0 \) in Si at 433 K. As shown in Fig. 1, the temperature dependence of these two results is qualitatively similar to that of the reported ballistic thermal conductance of a monatomic chain [20,25], where the atomic mass, interatomic bonding and spacing are assumed to be similar to those in bulk Si, and atomic motions are restricted to be longitudinal or dilational modes. In a realistic Si chain or wire, there exist two additional transverse or flexural polarizations, as well as a torsional polarization if the chain cross section consists of several or more atoms. The \( x_{\text{max}} \) of these polarizations is considerably lower than the longitudinal modes. In addition, surface effects can reduce the \( x_{\text{max}} \) values for each of the three of four lowest 1D acoustic subbands in a realistic Si chain with decreasing diameter [30–34]. For a Si nanowire of a cross section width of 2 nm [32], \( x_{\text{max}} \) for the dilatational modes with the highest \( \omega_{\text{max}} \) is only about 0.137 (0.198) at \( T = 433 \text{ (300) K} \). Consequently, the \( 4G_0 \) value is a factor of 24.3 larger than the ballistic thermal conductance contribution from the four lowest lying acoustic 1D modes calculated from Eq. (2) at \( T = 433 \text{ K} \) for the 2 nm width Si nanowire, and a factor of 17.8 larger at 300 K.

In addition, the \( G_0 \) expression of Eq. (3) has been derived for the case of strictly 1D phonon transport at low temperature, and can become inaccurate for the atomic contact geometry. For a constriction with the width in the range between \( \lambda_F/2 \) and \( \lambda_F \) of electrons, where \( \lambda_F \) is the Fermi wavelength, a calculation has shown that the ballistic electrical conductance is the quantum electrical conductance when the constriction length is about \( \lambda_F \) or longer [35]. As the constriction length is reduced to zero, the calculated electrical conductance can increase to be up to a factor of two higher than the quantum electrical conductance at the same constriction width range, while still exhibiting quantization steps with increasing constriction width. This increase can be attributed to partial transmission of additional modes with finite \( k_z \) and \( k_L \) incident on the constriction from different angles. Although transmission of additional phonon modes with finite \( k_z \) and \( k_L \) can help to increase the thermal conductance across an atomic contact, the thermal conductance calculated by Panzer and Goodson [23] and the conduction electron thermal conductance across the junction between a 3D Si-like lattice and a 1D Si-like monatomic chain with three degrees of freedoms is still a factor of 11.8 lower than the \( 3G_0 \) value at room temperature, because of a transmission coefficient that generally decreases with decreasing frequency in addition to finite \( x_{\text{max}} \) values for Si at room temperature.

In the constriction model [15], all 1D subbands with nearly continuous \( k_z \) and \( k_L \) distributions in the thermal reservoirs are allowed to be transmitted through the constriction with


Experimental Method

In order to measure the thermal resistance of a nanoscale point contact, we have modified a commercial atomic force microscopy (AFM) probe (Veeco MSNL-10, Cantilever Type C), which consists of a Si tip on a 510 nm thick SiN cantilever and coated on the back-side with a thin Ti adhesion layer and 50 nm Au. Using a focused Ga\(^+\) ion beam, the metal back-side of the cantilever was patterned into two separate leads, between which a \(\sim 100\) nm thick layer of Pt–C was deposited by ion-beam induced metal deposition, as shown in Fig. 2. The electrical resistance of the Pt–C resistor, \(R_{\text{Pt-C}}\), is 1.55 \(\Omega\) and the resistance of both Au leads, \(R_{\text{Au}}\), is about 37 \(\Omega\). The temperature-dependence of the electrical resistance was measured with thermocouples attached to the cantilever mount inside a box furnace to ensure isothermal conditions. The total electrical resistance \(R\) is thus dominated by \(R_{\text{Pt-C}}\) and decreases linearly with increasing temperature (Fig. 2). During the thermal measurement, the AFM cantilever was placed into an Omicron AFM chamber under UHV conditions (\(\sim 10^{-8}\) Pa) to eliminate heat transfer through the air and liquid meniscus layers present under atmospheric conditions. We first measured the total Joule heat dissipation, \(dQ_{\text{th}}/dT\), that is, \(R \left( V_{\text{th}}^2 - Q_{\text{th}} \right)\), using its use as both an electrical heater and resistance thermometer (RT). Before a small gap was cut in the Au leads, we have measured the resistance of the Au leads inside the box furnace at different temperatures to obtain \(dR_{\text{Au}}/dT = 0.073\) \(\Omega\) \(K^{-1}\). After the cutting and the deposition of the Pt–C resistor, we obtained the total \(dR/dT = -1.074\) \(\Omega\) \(K^{-1}\). The difference of these two values can be used to calculate \(dR_{\text{Pt-C}}/dT = -1.147\) \(\Omega\) \(K^{-1}\).

