Experimental test of the planar tunneling model for ballistic electron emission spectroscopy

Ian Appelbaum,[1,2] Rahul Sheth,[2] Ilan Shalish,[2] K. J. Russell,[2] and V. Narayanamurti[2]
[1]*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*
[2]*Division of Engineering and Applied Sciences, Harvard University, Cambridge, Massachusetts 02138*
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Using planar theory of ballistic electron emission spectroscopy with the addition of scattering at the metal-semiconductor interface, we calculate an expected change in the ratio of the collector current (I_c) to the tunnel current (I_t) as I_t is varied in the well-known system Au/GaAs(100). This alternative spectroscopy is performed experimentally and is shown to differ drastically from the theory, which nevertheless agrees well with standard voltage spectroscopy. From this discrepancy, we question the applicability of one-dimensional (1D) planar theory to an inherently 3D system.

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Ballistic electron emission spectroscopy (BEES) is a technique where a metal-vacuum-metal tunnel junction serves as a ballistic electron injector from a metal scanning probe emitter, through a metal base, over a Schottky barrier, and into a semiconductor collector.[1,2] As the emitter-base voltage is increased, the ballistic electrons originating in the tip emitter have increasing energy to couple with the available states in the semiconductor. The collector current is zero until this energy is above the Schottky barrier, after which it increases according to available conduction channels. This thresholded response has been used to measure Schottky barrier heights and buried heterostructure band offsets.[3–5].

Although the existence of thresholds in this spectroscopy is clear from any rudimentary semiconductor theory, there has been much discussion in the literature concerning the interpretation of the shape and magnitude of the spectra past threshold.[1,2,6–8] Much of this debate has been due to the assumed parallel momentum distribution of ballistically injected electrons. Since the tunneling probability increases with perpendicular momentum, it has been assumed that the vacuum tunnel barrier acts as a filter that passes forward-directed electrons. These electrons have relatively little parallel momentum, and so cannot couple with conduction valleys that lie far away from the interface Brillouin zone (IBZ) center. Au/Si Schottky diodes provided an early example.[9] Since the conduction-band minimum lies near the X point in the (100) direction, the (100) crystal orientation has states that lie at the zone center. With the (111) orientation, all states require nonzero parallel momentum. Therefore, BEES on the (100) crystal orientation should yield a larger I_c than (111). However, experiment has shown repeatedly that the two orientations yield virtually the same spectra.[10]

A similar difficulty arose in the interpretation of BEES spectra from Au/GaAs(100). Since the GaAs conduction-band minimum (at Γ) lies at the zone center, one expects the contribution from this valley to dominate over any additional thresholds from higher conduction-band minima such as L, which in this crystal orientation lies near the perimeter of the IBZ. Contrary to this expectation, the contribution from L is typically four to five times stronger than Γ.

To explain this discrepancy, the standard planar tunneling model was modified to include s-wave scattering at the base metal-semiconductor interface.[7] Electrons initially highly forward directed are scattered outside of the IBZ center, where they can couple with states in the L valley. The scattering probability (SP), the probability that an individual electron is scattered out of the zone center, was determined to be approximately 0.9 by fitting the model to the data.

The scattering probability is essentially a parameter used to coerce the theory into agreement with experiment; the parallel momentum conservation imposed by considering planar tunneling forces us to accept this parameter without rigorous justification. An independent means of testing this model would be helpful in identifying the actual physics underlying BEES. In this paper, we present a spectroscopy providing experimental means to test the planar tunneling model.

In the planar theory, the vacuum barrier determines the distribution of parallel momentum. Hence, one can obtain control over the distribution of parallel momentum by manipulating the vacuum gap. Experimentally, this parameter is controlled by the tunnel current. At constant voltage, the tunnel current varies inversely to the vacuum gap. Scanning the tunnel current from low to high at constant voltage, thus, widens the distribution of parallel momentum. At a voltage just below the L valley in Au/GaAs(100) (≈ 1.2 V), the ratio of collector current to tunnel current should decrease as the tunnel current increases. This is because as the tunnel current increases, the emitter-base distance decreases and the preference for forward-directed electrons becomes weaker. As this happens, a greater and greater fraction of electrons have more parallel momentum than the available states in the Γ valley near the IBZ center, and so the ratio I_c/I_t decreases.

