Evidence of Momentum Conservation at a Nonepitaxial Metal/Semiconductor Interface Using Ballistic Electron Emission Microscopy

L. D. Bell

Center for Space Microelectronics Technology, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91109

(Received 13 May 1996)

Ballistic-electron-emission microscopy (BEEM) spectroscopy has been performed on Au/Si(111) structures as a function of Au thickness and temperature. At 77 K a direct signature of parallel momentum conservation at the Au/Si interface is observed in the BEEM spectra. The variation in spectral shape with both Au thickness and temperature places restrictions on allowable values of inelastic and elastic mean-free paths in the metal, and also requires the presence of multiple electron passes within the Au layer. An independent indication of multiple reflections is directly observed in the attenuation of BEEM current with Au thickness. [S0031-9007(96)01516-5]

PACS numbers: 73.50.Gr, 61.16.Ch, 73.30.+y, 73.61.At

The verification of parallel momentum ($k_\parallel$) conservation at a metal/semiconductor (*M/S*) interface is of fundamental importance to the operation of many novel device structures, such as metal-base transistors and quantum well photodetectors, and to transport models used to characterize them. In epitaxial *M/S* structures the question is less controversial, since atomically abrupt interfaces can be achieved between materials with matching lattice nets. The problem of identifying $k_\parallel$ conservation in the case of a nonepitaxial evaporated metal film has been the subject of much research and is conceptually less straightforward. Contributing to the difficulty is the insensitivity of conventional measurements to this process. In general, the problem is one of separating a lack of $k_\parallel$ conservation, in the form of elastic interface scattering, from other scattering processes.

Ballistic-electron-emission microscopy [1] (BEEM), based on scanning tunneling microscopy [2] (STM), provides a nanometer-scale method for probing transport and interface properties. BEEM uses an STM tip to inject hot electrons into a *M/S* structure, where the collector current (I_c) which enters the semiconductor is measured. Even BEEM measurements, however, have been inconclusive in determining the degree of $k_\parallel$ conservation at nonepitaxial *M/S* interfaces. One early prediction [3] based on this idea was the BEEM spectrum for metal/Si(111). This was expected to differ dramatically from that of metal/Si(100), showing a much more slowly increasing threshold region and a substantially different spectral shape. This is due to the mismatch between the off-axis Si conduction-band minima and the forward-focused electron distribution in the metal produced by tunneling.

This predicted behavior was not observed for Au/Si(111). Instead, previously reported BEEM spectra [3] are nearly identical to those for Au/Si(100). This observation, while not confirming $k_\parallel$ conservation, does not disprove it. Elastic scattering in the metal film can provide the necessary momentum for electrons to enter the Si(111) conduction band, even if $k_\parallel$ is conserved at the *M/S* interface. A measurement is needed which separates the various scattering components and allows interface processes to be assessed independently. This Letter describes the observation of $k_\parallel$ conservation at a *M/S* interface by BEEM, even under conditions in which standing waves and coherent transport within the metal may not be observed.

A series of BEEM spectra was obtained for Au/*n*-Si(111) samples with varying Au thickness, both at room temperature and at 77 K. Sample preparation has been described elsewhere [1]. Several samples were fabricated for each Au thickness, and many spectra from these samples were averaged together for analysis. BEEM results were reproducible between similar sets of averaged spectra. Measurements were performed in a nitrogen-purged glovebox, and low-temperature spectra were acquired by direct immersion of the system in liquid nitrogen.

A summary of the results for two Au thicknesses is present in Fig. 1. Spectra from samples with intermediate thicknesses are not shown; these display a smooth transition of spectral shape with Au thickness at both temperatures. Note that, at room temperature, the shape near the threshold remains constant, as does the threshold position V_{th}. These spectra agree with those previously reported for Au/Si(111) [3] and with those obtained for Au/Si(100). The increasing inflection of the data at higher voltages as Au thickness increases results from an increasing contribution from inelastic scattering in the Au.

