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Minority carrier effects in nanoscale Schottky contacts

Lifeng Hao1 and P A Bennett1,2

1 School of Materials, Arizona State University, Tempe, AZ 85287, USA
2 Department of Physics, Arizona State University, USA

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Abstract
We report the current–voltage behavior for nanoscale point contacts to Si(111) obtained in ultrahigh vacuum using scanning tunneling microscopy. Epitaxial CoSi2 islands provide single-crystal contacts with well-defined size and shape. The zero bias conductance is found to be independent of the island size (102–104 nm2) and shape, but varies strongly with the surface Fermi level position. This behavior is explained by the recombination–generation current from minority carriers at the free surface, which may be orders of magnitude larger than the majority carrier thermionic or tunnel currents across the contact interface. This can give rise to large shifts of the apparent ideality factor and Schottky barrier height for the point contact.

As electronic devices shrink to the nanoscale, the role of electrical contacts becomes increasingly important. Indeed, the contacts become an intrinsic part of the functional unit, and can dominate the device operation [1, 2]. Some devices, such as nanowire transistors rely explicitly on contact effects rather than channel effects to control current flow [3].

Point contacts date from 1874, and provided the first solid state rectifiers, free from interface oxide effects [4]. Point contacts remain important today, since they can operate at very high frequency, and with very high sensitivity [5]. They may also be utilized in large arrays for efficient solar cell devices [6]. The geometry of the point contact creates an intense electric field that gives rise to strong tunneling and associated ‘leakage’ effects. Such effects may arise in multicomponent nanoelectronic structures, where they are difficult to control or even to identify. In this sense, the point contact is a prototype structure that allows the study of such effects in a controlled manner.

The current–voltage (I–V) behavior for an ideal Schottky diode may be written as

\[ I(V) = A* T^2 \exp \left( \frac{q \Phi_{SB}}{kT} \right) \left[ \exp \left( \frac{q V}{nkT} \right) - 1 \right], \]

where \( A* \), \( n \) and \( \Phi_{SB} \) are the Richardson constant, the effective ‘ideality factor’ and Schottky barrier height, respectively [7]. Several groups have investigated the I–V behavior of metal–semiconductor point contacts, and have reported anomalous values for \( n \) and \( \Phi_{SB} \) obtained by fitting the data to equation (1). This behavior has been variously attributed to tunneling or to ohmic conduction through surface states or to screening by a strongly pinned surface Fermi level adjacent to the contact [8–12].

In this paper, we report in situ I–V measurements of nanometer-sized metal contacts to a Si(111) substrate using UHV-STM. Epitaxial CoSi2 islands provide well-defined contacts with variable size in the range of 102–104 nm2. We find that the conductance near zero bias, \( G_0 \), is large and independent of contact size or Schottky barrier height, while the I–V curves show large and voltage-dependent ideality factors ‘\( n' \), in accord with similar earlier measurements [8–12]. Furthermore, \( G_0 \) is found to vary strongly with temperature and with surface Fermi level position, which is adjusted by submonolayer coverages of Co. This behavior is explained by a surface recombination–generation (RG) current of minority carriers at the surrounding free surface. This current is much larger than the majority carrier current across the metal–semiconductor interface itself. This mechanism, which appears only for nanometer-sized contacts, has not been considered in earlier point contact work, and provides a physical origin for anomalous \( n \), \( \Phi_{SB} \) values that have been widely observed. It also provides new insight into surface conductivity measurements using nanoprobes. This effect may arise for any small metallic feature in contact with a semiconductor surface or interface.

All experiments were performed in a UHV system with base pressure of \( 1 \times 10^{-10} \) Torr. Si(111) substrates (n-type,
\( \rho \sim 1 \ \Omega \ cm \) were degassed at 600°C for 12 h followed by repeated brief heating to 1200°C and slow cooling to yield a clean 7 × 7 surface. Epitaxial single-crystal CoSi2 islands were grown by depositing 0.4 monolayer (ML) Co and annealing at 600°C for 5 min. Different-shaped islands (triangle, hexagonal) with size ranging from \( 10^2 \) to \( 10^3 \) nm\(^2\) were obtained in a single growth cycle with identical surface condition [13]. For some experiments, the surface Fermi level was adjusted by depositing Co at 650°C, which produces a 1 × 1 structure with saturation coverage of 1/7 ML [14, 15]. The surface Fermi level is assumed linear with coverage from 0.65 to 0.42 eV, as shown in figure 2. Data from Smit et al [16, 17]. The surface Fermi level was adjusted by depositing Co at 650°C, which produces a 1 × 1 structure with saturation coverage of 1/7 ML [14, 15]. The surface Fermi level is assumed linear with coverage from 0.65 to 0.42 eV, as shown in figure 2. Data from Smit et al [16, 17]. The surface Fermi level was adjusted by depositing Co at 650°C, which produces a 1 × 1 structure with saturation coverage of 1/7 ML [14, 15]. The surface Fermi level is assumed linear with coverage from 0.65 to 0.42 eV, as shown in figure 2. Data from Smit et al [16, 17].

