Observation of Interface Band Structure by Ballistic-Electron-Emission Microscopy

L. D. Bell and W. J. Kaiser
Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91109
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A unique ballistic-electron spectroscopy technique has been employed to measure directly semiconductor-band-structure properties at a subsurface interface for the first time. Further, the method, based on scanning tunneling microscopy, enables spatially resolved carrier-transport spectroscopy of interfaces. A theoretical treatment has been developed which accurately accounts for the observed spectroscopic features.

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Semiconductor interface band structure is critical in determining important electronic properties of semiconductor structures such as superlattice carrier mobilities, quantum-well depths, and optoelectronic response. Detailed surface and interface band structures have been investigated by several methods including photoemission, but not by direct electrical measurement of heterostructures.[1] Several important ballistic-electron spectroscopy methods based on semiconductor heterostructures have recently been developed.[2,3] However, because of limitations of the heterostructures employed, only a narrow range of electron energy may be probed and band-structure effects are not directly observed. Also, because of uncertainty in the electronic properties of the heterostructure, detailed analysis of the ballistic-electron spectra is complicated. Conventional surface analytical techniques are limited in their capabilities for probing buried interfaces. Further, these and other conventional interface characterization methods do not offer high spatial resolution.

We report an advanced ballistic-electron spectroscopy method based on ballistic-electron-emission microscopy (BEEM),[4] which enables the first observation of local interface band structure. Two important semiconductor interface systems having contrasting band structures are investigated by this method: Au-Si and Au-GaAs. The important features of the conduction-band structure at the subsurface interface are investigated for both interfaces. A theoretical description is presented which accounts for the resulting spectroscopic features, and predicts high spatial resolution for interface electronic properties by BEEM.

In the present work, BEEM, based on scanning tunneling microscopy,[5] is implemented in a three-terminal configuration, as shown in Fig. 1(a). The scanning-tunneling-microscopy tip emits ballistic electrons into a metal-semiconductor structure via vacuum tunneling. These low-energy electrons have attenuation lengths of greater than 100 Å in metals,[6] and some of the electrons reach the metal-semiconductor Schottky-barrier (SB) interface with no energy loss. If base-tip bias V is greater than the SB height V_b, many of these electrons may cross the interface and enter the semiconductor, where they are measured as a collector current I_c. For V less than V_b, electrons cannot enter the collector and I_c is zero. BEEM spectra are acquired by sweeping tunnel voltage while feedback controlling the tunnel gap, S, at a predetermined tunnel current. The I_c-V spectrum is a direct probe of the SB interface electronic structure and of the bulk transmission properties of the base film. By scanning the tip over the heterostructure surface, simultaneous spatial imaging of subsurface properties and surface topography is achieved.[4]

A simple theoretical treatment has been developed which describes subsurface interface band-structure spectroscopy and imaging by BEEM. Conservation laws involving energy and transverse momentum have been

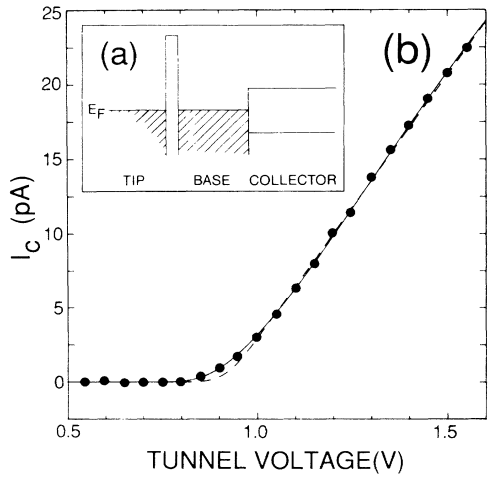

FIG. 1. BEEM probing of the Si conduction-band minimum at the Au-Si interface. (a) Energy-band diagram of the three-terminal BEEM configuration. The tunnel tip, separated by a vacuum barrier from the base electrode, serves as emitter of ballistic electrons into the base-collector structure. If the applied tip-base voltage V is greater than the SB height V_b, electrons may cross the SB interface and be collected. (b) The BEEM I_c-V spectrum (dots) for the Au-Si structure recorded at a tunneling current I_t of 0.87 nA. The dashed line is a calculated spectrum for the simple 1D theory. The solid line is a calculated spectrum for the theory given in Eq. (5), yielding a threshold of value of 0.82 eV.

invoked in this treatment. Also, a free-electron dispersion relation in the tip and base, and a parabolic conduction-band minimum in the semiconductor are treated. The theoretical treatment predicts the detailed behavior of the collector current at threshold which is independent of fitting parameters and is found to be in excellent agreement with experiment.