During the thermal measurement, the AFM cantilever was placed into an Omicron AFM chamber under UHV conditions (\(\sim 10^{-8}\) Pa) to eliminate heat transfer through the air and liquid meniscus layers present under atmospheric conditions. We first measured the thermal conductance of the cantilever when the tip was not in contact with the substrate. In the measurement, a direct current, \(I_{\text{dc}}\), is supplied to the Pt–C resistance thermometer at the tip of the cantilever, dissipating a Joule heat \(Q_b = I_{\text{dc}}^2 (R_{\text{Pt-C}} - R_{\text{Au}})\) in the Pt–C resistance thermometer, and \(Q_b = I_{\text{dc}}^2 R_{\text{Au}}\) in the two Au leads leading to the Pt–C resistor, each on top of a 266 \(\mu\)m-long cantilever beam. The voltage drop, \(V_{\text{dc}}\), and current are measured as \(I_{\text{dc}}\) is ramped from 0 to \(-I_{\text{dc,max}}\) to \(+I_{\text{dc,max}}\) and back to 0 (Fig. 3(a)). The current-voltage data can be fit with a third-order polynomial, \(V_{\text{dc}}(I_{\text{dc}}) = a_0 + a_1 I_{\text{dc}} + a_2 I_{\text{dc}}^2 + a_3 I_{\text{dc}}^3\), which is used to determine \(R\) as a function of \(I_{\text{dc}}\), that is, \(R = [V_{\text{dc}}(I_{\text{dc}}) - a_0]/I_{\text{dc}}\). The resistance obtained by fitting \(V_{\text{dc}}(I_{\text{dc}})\) match well with those obtained directly as \(V_{\text{dc}}/I_{\text{dc}}\) as shown in Fig. 3(b). The parabolic dependence of the resistance on the heating current verifies that the measured electrical resistance change is caused by the temperature-dependence of the electrical resistance. At different \(I_{\text{dc}}\) values, the total measured resistance change,
\[ \Delta R = R(l_{dc}) - R(l_{ac} = 0), \] 

is comprised of changes in the Pt–C RT and in the Au leads

\[ \Delta R = \frac{dR_{Pt-C}}{dT} \Delta T_b + \frac{dR_{Au}}{dT} \Delta T_b \]  

(6)

where \( \Delta T_b \) is the temperature rise at the Pt–C RT and \( \Delta T_b \) is the average temperature rise along the cantilever beams.

