Ballistic Electron Emission Microscopy for Nonepitaxial Metal/Semiconductor Interfaces

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We present a model of ballistic electron emission microscopy (BEEM) that includes elastic scattering at nonepitaxial metal/semiconductor interfaces. In the weak scattering limit, the model reduces to the traditional description of BEEM. In the strong scattering limit, the model quantitatively describes (1) the relative magnitudes of BEEM currents into the Γ, L, and X channels for Au/GaAs(100); (2) the relative magnitudes of the currents for Au/Si(100) and -(111); (3) the relative magnitudes of currents for Au/GaAs and Au/Si; and (4) the absolute magnitudes of the currents for these materials. [S0031-9007(98)05473-8]

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The transport of electrons across nonepitaxial metal/semiconductor interfaces is of interest in a wide range of contexts. Ballistic electron emission microscopy (BEEM) is a good way to study such processes because BEEM directly measures the current across interfaces for a well characterized distribution of incident electrons [1–4]. The original theoretical description of BEEM assumes that both energy and the interface parallel component of the wave vector are conserved as an electron traverses an interface [2]. This theory gives a description of BEEM current as a function of tunneling tip to metal film bias which has been used extensively to fit BEEM data near the threshold of a transport channel [5–11].

The materials systems studied most extensively by BEEM are Au/GaAs and Au/Si. Au/GaAs and Au/Si are prototypes for nonepitaxial metal interfaces on direct and indirect band gap semiconductors, respectively. In BEEM on GaAs, there are three transport channels corresponding to electrons going into the Γ, L, and X conduction band minima. Six fitting parameters are commonly used to describe GaAs BEEM data, one threshold energy and one magnitude factor for each of the three channels [2,5–7]. GaAs has been studied extensively and the material parameters necessary to determine the quantities usually taken as fitting parameters are known. When the expected values are compared with those required to fit BEEM data, one finds that the three fit threshold energies are close to the expected values, but that the three fit magnitude factors differ significantly from what is expected. Specifically, for BEEM measurements on Au/GaAs(100), the fit magnitude factors for the Γ and X channels are much smaller than expected and the fit magnitude factor for the L channel is much larger than expected. Tunneling predominantly injects forward directed electrons with small interface parallel wave vector components into the metal film. Because the parallel wave vector is assumed to be conserved, the calculated current into valleys with zero parallel wave vectors at the minimum [e.g., the Γ and one of the three X valleys for GaAs(100)] is much larger than the calculated current into valleys with large parallel wave vectors at the minimum [e.g., the L valleys for GaAs(100)]. This predicted difference is not observed experimentally [2,5–7]. For the same reasons, the calculated current for Si(100), for which two of the Δ conduction band minimum valleys have zero parallel wave vectors, is much larger than the calculated current for Si(111), for which all of the conduction minima have large parallel wave vectors. The measured BEEM currents do not show the predicted dependence on orientation for Si; in fact, the measured BEEM currents for (100) and (111) oriented Si are very similar [2,8–11].

It has long been recognized that elastic scattering of electrons, either at the metal/semiconductor interface or in the metal film, might account for the relative magnitude factors for the three channels in GaAs and the observed weak dependence on orientation in Si [6,9,11–13]. To date, however, no unified model quantitatively describing the BEEM data in these prototypical nonepitaxial materials has been proposed. Here, we present a model which starts with eigenstates of an ideal interface Hamiltonian and then allows interfacial elastic scattering to redistribute the electrons injected by tunneling among these eigenstates. In the weak scattering limit, this model reduces to the traditional description of BEEM with the inclusion of quantum mechanical reflection at the metal/semiconductor interface. In the strong scattering limit, it quantitatively describes the BEEM data on Au/GaAs and Au/Si.