At 77 K the spectrum shape, even near threshold, changes dramatically with increasing Au thickness; because of this changing shape, the apparent threshold increases substantially. Near-threshold phase-space fits are also shown for these spectra, with the derived threshold values; while the fit is adequate for thin Au, it is clearly unsatisfactory for spectra obtained with thick Au layers. However, these fits provide a qualitative means of tracing the change in spectral shape and the increase of the apparent threshold. It is important to emphasize that this simple model fits low-temperature Au/Si(100) spectra extremely well, independent of Au thickness.

0031-9007/96/77(18)/3893(4)$10.00

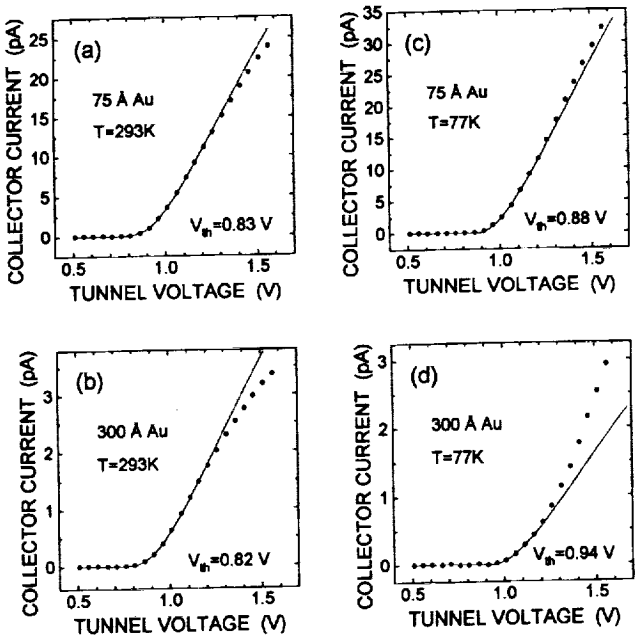

FIG. 1. Experimental BEEM spectra (circles) obtained for Au/Si(111) samples at a tunnel current of 1 nA. Solid lines are fits to the data using the original BEEM phase-space model. Fitting is only to data points at $V \leq 1.2$ V.

This change in spectral shape is a remarkable result. The 77 K Au/Si(111) spectra for the thickest Au layers closely match those calculated for no elastic scattering and for $k_{\|}$ conservation at the *M/S* interface. Surprisingly, this behavior appears only for thicker Au layers, while it might be expected that increased scattering in thick layers would preclude this observation.

There are several points concerning these observations which should be emphasized. First, this behavior appears for only thick Au and only at low temperature. Second, spectra for Au/Si(100) do not exhibit this low-temperature behavior. Therefore, the evolution of spectrum shape at low temperature cannot be attributed to a modification of the electron distribution by increased scattering in the Au. Moreover, spectra obtained at room temperature, where scattering is stronger, do no exhibit this behavior for either substrate orientation.

It is also important to note that Au band structure effects are unlikely to be responsible for this effect. Evaporated Au has been observed to be primarily of (111) orientation on both Si(100) and Si(111) [4,5], but only the 77 K Si(111) results display this changing spectral shape. A recent calculation [6] suggested that the Au band structure might be responsible for the previously observed similarity of Au/Si(100) and Au/Si(111) BEEM spectra. However, such effects would not produce the observed gradual evolution of spectral shape at such thick Au layers, nor would they be expected to be sensitive to temperature. Thus the observed low-temperature spectra are correlated solely with the change to the (111) substrate orientation.