As a general solution, we can express the temperature profiles for the case that the tip is in contact with the substrate. As illustrated in Fig. 4, heat flows to the substrate through this thermal resistance, \( R_s \), and to the cantilever mount through both supporting beams, \( R_b = L/(2\kappa_b A) \), where \( L, A, \) and \( \kappa_b \) are the length, cross section, and thermal conductivity of one cantilever beam. Due to heat generation in the leads and the Pt–C RT, the temperature rise of the Pt–C RT and the average temperature rise in the beams can be expressed as

\[ \Delta T_b = \left( Q_b + \frac{1}{2} Q_h \right) \left( R_b^{-1} + R_c^{-1} \right)^{-1} \]  

(7a)

\[ \Delta T = \frac{Q_b (R_c^{-1} + R_b^{-1})^{-1}}{2} + \frac{Q_b R_b}{12} \left( \frac{R_b + 4R_c}{R_b + R_c} \right) \]  

(7b)

respectively. For the out-of-contact case \( R_s = \infty \), and we can obtain the thermal resistance of the two cantilever beams from the measured electrical properties and Joule heat dissipation as

\[ R_b = \frac{\Delta R}{\frac{dR_{Pt-C}}{dT} \left( Q_b + \frac{1}{2} Q_h \right) + \frac{dR_{Au}}{dT} \left( \frac{1}{2} Q_b + \frac{1}{3} Q_h \right)} \]  

(8)

We have used this approach to measure thermal resistance of the cantilever to be \( R_b = (6.24 \pm 0.02) \times 10^4 \text{K W}^{-1} \), in agreement with the thermal conductivity values reported in the literature for SiNx and Au thin films [8,36–38].

To measure the temperature drop at the cantilever end when the tip is brought into contact with a bare \( p \)-type Si (100) substrate at \(~300 \text{K} \), we couple a small sinusoidal current, \( i_{ac} = 0.5 \mu \text{A} \) at frequency \( f = 2.5 \text{kHz} \) to a fixed \( I_{dc} \) in the Pt–C resistor. The resistance of the Pt–C sensor and its two lead wires is obtained as \( R = v_{ac}/I_{ac} \), where \( v_{ac} \) is the measured first-harmonic (1\( f \)) component of the voltage drop of the Pt–C resistor. The as-measured \( R = v_{ac}/I_{ac} \) can vary with \( I_{dc} \) because of the product between \( i_{ac} \) and the steady-state component in the heating-induced resistance change (\( \Delta R \)), as well as that between \( I_{dc} \) and the 1\( f \) component in \( \Delta R \) caused by the 1\( f \) component in the temperature rise [39]. We have measured the resistance change as a function of frequency and determined 2.5 kHz to be faster than the thermal response of the cantilever (Fig. 5), estimated to be on the order of 1 ms. At this high frequency, the \( i_{ac} \) component caused negligible 1\( f \) component in the cantilever temperature rise, so that the as-measured \( R \) can be used to obtain the steady-state component of \( \Delta R \) [39].

Concurrent with the thermal conductance measurement, we measure the cantilever beam deflection using a laser beam. We have measured the resistance change induced in the cantilever by the laser and find that there is a negligible temperature rise \( [\Delta T_b = \Delta R/(dR_{Pt-C}/dT + 1/dR_{Au}/dT) < 75 \text{mK}] \) for laser power set points below 22% of maximum power \( (P_{laser,max} < 7 \text{mW}) \), as shown in Fig. 6. For this experiment, we use a laser power set point of 17%. Figure 7 shows the normal force and electrical resistance change versus vertical height measured concurrently for a fixed heating power of 53 \( \mu \text{W} \) on a single probe, corresponding to an out-of-contact temperature rise of 33 K. To ensure steady-state conditions, the vertical height, \( z \), is held constant for 10 s before \( R_s \), the normal force, \( F_z \), and values are recorded. The vertical height is changed by 4 nm between adjacent measurement points. The electrical resistance of the electrically heated Pt–C RT changes abruptly when the Si tip is brought into and out of contact with the flat Si substrate.