The model starts with a Hamiltonian consisting of two parts: $H = H_0 + \delta H$, where H_0 describes an ideal interface for which the interface parallel component of the wave vector is a good quantum number, and δH describes interfacial scattering centers. H_0 has the form $H_0 = [H^m\Theta(-z) + H^{sc}\Theta(z)]$, where H^m describes the metal, H^{sc} describes the semiconductor, and the interface

is located at $z = 0$. The eigenstates of H_0 have the form $\Psi_0 = (\Psi^m_{k_\perp,k_\parallel} + \alpha\Psi^m_{-k_\perp,k_\parallel})\Theta(-z) + \beta\Psi^{\rm sc}_{k'_\perp,k_\parallel}\Theta(z)$, where Ψ^m is an eigenstate of H^m, $\Psi^{\rm sc}$ is an eigenstate of $H^{\rm sc}$ which may be evanescent, and the coefficients α and β are determined by interface matching conditions. For each state Ψ_0, there is electron flux transmitted into the semiconductor. (This flux is zero if $\Psi^{\rm sc}$ is evanescent.) The transmission coefficient T for the state Ψ_0 is the ratio of the transmitted flux in the semiconductor to the incoming flux in the metal for that state. In BEEM, a distribution of H_0 eigenstates is populated by tunneling. If there were no scattering, the BEEM current in the semiconductor would be a sum over the populated states of the incident electron flux times the transmission coefficient of the state. δH leads to transitions between the eigenstates of H_0, so the BEEM current becomes

$$I_B = eA\sum_{\vec{k}^i} F^i_\perp\left[T^i\left(1 - \sum_f P_{i\to f}\right) + \sum_f P_{i\to f}T^f\right].$$

Here, $\vec{k}^i$ is a wave vector in the metal which labels the eigenstates of H_0, $F^i_\perp$ is the interface normal flux in that state induced by tunneling, T is a transmission coefficient, $P_{i\to f}$ is the probability that a transition is induced by δH from state i to state f, both eigenstates of H_0, and A is the area in the planar tunneling model. The first term in brackets corresponds to electrons which are not scattered by δH and the second term corresponds to scattered electrons. The eigenstates of H_0 consist of an incident and reflected part in the metal and a transmitted part (perhaps evanescent) in the semiconductor. The three components of the eigenstate have the same interface parallel wave vector which, because tunneling preferentially weights forward directed states, is small for the likely populated initial states. δH scatters electrons between the eigenstates of H_0. The scattering conserves energy, but not interface parallel wave vectors. In the final state of the scattering process, states with large interface parallel wave vectors can be occupied with reasonable probability.

The perturbing Hamiltonian results from interfacial scattering centers. Let $\Pi^j_{i\to f}$ be the probability of scattering from state i to state f from the j'th scattering center (a number small compared to unity) if there were no other scattering centers to interfere with this process. This probability is the ratio of the scattering transition rate divided by the rate at which electrons are incident on the interface.

$$\Pi^j_{i\to f} = \frac{(2\pi/\hbar)\,(|M|^2/\Omega^2)\delta(\varepsilon_i - \varepsilon_f)}{A(\hbar k^i_\perp/m)\,(1/\Omega)},$$

where Ω is the normalization volume, $(|M|^2/\Omega^2)$ is the squared scattering matrix element (it is convenient to display the Ω dependence of the matrix element explicitly), $\delta(\varepsilon_i - \varepsilon_j)$ is the energy conserving delta function, A is the interface area, and $\hbar k^i_\perp/m$ is the velocity at which the electron in state i approaches the interface (evaluated in a free electron model). The total probability for scattering from state i to state f is

$$P_{i\to f} = \left(\sum_j \Pi^j_{i\to f}\right)(1 - S),$$

where S is the probability of any scattering event $S = \sum_f P_{i\to f}$ and the factor $(1 - S)$ accounts for interference from other scattering events. Solving for S gives

$$P_{i\to f} = \frac{\sum_j \Pi^j_{i\to f}}{1 + \sum_{j,f}\Pi^j_{i\to f}}.$$

We take the scattering matrix element to be independent of the initial and final states of the process corresponding to scattering from a hard core potential. An electron in the initial state is then randomly distributed among the H_0 eigenstates of the same energy after a single scattering event, so it is not necessary to explicitly include multiple scattering effects.

