Thermovoltaic Evidence for Electronic Knudsen Flow through Silicon Microcontacts

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Asymmetric heat generation is detected by Seebeck-voltage measurements in current-carrying microcontacts, produced by adjoining two wedges of n-type silicon in ultrahigh vacuum. Decreasing the contact dimensions increases this asymmetry, which arises in the Knudsen regime of ballistic electron transport when the geometric dimensions of the contacts are sufficiently reduced to become comparable to the electron mean free path.

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Electronic transport is severely affected by reduction of the sample dimensions. New phenomena arise whenever characteristic lengths of a transport-sustaining structure approach the mean free path of the carriers. Charge transport through solid-state configurations of reduced geometry has recently attracted much interest.[1-3] Less attention, however, has thus far been devoted to the interplay of thermal and electrical transport in such small structures.[4,5] Yet, novel effects can be expected here, such as those concerning the solid-state analog to the Knudsen flow of rarefied gases. The Knudsen regime arises when orifice dimensions become small enough to approach the mean free path of the gas molecules, leading to free molecule flow rather than continuum behavior.[6] Similar phenomena in solids will provide new information, for example, concerning electron-phonon interactions or boundary scattering, and might entail novel applications such as improved thermoelectric converters with reduced geometrical dimensions.

This Letter reports the results of a series of elementary experiments on microcontacts of silicon under highly controlled conditions. The existence of a regime of ballistic Knudsen flow is proved by the detection of asymmetric heat generation. As the contact area between two semiconductor specimens of like conductivity type is reduced, the majority-carrier current traversing the contact produces heat predominantly within the downstream part of a contact. The asymmetry can be detected by measuring the thermoelectric Seebeck voltage and is explained quantitatively.

Our experiments consist in producing well-defined small-area contacts between two wedge-shaped pieces of highly doped (3×10^{-3} Ω cm, phosphorus doping), n-type silicon. The wedges are arranged facing crosswise in ultrahigh vacuum and are cleaned by ion bombardment as well as analyzed for purity by Auger spectroscopy before they are pressed against each other piezoelectrically; the mechanical compressing force is measured capacitively. The details of the equipment are described elsewhere.[7] Variation of the contact pressure determines the contact area, which is monitored via the electrical resistance of the contact. Current is then passed (in either polarity) across the contact. After passage of the current for approximately 10 min, a steady-state temperature profile is reached, and then (within less than 0.2 sec) the Seebeck thermoelectric voltage is measured, which directly detects any temperature imbalance between the two legs of the microcontact. A schematic view of the arrangement is shown in the inset of Fig. 1.

The electrical resistance R of a small constricting circular orifice of radius a is[8,9]

$$R=(2\sigma a)^{-1}+K/2\sigma a=R_{\rm M}+R_{\rm K}\,, \tag{1}$$

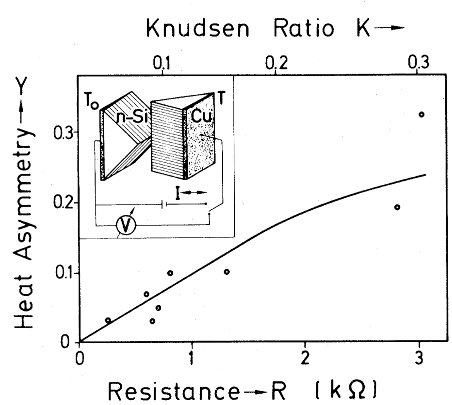

FIG. 1. Inset: Experimental arrangement. Two wedges of n-type Si are mounted on Cu blocks. One is kept at room temperature T_0, and the other may rise to T as a result of the current I traversing the contact. After current flow, the switch is thrown to measure $T-T_0$ via Seebeck voltage. The plot shows the heat asymmetry Y as a function of resistance R, which can be converted to a Knudsen ratio K. The curve represents theory, assuming an electron mean free path of $l=2$ nm.

with the Knudsen ratio[10]

$$K = l/a, \tag{2}$$

where σ denotes the electrical conductivity and l the mean free path of the carriers.[2,8,9] The term R_M describes the well-known "Maxwell" spreading resistance[9,11] for contact radii $a \gg l$. If $a \ll l$, the Knudsen ratio K becomes so large that R_K dominates the resistance. Equation (1) treats the carriers as classical particles similar to a molecular gas in the standard Knudsen description; we thus call R_K the "Knudsen resistance." The multiplication by K cancels in R_K the characteristic mean free path contained in σ, assessing the scattering. The Knudsen resistance thus describes a ballistic transport controlled by the small geometry. If a voltage is applied across a microcontact with large Knudsen ratio K, then the electric field is confined to regions of dimension a of the contact. Carriers are accelerated within this field region, propagate ballistically, i.e., without scattering, and begin to lose their kinetic energy to the lattice only after having traversed distances of order $l > a$. Thermoelectric conversion into heat is thus restricted to the downstream part of a contact couple. Although the contact construction is entirely symmetrical and also contains no p-n junction, its dimensional restriction causes it to become increasingly asymmetrical in electron-phonon interaction, leading to a unidirectional injection of lattice heat.