A typical \( I-V \) curve is shown in figure 1 for a 420 nm\(^2\) island. This curve shows rectifying behavior, and may be characterized by a model of a Schottky Barrier (described by equation (1)) plus parallel resistor, with \( R_b = 4 \times 10^9 \ \Omega \), \( n = 2-3 \) and \( \Phi_{SB} = 0.42 \ \text{V} \) (ideal values are \( R_b = \infty, n = 1 \) and \( \Phi_{SB} = 0.67 \ \text{V} \) [18]). \( R_b \) is much smaller than the resistance of the Schottky diode, indicating a large leakage current. The \( I-V \) curves for a whole set of islands with size ranging from \( 10^2 \) to \( 10^4 \) nm\(^2\) are similar in shape and magnitude. For ease of reference in the reminder of his paper, we will characterize these curves by their zero bias conductance, \( G_0 \), obtained from the slope of the \( I-V \) curve in the range ±0.05 V. We find that \( G_0 \) is independent of island size and shape, with a constant value of \( G_0 \sim 2.5 \times 10^{-10} \ \Omega^{-1} \) at 25°C and \( G_0 \sim 2 \times 10^{-14} \ \Omega^{-1} \) at 100°C, as shown in figure 2. Data from Smit et al for the same CoSi2/Si(111) system show a similar constant value of \( G_0 \sim 1 \times 10^{-10} \ \Omega^{-1} \) at 25°C, for low-doped samples (inset to figure 1 in [19]). This current cannot be due to thermionic emission, which would yield \( G_0 \sim 2 \times 10^{-14} \ \Omega^{-1} \) for an island size of \( 10^3 \) nm\(^2\) and \( \Phi_{SB} = 0.67 \ \text{eV} \) at 25°C. This current cannot be due to tunneling either, since that contribution is far too small. This may be directly calculated for a spherical contact embedded in bulk silicon, and is shown in the figure. Finally, \( G_0 \) cannot be due to ohmic surface conductance, since that would be independent of \( T \), unlike the measurement.

The discussion above suggests that the point contact conductance is dominated by an additional (parallel) non-ohmic component. To explore this hypothesis, the surface was altered by adding a submonolayer of Co atoms at 650°C, changing the reconstruction from \( 7 \times 7 \) to \( 1 \times 1 \), and also shifting the surface Fermi level from 0.65 to 0.42 eV, as indicated on the top axis of figure 3. Here \( \theta \) is the fraction of saturation coverage of 1/7 ML. The inset shows an STM
characterized by the surface recombination velocity, $s$, that surrounds the point contact. Surface R–G events are dominant over net current flow. This field drives a thermionic current (majority carriers tunneling through the Schottky barrier) as well as a thermionic injection current. These currents are small compared with the total tunneling current (majority carriers tunneling through the near-surface space–charge layer, which depends on band bending and surface Fermi level, but in a monotonic way). We propose instead that this behavior is due to a large R–G current. For zero bias condition, we have $n_s = n_i \exp[(E_{Fs} - E_i)/kT]$ and $p_s = n_i \exp[−(E_{Fs} - E_i)/kT]$ in which $E_{Fs}$ is the surface Fermi level and $E_i$ is the intrinsic Fermi level. We note that $s$ depends on $D_a$ linearly and on $E_{Fs}$ in a complicated way. Actually, equation (2) shows that $s$ varies exponentially with $E_{Fs}$, being sharply peaked near $E_i$ (near mid-gap), as illustrated in the inset of figure 3. The measured current clearly follows the general trend. This indicates that $E_{Fs}$, instead of $D_a$, dominates the variation of $s$ and $G_0$, although $D_a$ might be changed with Co coverage as well.