Although the preceding argument predicts the negative sign of the effect in this system at voltages below the L valley, the magnitude remains undetermined. To estimate the magnitude of this effect over this range, we have developed a BEES simulator using the Monte Carlo method.

Individual momentum states in a free-electron metal emitter are sampled at random and followed through the system. Electrons with enough energy to fill unoccupied states in the base metal tunnel across a trapezoidal barrier to form a tunnel current

$$I_t = 2Ae\sum \frac{\hbar}{m} k_\perp T^{WKB}(k_\perp, V) F(T,E) \times [1 - F(T, E+eV)]\Delta k^3. \quad (1)$$

The sum is over all states in the emitter, of which only those with positive $k_\perp$ will contribute to the sum. This sum substitutes an integral of the electron flux $[2(\hbar/m)k_\perp \Delta k^3]$ times the Wentzel-Kramers-Brillouin (WKB) tunneling probability (T^{WKB}), and thermal occupation ($F(T,E)[1-F(T,E+eV)]$), where T is the temperature, E is the electron energy in the emitter, and V is the applied voltage. A is the effective tunneling area, and the factor of 2 accounts for spin degeneracy. The phase-space volume Δk^3 is determined by the sampling density and the normalization condition

$$n = 2\int F(T,E)\frac{dk^3}{(2\pi)^3} \rightarrow 2\sum F(T,E)\Delta k^3,$$

where n is the electron number density in the emitter metal, F is the Fermi function, and k_F is the Fermi wave vector.

In the base metal, inelastic attenuation is modeled after Ref. 7. Elastic interfacial scattering, occurring with probability SP, is modeled by a random reorientation of the electron's momentum while conserving the norm of the momentum vector. If the parallel momentum in the base is equal to an available state with equal energy (modeled with spherical, energy dependent effective masses) in the semiconductor, the electron contributes to the collector current with a probability determined by the quantum-mechanical transmission of a step potential over the Schottky barrier, E_{SB}. The collector current for each conduction valley is then

$$I_c = 2Ae\sum \frac{\hbar}{m} k_\perp T(k_\perp, V) F(T,E)[1 - F(T,E+eV)] \times M_{inel}(E+eV) Q(E+eV, E_{SB}) \times \left(\int \delta(\vec{k}_\parallel^{sc} - \vec{k}_\parallel^{base}) dk^2 \right) \Delta k^3, \quad (2)$$

where $M_{inel}(E+eV)$ is the inelastic attenuation coefficient, $Q(E+eV, E_{SB})$ is the quantum-mechanical transmission coefficient, and the integral over a δ function accounts for parallel momentum conservation from the base to the semiconductor.

At every voltage point in a spectrum, the vacuum gap is adjusted to keep the tunnel current constant to within a fraction of $\approx 10^{-3}$, matching experimental conditions. This is done by numerical integration of an analytic expression for the tunnel current, and application of a bisection root-finding algorithm.

To demonstrate the accuracy of the Monte Carlo model, we simulate the voltage spectroscopy of a 60 Å Au/GaAs(100) Schottky diode. It is useful to compare the second derivatives of the BEES spectra (SD-BEES) because it allows fitting the data with the results of the simulation in a more sensitive fashion than comparing raw spectra. In Fig. 1, we show both the experimentally determined SD-BEES and fitted simulation results. Both spectra are normalized for comparison. Experimental conditions are in air at room temperature with a tunnel current of 1 nA. The measurements were performed in a surface/interface AIVTB-4 BEEM/STM using a Au tip. In the simulation, we used SP = 0.88. We chose the effective tunneling area to be 10 nm^2, an order-of-magnitude estimate based on the image resolution obtained during microscopy mode. In order to obtain high signal to noise in the second derivative, we sample electron k space 10^8 times per voltage point. The agreement between experiment and theory is comparable to previous efforts.[7,8]