As shown in Fig. 8, the sudden total electrical resistance change at the exact points where the Si tip snaps-to and pulls-off contact \( (\Delta R_{contact} = \Delta R_{snap} – \Delta R_{pull-off}) \) for different Joule heating powers extrapolates to 0.20 \( \Omega \) at 0 W, in accordance with our observation that \( \Delta R_{contact} \) is less than the noise in the measured resistance when an unheated tip makes contact with the substrate. Hence, the observed resistance change can be attributed to the temperature change due to additional heat transfer from the tip to the sample. When the silicon tip is in contact with the silicon substrate, the Joule heat generated in the Pt–C RT and Au leads is conducted through the cantilever beams to the scanning probe chip and through the nanoscale point contact between the Si tip and the Si sample. As the cantilever is further pushed down while in contact, the effective tip-substrate contact area is expected to increase due to the increase of contact force \( (F_z) \), roughly proportional to \( F_z^{2/5} \) for a sphere-plane contact. The dependence of constriction thermal resistance on applied force was not detectable during experiments as the applied force is low \( (<10^{-8} \text{ N}) \) and the fluctuation in the interface thermal

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**Fig. 4** Schematic diagram and thermal resistance circuit of the experimental method for in-contact thermal resistance measurement of a Si–Si nanopoint contact

**Fig. 5** Measured change in electrical resistance of the Pt–C RT, \( \Delta R \), when heated by a dc current and measured by a coupled ac current of frequency \( f \), normalized by the change measured using a frequency of \( f = 15 \text{ kHz} \)
conductance is relatively large in such low-pressure nanoscale point contacts (Fig. 7).

The contact thermal resistance, $R_c$, is comprised of the interfacial resistance of the Si–Si interface, $R_i$, the diffusive resistance in the Si tip and the Si substrate, $R_{d,\text{tip}}$ and $R_{d,\text{sub}}$, respectively, and the thermal resistance between the Pt–C RT and the base of the Si tip, $R_{\text{Pt}/\text{C},\text{tip}}$, as shown in the thermal resistance circuit of Fig. 4.

Since we have measured $R_b$, and the sudden total electrical resistance change at the exact points where the Si tip snaps-to and pulls-off contact (Δ$R_{\text{contact}} = \Delta R_{\text{in-contact}} - \Delta R_{\text{out-of-contact}}$) are plotted versus total heating power, $Q$, measured at the snap-to and pull-off contact points over several approach/retract cycles. The applied $Q$ corresponds to out-of-contact temperature rises of Δ$T_h = 22–33$ K above room temperature. Additionally, Δ$R_{\text{contact}}$ extrapolates to 0.2 Ω at $Q = 0$.

We note that the measured $R_c$ is an order of magnitude lower than the contact thermal resistance in Refs. [8,10], likely due to the larger apparent contact area obtained in this work due to the frontal contact case.

Discussion

In order to understand heat transfer through the point contact, information about the contact area is critical. We consider two cases for the upper and lower limits of the contact diameter, the frontal contact case and the apex contact case, respectively. The cantilever tip is shown in Fig. 9 and its radius at the apex is measured by scanning electron microscopy (SEM) to be $r_{\text{tip}} = 62.5$ nm after the thermal experiment was conducted. As apparent in Fig. 9(b), the tip is expected to have made contact either at the apex, or along the flattened portion, $d_2$, at the frontal face of the tip as the cantilever is tilted slightly toward the substrate in its holder.

The contact area in frontal contact case can be assumed to be made by an ellipse with a major diameter less than the tip diameter in the frontal profile (Fig. 9(a)), i.e., $d_1 < 165$ nm, minor diameter $d_2$. We thus estimate the maximum effective contact diameter for the nanopoint contact to be 122 nm. Surface roughness will reduce the actual contact area, and so we note that...
$$d_c = 122 \text{ nm}$$

is the upper limiting case for the nominal contact area.

The lower limit of the contact diameter is for the case where the tip makes contact with the substrate at its apex (apex contact case). In this case, the Derjaguin-Muller-Toporov [40,42] theory can be used to calculate the contact diameter as

$$d_{c,DMT} = \frac{3 \gamma_{tip}}{4E_{tip}} \left( F_N + 2 \Delta \gamma \pi r_{tip} \right)^{1/3}$$

(10)

where $E^* = E/[2(1-\nu^2)]$ is the effective elastic modulus, $\Delta \gamma$ is the work of adhesion, $F_N$ is the external applied normal force, and $\nu$ and $E$ are Poisson’s ratio and the elastic modulus of the two contacting Si surfaces, which are taken from the literature as 0.28 and $1.3 \times 10^{11}$ Pa [43], respectively.