To understand these observations it should first be noted that inelastic scattering in the metal will usually remove an electron from the collection process altogether, since the energy lost is large (averaging one-half of the electron's kinetic energy) [7]. Therefore, elastic scattering is the important process in the modification of the momentum distribution of collectable electrons. The only interpretation consistent with these observations is that, at 77 K, elastic scattering is *decreasing* as the Au layer thickens. The contributions of nearly all components of scattering (electron-phonon, electron-electron, impurity, and defect scattering) will increase with metal thickness. One contribution, elastic scattering from the metal film boundaries, will decrease with film thickness, since as the boundaries are separated the electrons encounter them less frequently. Thus the dominant source of elastic scattering and momentum randomization at low temperature must be diffuse reflection from the Au surface, implying multiple passes within the Au film. It is not required that the surface reflection be locally diffuse, since many BEEM spectra are averaged together. STM images of the Au surface reveal the typical polycrystalline structure of evaporated Au films; averaging over different surface gradients will provide an average diffuseness to the reflected distribution. Indeed, averages of smaller subsets of data show some variation in spectral character.

Specular reflection at the *M/S* interface is assumed, in order to be consistent with $k_{\|}$ conservation and specular transmission. High-resolution cross-sectional transmission electron microscopy (TEM) was performed in order to characterize the Au/Si(111) interface. Images reveal a large-height step structure, with large, flat terraces. The step risers often were observed to form (100) facets. This stepped topography is quite different from the interface character previously observed for (100) structures [8] where large areas of flat topography were seldom seen. The TEM results suggest that a Si(111) surface is more resistant to reaction with Au than the (100) surface. Similarly, in BEEM experiments on Au/Si(111)(7×7) Cuberes *et al.* [9] did not observe the effects of diffusion.

A description for the data can therefore be constructed as follows. At low temperature, the elastic mean-free path λ_e for electron-phonon scattering is greatly increased, and this process is neglected in the analysis for the 77 K data. In contrast, inelastic electron-electron scattering is largely independent of temperature [10]. For thin Au layers, electrons which are not initially collected reflect from the *M/S* interface and reach the surface, where they diffusely scatter. Because the Au is thin, these electrons are able to make several passes through the film before being removed by inelastic scattering. The electrons are randomized by the surface scattering, which allows many more to be subsequently collected. Thus the BEEM spectrum for Au/Si(111) resembles the Au/Si(100) spectrum.

As Au thickness increases, fewer electrons are able to make multiple passes through the Au before inelastical scattering, and the average momentum randomization decreases. For 300 Å Au layers, very few electrons survive to be reflected back to the surface and then be collected

so current is due primarily to electrons collected on their first attempt. Therefore the spectrum is that expected for Si(111) in the absence of elastic scattering. At room temperature, quasielastic scattering due to electron-phonon interactions also randomizes the injected electrons, especially for thicker Au layers. Surface scattering is no longer required for randomization in thick layers, although multiple passes still occur for thinner layers.

The low-temperature observations place limits on the allowable value of the inelastic mean-free path λ_i. This must be long enough to allow multiple electron passes for 75 Å Au, but short enough so as to usually allow only one attempt at 300 Å Au. An additional restriction is imposed by the observed total attenuation length λ_{tot} of about 130 Å for Au, measured by BEEM at room temperature, [11] which has been reproduced by several groups [12,13]. This is related to λ_i and λ_e by the expression $1/\lambda_{\text{tot}} = 1/\lambda_i + 1/\lambda_e$. The calculations discussed below indicate that this relation holds for thick Au layers, but not for thin layers.