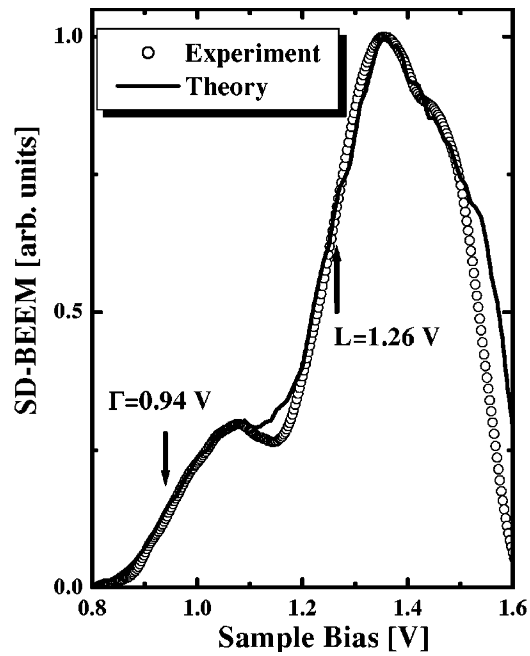

FIG. 1. Second derivative of BEES voltage spectroscopy on Au/GaAs(100). Results of the Monte Carlo simulation are superimposed on the experimental spectrum. The conduction-band thresholds used in the simulation are shown with arrows.

Having demonstrated the accuracy of the simulation, we now use the same model to examine the magnitude of the change in I_c/I_t as I_t changes over a realistic range. Experimentally, we have a dynamic range of less than two orders of magnitude in the tunnel current. Keeping the voltage constant, just below the L-valley minimum at 1.2 V, we scan the simulated tunnel current from 0.2 nA to 5 nA. Figure 2(a) presents the results of this simulation. For the previously fitted value of SP = 0.88, the ratio I_c/I_t is expected to vary by approximately 25% over the specified range.

It is interesting to note that even in the case SP = 1.0, when the parallel momentum has been randomized by scattering, this calculated ratio will *still* decrease, by approximately 10%, as shown in Fig. 2(b). This effect is due to the changing energy distribution of the tunneling electrons. The ratio I_c/I_t can be written as

$$I_c/I_t = \frac{\sum C_i A_i}{\sum A_i + \sum A_j},$$

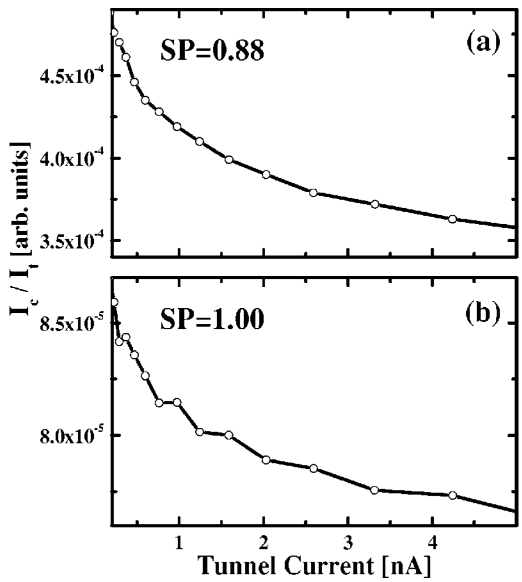

FIG. 2. Simulations of tunnel current spectroscopy for SP $=0.88$, (a); and SP$=1.00$, (b).

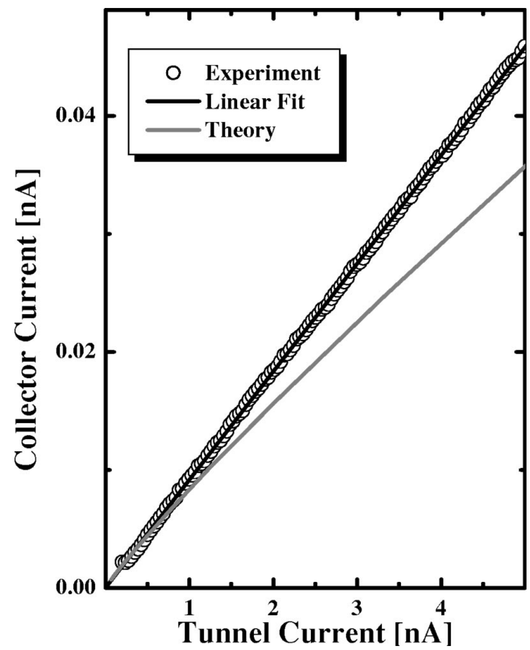

FIG. 3. Comparison of experimental and theoretical tunnel current spectroscopies. The parameters used in the simulation shown are the same as those in Fig. 1.