We have used a well-known formalism for tunneling between planar electrodes to describe the tunneling current I_t.[7] Electrons tunneling from the tip to the metal base occupy tip states within a shell of the Fermi sphere between $E=E_F$ and $E=E_F-eV$.[8] Defining the energies associated with the components of the electron wave vector normal and transverse to the interface as E_x and E_t, respectively, within the tip electrode, then

$$I_t=C\int_0^\infty D(E_x)\int_0^\infty [f(E)-f(E+eV)]dE_t\,dE_x\,, \quad (1)$$

where $D(E_x)$ is the transmission probability for an electron to tunnel through the vacuum barrier, $f(E)$ is the Fermi function, and C is a constant.[7] The expression from planar tunneling theory for a square barrier is used for $D(E_x)$.[7]

A similar expression can be directly obtained for the collector current by considering a shell in the Fermi sphere of the tip between $E=E_F$ and $E=E_F-e(V-V_b)$. However, well-known conservation laws at the metal-semiconductor interface[9,10] further constrain the allowed tip states. This can be seen by our considering an electron entering the semiconductor from the base at an energy just above that of a zone-centered band minimum in the semiconductor. The electron has a kinetic energy on the order of 7 eV in the Au base. As it enters the semiconductor near the bottom of the conduction band, it loses a large fraction of the normal component of its kinetic energy. However, following the treatment of photoresponse,[11,12] transverse momentum is conserved across the interface in the absence of scattering. This causes a "refraction" of the electron as it enters the semiconductor. An electron with large transverse momentum is unable to enter the semiconductor since there are not states satisfying the (E,k_t) relationship for the electron. Specifically, conservation of k_t defines a critical angle for electron propagation in the base outside of which electrons may not be collected:

$$\sin^2\theta_c=\frac{m_t}{m}\frac{V-V_b}{E_F+V}\,, \quad (2)$$

where m_t is the electron effective mass parallel to the interface within the semiconductor, and m is the free-electron mass.[9] The accompanying restriction on transverse energy within the tip for m_t less than m is simply

$$E_t\le\frac{m_t}{m-m_t}[E_x-E_F+e(V-V_b)]\,. \quad (3)$$

Only electrons within the tip with E_t given by Eq. (3) may be collected, in the absence of scattering.

The following expression may therefore be written for collector current:

$$I_c=RC\int_{E_{min}}^\infty D(E_x)\int_0^{E_{max}} f(E)\,dE_t\,dE_x\,, \quad (4)$$

where R is a measure of attenuation due to scattering in the base layer. R is taken to be an energy-independent constant, since ballistic-electron attenuation lengths in metals are nearly independent of energy for $E-E_F$ of less than 2 eV.[13] E_{max} is given by $[m_t/(m-m_t)]\times[E_x-E_F+e(V-V_b)]$, as in Eq. (3), and $E_{min}=E_F-e(V-V_b)$.

The collector current in terms of the tunnel current from Eqs. (1) and (4) is, therefore,

$$I_c=RI_t\frac{\int_{E_{min}}^\infty D(E_x)\int_0^{E_{max}} f(E)\,dE_t\,dE_x}{\int_0^\infty D(E_x)\int_0^\infty [f(E)-f(E+eV)]dE_t\,dE_x}\,. \quad (5)$$

Equation (5) is fitted to the experimental spectra by adjustment of V_b and R.[14] Most importantly, as a consequence of the parabolic conduction-band minimum and k_t conservation, Eq. (5) predicts that the I_c-V spectrum behaves as $(V-V_b)^2$ for voltages just above the threshold value V_b, independent of the fitting parameters.

An important consequence of transverse-momentum conservation at the interface and the existence of the critical angle defined in Eq. (2) is a focusing which provides high spatial resolution of interface properties. Since only electrons with small transverse momenta in the base may be collected, scattering in the base serves mainly to reduce the number of electrons collected, rather than to reduce resolution. For example, for GaAs with $m_t/m=0.067$,[15] only electrons within a few degrees of normal incidence may be collected, for $e(V-V_b)$ of a few tenths of an eV, yielding a lateral resolution of order 10 Å for a 100-Å-thick base layer. High spatial resolution has previously been obtained for BEEM images of the Au-GaAs interface,[4] in agreement with this treatment.