The total heat generation rate by the current I is also split into a Maxwellian and Knudsen part:

$$\dot{Q} = R_M I^2 + R_K I^2 = \dot{Q}_M + \dot{Q}_K. \tag{3}$$

While $\dot{Q}_M$ arises symmetrically around the orifice, the Knudsen part $\dot{Q}_K$ is created only in the downstream part, which the carriers are approaching, since their excess energy gained in the high-field region of the orifice is transferred to the lattice *after* the passage. We characterize this asymmetry of heat production by

$$Y = (\dot{Q}_1 - \dot{Q}_2)/(\dot{Q}_1 + \dot{Q}_2), \tag{4}$$

where $\dot{Q}_i$ is the rate of change of heat in leg i of the contact. If one assumes that all heat stays within the contact leg where it was generated, Eq. (4) simplifies to

$$Y = \dot{Q}_K/\dot{Q} = K/(K+1), \tag{5}$$

which tends to zero for bulk contacts and to unity for microcontacts of very small dimension (i.e., large Knudsen ratios). Equation (5) presents an upper limit for Y, since any heat flowing across the contact reduces the asymmetry Y.

A number of microcontacts are analyzed in detail. Current-voltage measurements reveal nonlinear behavior for large Knudsen ratios, which is probably caused by carrier multiplication in the high-field region near the contact. For the thermal measurements reported here, we use contacts of up to 3 kΩ resistance. The main source for the scatter of the experimental data is not the nonlinearity but an inevitable change of the contact resistance during the traversal of the current. This scatter increases with increasing R, i.e., with decreasing contact geometry. The average value of R during current passage is then used. From the resistance R, we calculate the contact radius a with Eq. (1), and hence the Knudsen ratio K, with the assumption of a value for l. Both R and K are plotted as abscissae in Fig. 1. The mean free path in the silicon is here chosen to be $l = v_t m^* \mu/e = 2$ nm, this fit being in good agreement with estimates for the room-temperature thermal velocity[12] $v_t = 5\times 10^4$ m/s, an average effective electron mass $m^* = 0.8 \times 10^{-30}$ kg, and an electron mobility[12] appropriate for heavy doping of $\mu = 8\times 10^{-2}$ m^2/V s.

For each contact, a series of measurements is performed to obtain the thermal asymmetry Y. The measured total Seebeck thermovoltage U_S is given by

$$U_S = \text{const}\times[(1\pm Y)RI^2/2 \pm \pi I], \tag{6}$$

where $\pm I$ denotes polarity and magnitude of the electric current. The term πI accounts for the Peltier heat created at the junction between the silicon sample and its copper block support; the Peltier coefficient π applies to the combination Si/Cu. Applying two polarities and two magnitudes each of the current I, one can determine both π and Y from the four experimental Seebeck voltages U_S. The Peltier coefficient which we thus obtain agrees well with the literature value, and thus provides a consistency check. The temperature differences, as measured by the Seebeck voltage, never exceed 1 °C. The values of Y thus obtained are plotted as the ordinate in Fig. 1.

Figure 1 clearly shows the expected increasing asymmetry of heat generation due to the ballistic traversal of the microcontact. The curve is a fit with $l = 2$ nm for Eq. (5), which neglects any reverse heat flow, such as by lattice or electronic thermal conductivity. This neglect seems justified, as the fit indicates. The deviation towards too large a value of Y for $R = 3$ kΩ might stem from two small contacts in parallel.

In conclusion, we have shown that elementary electrical and thermal measurements, done under well-defined conditions with semiconductor microcontacts, verify the existence of the solid-state equivalent of Knudsen ballistic flow and its consequences for asymmetric generation of lattice heat. Such thermoelectric measurements represent useful additions and valuable alternatives to the presently purely electrical current-versus-voltage analysis of microstructures such as by tunneling spectroscopy.[1,2] Determinations of carrier mean free paths, contact dimensions, and correlations of differential electrical resistance with the rate of lattice heating should, for example, provide new insight into solid-state microstructures. Current-carrying point contacts of defined small dimensions promise useful thermoelectric device applications of improved conversion efficiencies as a result of the principal possibility of spatially selective heat generation, as here demonstrated, and because small structures can be made to relax the strong relation—which is inevitable for bulk systems—between thermal and electrical resistances.

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