In order to determine $F_N$, we use the model that Clifford and Seah [44] developed based on the Neumann and Ducker method [45], which takes into account the non-uniform curvature of the cantilever beams and the location of the Si tip. The elastic modulus $E_{SiN}$ is taken to be the reported values for low pressure chemical vapor deposition grown low-stress SiN$_x$ $(2.18 \pm 0.72) \times 10^{11}$ Pa [46–48]. We account for the contribution of the Au layer to the spring constant, $c$, following Ref. [44] with the modulus of the Au layer taken to be $E_{Au} = 5.3 \times 10^{11}$ Pa [49]. For the cantilever in this work, we calculate $c = 0.0158 \pm 0.0049$ N m$^{-1}$, which is most sensitive to the 33% uncertainty in $E_{SiN}$, yet within the range specified by the manufacturer (0.005–0.02) N m$^{-1}$.

The pull-off force can be calculated based on the spring constant of the cantilever and the calibrated experimental force-distance curve as $F_{pull-off} = (-0.97 \pm 0.2) \times 10^{-10}$ N. Based on the measured pull-off force, the work of adhesion, $\Delta \gamma$, can be obtained from the DMT model as

$$\Delta \gamma = -\frac{F_{pull-off}}{2\pi r_{tip}}$$

(11)

which yields $\Delta \gamma = (2.5 \pm 0.5) \times 10^{-2} \text{ J m}^{-2}$. This value is on the order of minimum value reported for Si-Si interfaces [50] but orders of magnitude below that measured for covalently bonded Si $(\Delta \gamma = 2.13 \text{ J m}^{-2})$ [51] and bonded hydrophilic Si wafers $(\Delta \gamma = 0.21 \text{ J m}^{-2},$ unannealed) [52]. Based on the Lennard-Jones (LJ) model [53,54], the surface adhesion is related to the equilibrium interface separation, $z_0$, and $\Delta \gamma$ value corresponds to $z_0 = 1.3 \pm 0.3$ nm. For atomically smooth Si interfaces, the equilibrium separation is $z_0 = 0.149$ nm, which would yield $\Delta \gamma_{LJ} = 0.23 \text{ J m}^{-2}$ based on the LJ model. The rather small $\Delta \gamma$ and large $z_0$ values found from the measured pull off force in this work can be attributed to surface roughness of the tip and substrate [56]. We additionally note that the values corresponding to our measured $F_{pull-off}$ lead to a Tabor coefficient $(\approx \gamma_{tip}/N^2z_0^2) = 0.03$ [57], of ~0.003, for which the DMT model is deemed more appropriate [54,58] than the Johnson-Kendall-Roberts (JKR) model [41], which would be more appropriate for Tabor coefficients >5. For the $\Delta \gamma$ values calculated from the measured $F_{pull-off}$, we can now use the DMT model (Eq. (10)) to calculate $d_{c,DMT} = 3.4 \pm 0.7$ nm for the apex contact case. As a validation of our assumption of elastic contact, we use $d_{c,DMT}$ estimate the stress limits at the contact under maximum applied $F_N$ at $7.1 \times 10^3$ Pa, corresponding to a maximum strain of 0.005.