We evaluate the BEEM current at zero temperature using a free electron model for the metal and an effective mass model for the semiconductors with spherical but nonparabolic effective masses, $m^*(E) = m^*_0(1 + \alpha E)$, where α is the nonparabolicity parameter. The BEEM current for direct transmission into a valley is

$$I^D_B = eA\left[\left(\frac{1}{2\pi}\right)^2\frac{2m}{\hbar^3}\,e^{-\delta/\xi}\right]\int_0^{eV-E_b} dE_S\left(\frac{m^*}{m}\right)^2 \times (2E_i)\,\frac{1}{\pi}\int_0^{\pi} d\theta\int_0^{\lambda}\frac{dx(4ax^2)}{(a + x)^2}\,\frac{e^{-2gl}}{(1 + \eta/a)}$$

and the BEEM current for transmission into a valley with scattering is

$$I^S_B = eA\left[\left(\frac{1}{2\pi}\right)^2\frac{2m}{\hbar^3}\,e^{-\delta/\xi}\right]\int_0^{eV-E_b} dE_S\left(\frac{m^*}{m}\right)^2 \times \int_0^{E_i}\frac{d\varepsilon e^{-2gl}(\eta/Q)}{[1 + \eta/Q]}\,\frac{1}{\pi}\int_0^{\pi} d\theta\int_0^{\lambda}\frac{dx(4x^2)}{(a + x)^2}$$

where δ is the metal thickness, ξ is the hot electron attenuation length, l is the vacuum tunneling length, and g is the WKB tunneling factor [14]. Here, V is the tip bias, Φ is the work function and E_f is the Fermi energy, E_b is the threshold energy for the valley,

$$E_i = E_S + E_f + E_b, \qquad \lambda = \left(\frac{mE_S}{m^*E_i}\right)^{1/2},$$

$$\eta = \frac{N}{A}\,\frac{m}{\hbar^2}\,\frac{|M|^2}{2\pi},$$

$$a = \left[1 - \frac{\hbar^2 (k_\parallel^0)^2}{2mE_i} - \frac{m^*}{m}\left(\frac{E_S - \frac{m^* E_i}{m} x^2}{E_i} \right) - \frac{\hbar^2 (k_\parallel^0)}{mE_i}\left[\frac{2m^*}{\hbar^2}\left(E_S - \frac{m^* E_i}{m} x^2 \right) \right]^{1/2} \cos\theta \right]^{1/2},$$

$Q = (1 - \varepsilon/E_i)^{1/2}$, $k_\parallel^0$ is the parallel wave vector at the energy minimum, and N is the number of interfacial scattering centers.

For GaAs, we consider Γ, L, and X minima, and, for Si, the Δ minima. The required material parameters are known for these well studied materials [15]. For Au, we use a Fermi energy of 5.5 eV, a work function of 5.1 eV, and an attenuation length of 13 nm [11]. For GaAs, we use the following: For the effective masses, $m_\Gamma^* = 0.067m$, $m_L^* = 0.22m$, and $m_X^* = 0.41m$; for the nonparabolicity parameters, $\alpha_\Gamma = 0.69\ \mathrm{eV}^{-1}$, $\alpha_L = 0.65\ \mathrm{eV}^{-1}$, and $\alpha_X = 0.36\ \mathrm{eV}^{-1}$; for the Au Schottky barrier, 0.88 eV [16]; and for the Γ-L and Γ-X energy separations, 0.33 and 0.52 eV, respectively. For Si, we use, for the effective mass, $0.33m$; for the nonparabolicity parameter, $0.50\ \mathrm{eV}^{-1}$; and for the Au Schottky barrier, 0.80 eV [16]. l is adjusted as a function of tip bias to give a constant tunneling current density chosen so that the tip-to-metal film separation is close to 1 nm. In the strong scattering limit, there is essentially no dependence of the calculated ratio of BEEM to tunneling current on l. The strength of the interface scattering η determines the probability that an electron scatters at the interface, which is $\eta/(1 + \eta)$, and the probability that it does not scatter, which is $1/(1 + \eta)$. In the weak scattering limit $\eta \to 0$, the result reduces to the traditional description of BEEM with the inclusion of quantum mechanical reflection at the metal/semiconductor interface. In the strong scattering limit $\eta \to \infty$, all of the electrons scatter.