In order to determine appropriate scattering parameters for the array of BEEM spectra in Fig. 1, standard Monte Carlo techniques were used. The goal of these calculations was to fit all spectra with a single set of scattering parameters. An energy dependence for λ_i is assumed; however, the theoretical $1/(E - E_F)^2$ dependence [7] is too strong to be consistent with the experimental spectra. Other BEEM experiments have also measured a weaker dependence [14]. For the calculations presented here, a weaker linearly decreasing energy dependence of $\lambda_i = 1.5\lambda_{i0}[1 - (E - E_F)/3]$ is used, where energies are in eV and λ_{i0} is the inelastic mean-free path for electrons at $E - E_F = 1$ eV. This empirical expression was found to provide a consistently good fit to the high-voltage portions of the BEEM spectra. The particular functional form is not critical to the modeling of the threshold region, since the choice primarily affects the higher voltage inflection of the spectra. λ_e is assumed to be energy independent for these energies [15]. Also, no elastic impurity or defect scattering, including grain-boundary scattering, is included. Such a contribution must be small to allow observation of the spectral behavior displayed by the 300 Å data at 77 K. It should also be noted that there was no observed change in Au grain size or texture with increasing Au thickness.

Quantum mechanical reflection, calculated for a step potential, is included in the model. Free-electron band structure is used for the Au layer, and an effective mass model is used for Si with ellipsoidal constant-energy surfaces centered near the X points. Planar tunneling [16] is used for electron injection from the STM tip. A more realistic treatment for tunneling has been introduced for the nonplanar STM geometry [17]. For a 3 eV work function, this yields a tunneling gap of $s \sim 6$ Å, and Lang *et al.* [18] have pointed out that an energy width of ~0.2 eV is expected for the tunneling distribution. In the planar tunneling model a value of $s = 15$ Å, which has been previously used [1] to fit BEEM spectra, reproduces this energy width. This value is used here.

In order to fit both the 75 and 300 Å data at 77 K, a rather narrow range of λ_{i0} proved to be suitable. The observed magnitude of I_c imposes a secondary restriction. For excessively long or short values of λ_{i0}, calculated currents are much larger or smaller than observed. It is encouraging that the range of λ_{i0} which provided the most consistent fit to the spectral shapes of the 77 K data also generated values of I_c which agreed with the observed currents. The best overall series of fits was produced using $\lambda_{i0} = 220$ Å. λ_e was then added to model the room-temperature spectra. A value of $\lambda_e = 400$ Å was used; this was dictated by λ_{i0} and by the observed $\lambda_{\text{tot}} = 130$ Å for moderate Au thicknesses (50–200 Å). These values are larger than those used for the modeling of Pd/Si BEEM results [14]; however, in that case the measured λ_{tot} was also much shorter.

Figure 2 shows the resultant fits for the BEEM spectra from Fig. 1. The calculations exhibit excellent agreement with the data. The change in shape at low temperature is reproduced, leading to an apparent increase in threshold. The addition of phonon scattering also reproduces the room temperature measurements. Furthermore, the calculated I_c magnitudes agree extremely well with the measured values. Fits to data from samples with intermediate Au thicknesses exhibited similar agreement. The