Interface band structure was investigated in two important metal-semiconductor interfaces: Au-Si and Au-GaAs. It is important to contrast the complex GaAs conduction-band structure with that of Si in the energy range probed by this experiment: GaAs has a direct conduction-band minimum at the zone center and two higher indirect minima at the L and X points of the Brillouin zone,[15] while Si has only a single conduction-band minimum along the [100] direction. The ballistic-electron spectroscopy of BEEM may probe the direct and indirect band minima of both systems. The interfaces were prepared by evaporating Au electrodes in ultrahigh vacuum on chemically prepared n-Si(100) ($n=2\times10^{15}$ cm^{-3}) and n-GaAs(100) ($n=3\times10^{16}$ cm^{-3}) substrates. The experimental apparatus has been described previously.[4,16]

A typical I_c-V BEEM spectrum for a Au-Si hetero-

structure is shown in Fig. 1(b). Also plotted are a fit by a simple one-dimensional (1D) theory including thermal broadening but neglecting transverse-momentum conservation,[4] and a fit by the theory developed above. A deviation of the 1D theory from the experimental spectrum is observed at the threshold region. With use of the theory developed above, however, excellent agreement is obtained for all data points. The threshold region of Fig. 1(b) is shown on an expanded scale in Fig. 2(a), emphasizing the agreement of the theory with the experimental spectrum in the threshold region. A stringent test of the agreement between theory and experiment may be made by our comparing the derivative dI_c/dV vs V for the data and for the theory, as shown in Fig. 2(b). The experimental dI_c/dV spectrum reveals the inflection of the I_c-V spectrum above threshold as a maximum in the derivative curve; the calculated spectrum also displays this behavior. The dI_c/dV spectrum also reveals a linear region above 0.8 eV corresponding to a square-law behavior of the I_c-V spectrum above threshold. Most importantly, the square-law behavior of the spectrum near threshold is independent of fitting parameters; it is a direct consequence of the parabolic conduction-band minimum of the Si interfacial band structure and the resulting restrictions on k_t.

The Au-GaAs spectra display features which are qualitatively different from those of the Au-Si spectra. These spectra display a threshold region which, in contrast to the Au-Si spectra, is apparently composed of multiple thresholds. This dramatic difference is seen by comparing a typical spectrum obtained for a Au-GaAs heterostructure shown in Fig. 3(a) with the spectrum obtained for a Au-Si heterostructure shown in Fig. 1.

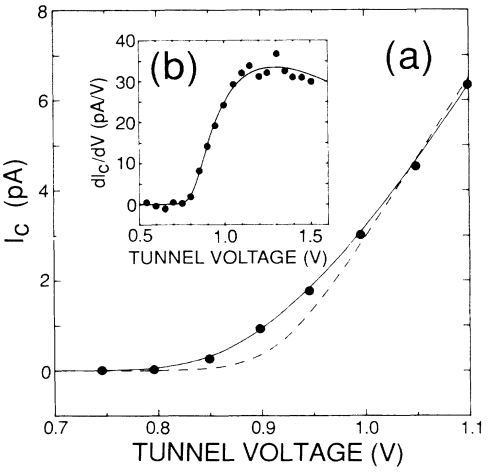

FIG. 2. (a) Expanded plot of the threshold region of the BEEM spectrum shown in Fig. 1(b), displaying the excellent agreement of Eq. (5) with experiment. Experimental points are shown as dots, with the dashed and solid lines as indicated in Fig. 1(b). (b) dI_c/dV vs V for the experimental BEEM spectrum and the calculated solid-line spectrum of Figs. 1(b) and 2(a).