Figure 1 compares the calculated ratio of BEEM to tunneling current in the strong scattering limit as a function of tunneling tip bias for Au/GaAs(100) with the experimental results of Ref. [7]. In the strong scattering limit, the injected flux distribution is redistributed by scattering and valleys with zero interface parallel wave vectors at their energy minimum are not preferentially weighted. The calculation in the strong scattering limit gives a reasonable description of the experimental results without fitting parameters. The inset of Fig. 1 compares the calculation in the weak scattering limit with the experimental results. In this limit, the calculated current in the Γ and X channels are much too large and in the L channel much too small to describe the data. Elastic scattering must both greatly reduce current in the Γ and X channels and greatly increase current in the L channel to describe the data. The scattering strength η must be large so that almost all of the electrons scatter at the interface in order to sufficiently reduce the current in the Γ channel. Because there was an oxide layer at the interface [7] of this sample, strong interface scattering is to be expected.

Figure 2 compares the calculated ratio of BEEM to tunnel current in the strong scattering limit as a function of tunneling tip bias for Au/Si with the experimental results of Ref. [11]. The calculated results in the strong scattering limit for Si(100) and Si(111) are very similar to each other as is observed experimentally [9,10] and give a reasonable description of the experimental results without fitting parameters. The inset of Fig. 2 compares the calculation in the weak scattering limit with the experimental results. In this limit, the calculated result for Au/Si(100) is too large and for Au/Si(111) is too small to describe the data. Elastic scattering must both greatly reduce current for Si(100) and increase current for Si(111) to describe the data. The scattering strength η must be large in order to sufficiently reduce the current for Si(100). The Au/Si interface is not epitaxial and scattering centers can arise from structural defects at the incommensurate interface. Hydrogen terminated Si surfaces were used in the sample fabrication of Ref. [11] to achieve a chemically clean interface.

Elastic scattering at the metal/semiconductor interface is specifically considered in this model. To describe the BEEM data, it is necessary to go to the strong scattering limit. Scattering simultaneously reduces the intensity of the calculated BEEM current in the Γ channel and increases it in the L channel of Au/GaAs(100) and, in the strong scattering limit, the calculated results agree well

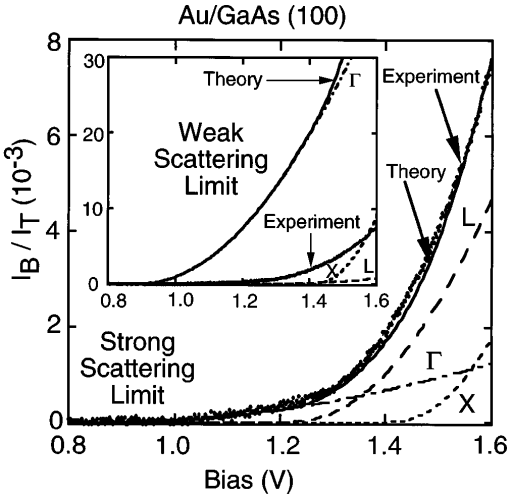

FIG. 1. Comparison of the calculation in the strong scattering limit for Au/GaAs(100) with the experimental results of Ref. [7]. The dot-dashed line shows the Γ, the long-dashed line the L, the short-dashed line the X contribution to the BEEM current, and the solid line the sum of the three. The inset compares the calculation in the weak scattering limit to the same experimental results.

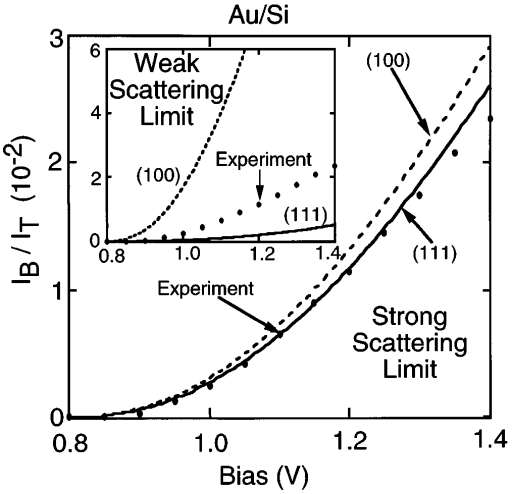

FIG. 2. Comparison of the calculation in the strong scattering limit for Au/Si(100) (dashed line) and Au/Si(111) (solid line) with the experimental results for Au/Si of Ref. [11]. These measurements were made on Au/Si(111) but measurements for Au/Si(100) are very similar to those for Au/Si(111) (see Refs. [9] and [10]). The inset compares the calculation in the weak scattering limit to the same experimental results.

with the experimental results. Both the reduction of the Γ channel current and the enhancement of the L channel by scattering are necessary for the calculated results to agree with the experiment. Scattering reduces the calculated BEEM current for Au/Si(100) and increases it for Au/Si(111) and, in the strong scattering limit, the calculated results agree well with the experimental results. Again, both the reduction of the current for the (100) orientation and the enhancement of the current for the (111) orientation are necessary to agree with the experiment.