where the tunnel current [Eq. (1)] has been broken up into two parts. The first sum is over emitter states that couple to the semiconductor and the second is over the remaining states that do not. A_i represents the summand in Eq. (1). C_i represents ballistic attenuation, quantum-mechanical reflection at the Schottky interface, and parallel momentum conservation as shown in Eq. (2).

In the case when I_t is relatively small, the vacuum gap is large and the tunneling process is very selective to high energy electrons that are more likely to couple with semiconductor states. Thus, the relative contribution of the second sum to the denominator is smaller than when the tunnel current increases. This is because for a smaller vacuum gap, the tunneling process becomes less selective of high-energy electrons. At 1.2 V, this effect, dependent on the energy distribution, adds to the previously discussed effect that relies on the changing distribution of parallel momentum.

We have modified the BEEM software so that we can perform the tunnel current spectroscopy at specified points in the topography. Figure 3 shows the average of over 13 000 scans of 128 tunnel current points between 0.2 nA and 5 nA on the same Au/GaAs sample as in Fig. 1. We do not show the ratio I_c/I_t because an undetermined collector current offset cannot be fully nulled during the measurement. Instead, we show I_c. We also show the calculated I_c for SP$=0.88$, normalized for comparison to match the experimental I_c at low I_t. While the simulation predicts a visibly nonlinear spectrum, the experimental data appear remarkably linear, corresponding to an unchanging I_c/I_t. Clearly, this indicates that the model that has been used with much success to simulate voltage spectroscopy cannot be successfully applied to tunnel current spectroscopy.

In order to account for the inadequacy of the model to explain tunnel current spectroscopy, we point to the questionable applicability of planar theory to real (nonplanar) systems.

Parallel momentum conservation across the tunnel gap will clearly break down when the assumption of planar tunneling is examined. Although poor microscopy resolution is often used as an indicator for a quasiplanar tunnel region, it may also be the case that tunneling occurs from many highly localized points at the end of a blunt tip. Each of these points breaks the local translational symmetry, destroying parallel momentum conservation. In this case, the parallel momentum of ballistic electrons in the base is determined only by energy conservation, resulting in a wider distribution immune to changes in the vacuum gap.

The unobserved decrease in I_c/I_t due to energy distribution changes is more difficult to explain. It may be that the effective tunneling area changes drastically when the tunnel current is ramped, which would lead to a more constant vacuum gap. Thus, the tunnel current changes over a wide range but the distribution of tunneling electrons does not.

An alternative explanation is suggested by the work of Garcia-Vidal *et al.*[11] and Reuters *et al.*[12] Using a Keldysh Green's function method to model electron transport through a Au(111) base metal crystal, they show that the ballistic current prefers to travel along directions determined by the metal band structure. These directions have parallel momentum compatible with the conduction valleys in Si(100) and (111), which resolves the similarity of BEES on these two orientations without invoking interfacial parallel momentum scattering.

A similar effect could be at work in the case of Au/GaAs(100): if the parallel momentum distribution of ballistic electrons is largely determined by the base metal, changing the tunnel current by manipulating the vacuum gap will only result in more ballistic electrons, without changing their momentum distribution. I_c will, therefore, vary linearly with I_t, as observed experimentally. This argument relies on a epitaxial Au film grown on GaAs(100); there is, however, no evidence that this is actually the case.

We have presented both simulation and experimental results of tunnel current spectroscopy on Au/GaAs(100). Using the standard planar tunneling theory, we have shown that although the model predicts the shape of the voltage spectroscopy with great success, experiment and theory disagree strongly for tunnel current spectroscopy. This highlights the inapplicability of planar theory to real systems.

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