For the lower and upper limits of contact area, respectively, we can analyze our measured $R_t$, and evaluate the constituent resistances. The total contact thermal resistance due to solid-solid heat conduction is comprised of an interfacial resistance, $R_i$, and the diffusive component of the two sides, $R_s$ [16,19]. Wexler [16] proposed an interpolation formula where the diffusive component is multiplied by a numerical factor depending on the Knudsen number, $\xi(K)$, before being added to the ballistic component. The factor $\xi(K)$ is a function of the Knudsen number, $K \equiv l_{ph}/d_c$, where $l_{ph}$ is the phonon mean free path, and limiting values of $\xi(K)$ are approximately 0.694 for Knudsen numbers approaching $\infty$ (i.e., $l_{ph} >> d_c$) and 1 for Knudsen numbers approaching 0 (i.e., $l_{ph} << d_c$) [16]. Including an additional thermal resistance from the Pt–C RT to the Si Tip, $R_{Pt-C,tip}$, the total thermal contact resistance can be expressed as

$$R_t = R_i + R_{d,tip} + R_{Pt-C,tip}, \quad \text{where} \quad (13a)$$

$$R_d = R_{d,tip} + R_{d,sub}, \quad \text{and} \quad (13b)$$

$$R_{d,tip} \quad \text{and} \quad R_{d,sub} \quad \text{are the diffusive components of the solid-solid thermal resistance of the Si tip and the Si substrate, respectively.}$$

To calculate the diffusive components of the solid-solid thermal resistance between the Si tip and Si substrate, $R_d$, we model the tip as a cone of half angle $\theta_{tip}$ and contact diameter $d_c$ (Fig. 10). We can calculate the thermal resistance from the Pt–C RT to the base of the tip, $R_{Pt-C,tip}$, and the diffusive components, $R_{d,tip}$ and $R_{d,sub}$ as [59]

$$R_{Pt-C,tip} = \frac{1}{2 \tan \theta} \left[ \ln(L_2/L_1) \right] \left( R_{tip} + R_{sub} \right) \left( R_{Pt-C,tip} \right)$$

(14)

where $A = 2.58 \times 10^{19} \text{ J}$ is the Hamaker constant for Si in vacuum [55]. The above $\Delta \gamma$ value corresponds to $z_0 = 1.3 \pm 0.3$ nm. For
Heat is transferred via both phonons and thermal radiation. The presence of quantized phonon transport at room temperature in this experiment results in the measurement of the thermal contact resistance through a nanoscale Si contact. Hence, it is clear that direct tip-sample heat conduction by phonons is the dominant mode of heat transfer in this experiment, so that $R_t = R_{ss}$.

With the additional assumption that the transmission coefficient ($x$) and phonon group velocity ($v$) are assumed to be independent of frequency, the nanoconstriction model of Eq. (5) can be simplified as

$$R_{hi} = \frac{4}{\pi x v r (d_c/2)^2}$$

where $C$ is the specific heat contribution from the acoustic phonon polarizations. Values of $C$ and $v$ from Ref. [67] are used. The transmission coefficient depends on the adhesion energy as well as the detailed atomic structure at the contact point, including the presence of native oxide on the tips and sample surfaces. An analytical model has been developed predicting that $x$ drops as much as three orders of magnitude for a van der Waals bonded Si-Si interface [24] compared to that for a covalently bonded Si-Si contact [51], which has been supported by recent experiments [68,69]. For the case that the tip makes contact across its frontal slope, the maximum effective $d_c$ must be less than 122 nm, and we calculate the minimum allowable transmission coefficient, $x = 0.125-0.439$. Therefore, the interface thermal resistance can be explained by a constriction model with a contact diameter of 122 nm and a transmission coefficient greater than 0.125.

Conclusions

This work demonstrates a method for simultaneous measurement of the thermal contact resistance through a nanoscale Si point contact and the adhesion energy in a UHV AFM at near room temperature. Phonon thermal conductance is deemed to dominate near-field radiation transfer through the point contact. It is found that the measurement result can be explained by a nanoconstriction model, which allows the transmission of phonons in the whole Brillouin zone of bulk Si with a finite average transmissivity of less than 0.125. Moreover, it is emphasized that the quantum thermal conduction expression is inaccurate for evaluating the thermal conductance of Si atomic contacts at above room temperature. The presence of quantized phonon transport at nanoscale contacts remains to be verified by further experimental observation of contact thermal conductance that exhibits either quantization steps with increasing contact pressure or a linear temperature dependence with the expected magnitude.