The current flow pattern for a point contact on a free surface is shown in schematic form in figure 4. Under equilibrium conditions, with zero applied bias, charged surface states pin the Fermi level and create a gradual variation of Fermi level and charge density. These currents are small compared with the total tunneling current. An external bias voltage applied to the tip creates an approximately radial electric field which acts as the driving force for net current flow. This field drives a thermionic current (majority carriers excited over the Schottky barrier) as well as a tunneling current (majority carriers tunneling through the barrier). These currents are small compared with the total observed current, as discussed above. The R–G current arises because the tip-induced voltage shifts the carrier density out of thermal equilibrium (np ≠ $n_i^2$). This causes generation or recombination processes which take place mostly on the free surface surrounding the tip.
For example, under reverse bias (tip negative, for n-type Si), the potential of the free surface near the tip is raised, causing $n_p r < n_i^2$, which in turn causes thermal generation of electron–hole pairs at recombination centers on the free surface. The generated electrons are swept out of the depletion region and into the bulk by the built-in field, while the generated holes go to the tip, driven by drift and diffusion forces. Under forward bias, the same process occurs in reverse: holes are injected from the tip into the surface states directly or into the surface space charge region, move across the surface and recombine there with electrons that arrive from the bulk. It should be noted that the built-in field holds minority carriers near the surface everywhere. The total R–G current then involves a series sum of minority current along the surface and majority current to/from the bulk, connected via the surface R–G processes.

The magnitude of current flow depends primarily on the degree of departure from equilibrium (separation of quasi-Fermi levels, which varies with distance from the tip) and the efficiency of the R–G process. Indeed, following Fitzgerald [20], the surface generation current for a fully depleted surface may be roughly estimated as

$$I_g = qsn_i A,$$  

(3)

where $A$ is the collection area. For the Si(111)-7 × 7 surface, we use $s \sim 2 \times 10^6$ cm$^{-1}$ [23], and $A \sim (100 \mu m)^2$ [24]. $A$ is large, since it is determined by the minority carrier diffusion length for Si which can be 100 $\mu$m. This geometry is similar to the gate-controlled diode configuration, in which surface generation current is collected from areas of this size [20]. Thus, the estimated surface generation current is 0.3 $\mu$A, which is close to the measured reverse bias current (0.5 $\mu$A) for direct W tip contact to clean 7 surface. The above simple estimate suffices to verify the dominance of surface R–G current over interface current for small contacts. A full calculation of the I–V behavior would have to include the variation of surface potential, carrier density and current flow.

The observed independence of $G_0$ on contact size, as shown in figure 2, can be easily understood since, for a small contact, the total contact is dominated by the surface R–G current which is not related to the contact. For large contacts, however, the thermionic and/or tunneling current will exceed the surface current, since they scale with island size. For our substrate, this occurs for island size $r > 1 \mu$m. This cross-over size will depend on doping level and surface recombination rate. Finally, we note that the R–G current increases rapidly with temperature since $n_i \sim \exp(-E_g/2kT)$, in accord with the data.

The dominance of minority current (via surface R–G process) for nanoscale Schottky contacts is in striking contrast to planar Schottky contacts. In a planar Schottky contact, the majority and minority currents are closely coupled, with the minority current generally negligible in relative size [7]. For the nanoscale Schottky point contact, however, these currents are decoupled: the majority current flows across the interface while the minority current may flow along the free surface. As a result, the minority current may strongly dominate if the surface is electrically active.

The surface R–G current will be present for any biased metallic contact on a semiconductor surface. In practical devices, the contact geometry is carefully designed to reduce R–G currents and other ‘leakage’ effects [7]. This requires careful control of the surface recombination velocity ‘$s$’. For Si/SiO$_2$, one can have $s < 1$ cm$^{-1}$, which would bring $G_0$ into an acceptable range of 10$^{-10}$ Ω$^{-1}$ [24, 25]. For multicomponent and/or prototype nanoelectronic structures, however, $s$ is not well known or controlled, and may be very large.

Surface R–G effects may also be important in electrical nanoprobe measurements, such as ‘scanning spreading resistance’, which is widely used to measure substrate conductivity [26, 27], or multi-tip STM, which is used to measure conductance of surface layers. The surface R–G currents can significantly alter the potential distribution and current flow, and must be included in a proper model of the probe. This has not been done, to date, which may explain the orders of magnitude variation in the reported conductance for intrinsic surface states on clean silicon [28–31].

In summary, we have shown that the current flow for nanoscale Schottky contacts on Si(111) is strongly dominated by minority carrier recombination–generation current at the free surface. This current will occur for any small metal contact to a semiconductor surface and can be magnitudes larger than the majority carrier thermionic or tunnel currents across the metal–semiconductor interface. This may be misinterpreted as large shifts of the apparent ideality factor, Schottky barrier height or spreading resistance for small contacts and may also perturb multi-probe surface conductivity measurements.

Acknowledgments

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References

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