In Ref. [11], the attenuation of BEEM current with metal thickness was shown to be nonexponential at low Au thickness, and the shape of the BEEM I-V curve in Au/Si(111) for thick Au layers was found to change with temperature. Elastic scattering in the metal and multiple reflections between the metal surfaces were considered to interpret these results. The electron attenuation length in Au was measured to be 13 nm and the elastic mean free path at room temperature was estimated to be 40 nm. If only elastic scattering in the metal and multiple reflections are considered, it is necessary that almost every electron scatter elastically before it hits the interface to describe the small BEEM current in the Γ channel for Au/GaAs(100) and the small threshold current for Au/Si(100). This would require an elastic mean free path much less than the film thickness, which is typically 5–10 nm. Very short elastic mean free paths are not consistent with the observed nanometer spatial resolution in BEEM imaging of these interfaces [1,8,10].

In summary, we present a model to describe BEEM on nonepitaxial metal/semiconductor interfaces that starts with eigenstates of an ideal interface Hamiltonian and allows elastic scattering processes to redistribute the incident electrons injected by tunneling among these eigenstates. In the weak scattering limit, the results of the model reduce to the traditional description of BEEM which assumes interface parallel wave vector conservation at the interface. In the strong scattering limit, it quantitatively describes the BEEM data on Au/GaAs and Au/Si.

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[1] W. J. Kaiser and L. D. Bell, Phys. Rev. Lett. **60**, 1406 (1988).
[2] L. D. Bell and W. J. Kaiser, Phys. Rev. Lett. **61**, 2368 (1988).
[3] M. Prietsch, Phys. Rep. **253**, 163 (1995).
[4] L. D. Bell and W. J. Kaiser, Annu. Rev. Mater. Sci. **26**, 189 (1996).
[5] J. J. O'Shea, T. Sajoto, S. Bhargava, D. Leonard, M. A. Chin, and V. Narayanamurti, J. Vac. Sci. Technol. B **12**, 2625 (1994).
[6] M.-L. Ke, D. I. Westwood, C. C. Matthai, B. E. Richardson, and R. H. Williams, Phys. Rev. B **53**, 4845 (1996).
[7] J. J. O'Shea, E. G. Brazel, M. E. Rubin, S. Bhargava, M. A. Chin, and V. Narayanamurti, Phys. Rev. B **56**, 2026 (1997).
[8] H. D. Hallen, A. Fernandez, T. Huang, J. Silcox, and R. A. Buhrman, Phys. Rev. B **46**, 7256 (1992).
[9] L. J. Schowalter and E. Y. Lee, Phys. Rev. B **43**, 9308 (1991).
[10] A. M. Milliken, S. J. Manion, W. J. Kaiser, L. D. Bell, and M. H. Hecht, Phys. Rev. B **46**, 12 826 (1992).
[11] L. D. Bell, Phys. Rev. Lett. **77**, 3893 (1996); J. Vac. Sci. Technol. A **15**, 1358 (1997).
[12] R. Ludeke and A. Bauer, Phys. Rev. Lett. **71**, 1760 (1993).
[13] A. Bauer, M. T. Cuberes, M. Prietsch, and G. Kaindl, Phys. Rev. Lett. **71**, 149 (1993).
[14] Expressions for g, etc., in the present notation are given in D. L. Smith and Sh. M. Kogan, Phys. Rev. B **54**, 10 354 (1996).
[15] There is, of course, some variation in the precise values quoted for the material parameters. The values used here are typical, and minor variations of these do not significantly change the calculated results.
[16] See, for example, S. M. Sze, *Physics of Semiconductor Devices* (Wiley, New York, 1981), 2nd ed.