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Nomenclature

- \( i_{dis} \): alternating electrical current (A)
- \( k_B \): Boltzmann constant (K \( \text{J} \cdot \text{K}^{-1} \))
- \( d_c \): contact diameter (m)
- \( R_c \): contact thermal resistance (K \( \text{W}^{-1} \))
- \( \xi \): correction factor for diffusive thermal transport
- \( R_R \): diffusive thermal resistance (K \( \text{W}^{-1} \))
- \( R_{ab,sub} \): diffusive thermal resistance of the Si substrate (K \( \text{W}^{-1} \))
- \( R_{direct} \): direct electrical current (A)
- \( E \): elastic modulus (Pa)
- \( R_{Au, c} \): electrical resistance of electrical resistance of both Au leads (\( \Omega \))
- \( R_{Pt, C} \): electrical resistance of the Pt–C resistance thermometer (\( \Omega \))
- \( d_1 \): ellipse major diameter for frontal contact case (m)
- \( d_2 \): ellipse minor diameter for frontal contact case (m)
- \( v_0 \): first-harmonic (1f) component of the voltage drop of the Pt–C resistor (V)
- \( f \): frequency of alternating current (Hz)
- \( \theta_{half} \): half angle of cantilever (rad)
- \( \beta \): half angle of cantilever tip (rad)
- \( A \): Hamaker constant (J)
- \( H \): height of Si tip (m)
- \( R_d \): interface thermal resistance (K \( \text{W}^{-1} \))
- \( Q_{b, dissipation} \): Joule heat dissipation in both cantilever beams (W)
- \( Q_s \): Joule heat dissipation in the Pt–C resistance thermometer (W)
- \( K \): Knudsen number
- \( L \): length (m)
- \( b \): minor diameter in the frontal contact case (m)
- \( F_{pull-off} \): normal force required to separate the Si tip from the Si substrate (N)
- \( F_{pull-off} \): normal force required to separate the Si tip from the Si substrate (N)
- \( N \): number of acoustic phonon polarizations with zero energy at the Brillouin zone center
- \( \omega \): phonon angular frequency (rad s \(^{-1} \))
- \( v \): phonon group velocity (m s \(^{-1} \))
- \( \nu \): phonon mean free path (m)
- \( p \): phonon polarization
- \( \nu \): phonon transmission coefficient through nanopoint contact
- \( n \): Poisson’s ratio
- \( G_0 \): quantum thermal conductance of a 1D phonon waveguide (W K \( \text{m}^{-1} \))
- \( r_{tip} \): radius of the Si tip (m)
- \( \hbar \): reduced Planck constant (s m \( \text{K} \))
- \( C \): specific heat (J m \(^3\) K \(^{-1} \))
- \( c \): spring constant of the cantilever (N m \(^{-1} \))
- \( R_{contact} \): sudden resistance change of the Pt–C resistance thermometer as it is brought into contact with the Si substrate (\( \Omega \))
- \( T_0 \): temperature of the cantilever mount (K)
- \( T_G \): temperature of the cantilever tip (K)
- \( \kappa \): thermal conductance (W K \(^{-1} \))
- \( \Delta R_{contact} \): thermal resistance due to solid–solid conduction through the interface (K \( \text{W}^{-1} \))
- \( R_p, t, C, t, \kappa \): thermal resistance of the two cantilever beams (K \( \text{W}^{-1} \))
- \( b_s \): thickness of the cantilever beam (m)
- \( \epsilon \): total electrical resistance (\( \Omega \))
- \( \Omega \): total Joule heat dissipation (W)
- \( \gamma \): vertical height above substrate (m)
- \( \Delta \gamma \): work of adhesion (J m \(^{-2} \))

References