The multiple-threshold structure observed in the Au-GaAs BEEM spectroscopy was investigated by our fitting the theory of Eq. (5) with three threshold values; the resulting spectrum is plotted in Fig. 3(a). For comparison, theoretical spectra for one and two thresholds are also displayed. For the case of three thresholds, the agreement between theory and experiment is excellent, yielding threshold values of 0.89, 1.18, and 1.36 eV. The first threshold value is in agreement with the commonly accepted value for the Schottky-barrier energy for Au-GaAs, 0.9 eV.[1] The differences between the upper thresholds and the lower one, 0.29 and 0.47 eV, agree well with the expected relative energies of the three lowest conduction-band minima in GaAs; 0.29 and 0.48 eV for the separation between the direct minimum and the satellite minima at the L and X points, respectively.[15] The thresholds are therefore assigned to ballistic-electron injection into the Γ, L, and X minima, respectively. As a sensitive test of the agreement between experiment and theory the experimental and theoretical derivative spectra, dI_c/dV vs V, are compared in Fig. 3(b). The thresholds, marked by arrows, appear as steps in the derivative spectra and the theory agrees well with the experimental BEEM spectrum. The changes in slope at the thresholds show relative magnitudes which are in agreement with the ordering of the different effective masses of the three minima.[15] It is useful to compare the multiple thresholds seen in the Au-GaAs dI_c/dV spectra of Fig. 3(b) with the single threshold observed for Au-Si in Fig. 2(b).

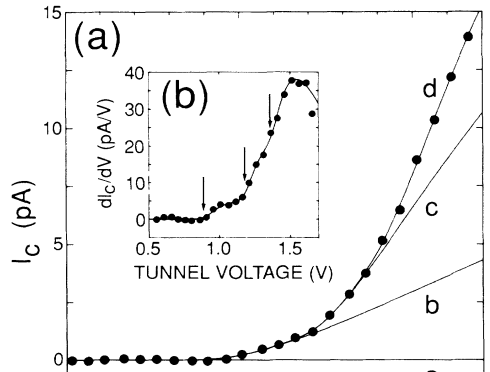

FIG. 3. BEEM probing of the direct minimum and satellite minima of the GaAs conduction band at the Au-GaAs interface. (a) BEEM I_c-V spectrum (dots) for a Au-GaAs heterojunction recorded at $I_t = 1$ nA. Curve a is a zero-current reference; curves b, c, and d are calculated spectra treating one, two, and three thresholds, respectively. Spectrum d yields threshold values of 0.89, 1.18, and 1.36 eV. (b) Derivative dI_c/dV vs V for the data (dots) and the calculated spectrum d shown in part (a). The three threshold values are indicated by arrows.

Many I_c-V spectra were measured at different locations on many Au-GaAs structures. The multiple thresholds were observed in all spectra obtained. The spectrum shown in Fig. 3 is representative of the average values for the thresholds observed. However, spatial variations as large as 0.1 eV in the relative energies of the three thresholds were detected, providing a direct measure of the local variation of the GaAs conduction-band structure. Variation in local interface band structure may result from variation in interfacial strain[15] or diffusion-induced nonstoichiometry.[1]

In conclusion, ballistic-electron spectroscopy methods have been employed to directly observe interface band-structure properties. Also, a simple theory has been developed which accurately describes the observed spectroscopic behavior. Two important interface systems having contrasting band structure have been investigated: Au-GaAs and Au-Si. The Au-Si spectra, reflecting the simple band structure of Si, provide a stringent test of the proposed theory, and it is shown that the agreement between data and theory is excellent. The Au-Si spectra indicate that the detailed spectral shape is directly determined by the interfacial semiconductor band structure. For the Au-GaAs interface, BEEM spectra clearly reveal properties of the satellite conduction-band minima of GaAs. Further, BEEM has yielded the first direct measure of local variation in the GaAs conduction-band structure. Since for certain interface systems spatial variations may induce smearing of spectral features in large-area measurements, only a local probe such as BEEM may enable observation of interface band structure for such interfaces. The ballistic-electron spectroscopy methods discussed here are applicable to the investigation of many systems, including semiconductor-semiconductor strain-layer interfaces, where the local variation in band structure plays an important role in determining the interface electronic properties.

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[14]All fits of Eq. (5) to experimental spectra were performed with values of barrier height $\phi = 3$ eV and $S = 15$ Å. The approximation of constant S is justified since the small variation in S occurring during the sweep of V produces less than a 3% variation in the collector current calculated from Eq. (5) over the entire spectral range. It is important to note that the quality of the agreement between theory and experiment is not sensitive to variations of ϕ in the range 2–4 eV or S in the range 12–18 Å.

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