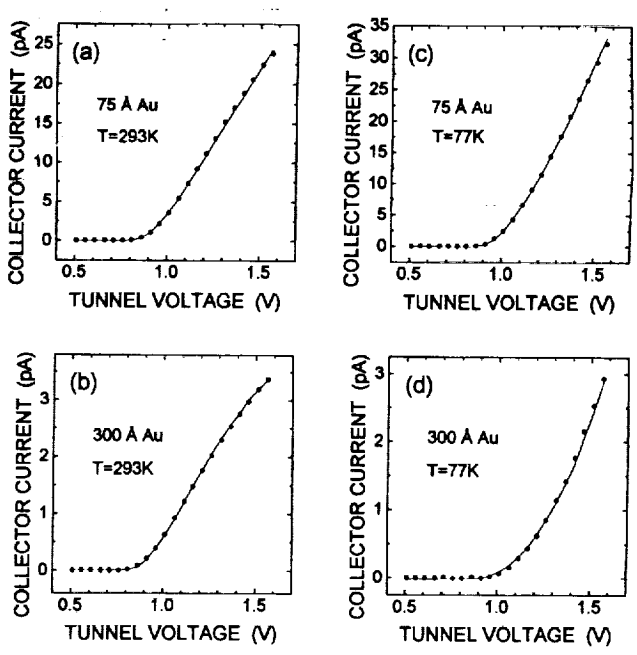

FIG. 2. Experimental BEEM spectra (circles) from Fig. 1. Solid lines are fits to the data using the model described in the text. $V_b = 0.82$ eV was used at room temperature; 0.86 eV was used at 77 K. These values are derived from BEEM measurements on Au/Si(100); the increase at low temperature results from the change in the Si band gap. The calculated curves have been adjusted only slightly by an overall scale factor in order to obtain a best fit to the data. This scale factor ranges from 0.98 to 1.04 for the four spectra.

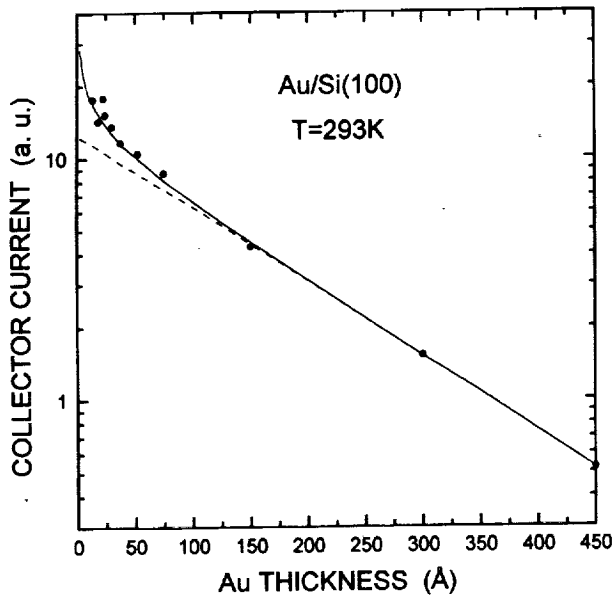

FIG. 3. Experimental BEEM attenuation length measurement (circles) for Au/Si(100) samples. I_c was measured at $V = 1.2$ V. The solid line is the dependence calculated from the same model used to fit the data in Fig. 2. The dashed line is the dependence which results if boundary reflections within the Au film are not allowed.

estimated error in the values of λ_e and λ_i is $\pm 20\%$; a variation by this amount produces a noticeable disagreement with the experimental spectra.

There is a powerful additional indicator of multiple reflections and of the validity of this model, obtained from an independent measurement over a different Au thickness range. A series of Au/Si samples was fabricated using Si(100) substrates. This series included samples with Au layers as thin as 14 Å. A plot of I_c versus Au thickness for these samples yields a dependence which deviates from simple exponential behavior for thinner Au layers, as shown in Fig. 3. Using the same model which was used to fit the individual BEEM spectra of Fig. 2, an attenuation curve was calculated which is also plotted in Fig. 3. Since λ_e and λ_i were chosen to reproduce the measured λ_{tot} for thick layers, the agreement there is expected. The notable feature is that the calculation reproduces the deviation at thin layers extremely well. This behavior is a direct indication of the presence of multiple electron reflections within the Au layer. The width and shape of this "peaking" at small Au thicknesses is fixed by λ_e and λ_i and depends on no adjustable parameters. When multiple reflections are not allowed, the calculated dependence lacks this feature, as shown by the dashed line in Fig. 3.

Interestingly, Niedermann *et al.* [19] observed a regime of apparent shorter λ_{tot} for thinner PtSi layers in BEEM measurements of PtSi/Si(100). Although this was interpreted as an interfacial layer with a shorter attenuation length, it appears possible that this was also an observation of multiply reflected electrons.

In conclusion, BEEM measurements have directly revealed a strong degree of $k_\parallel$ conservation for hot electrons crossing the Au/Si(111) interface. The dependence of BEEM spectral shape on Au thickness indicates that multiple electron passes within the metal layer contribute to collected current. In addition, a direct and independent signature of multiple electron passes has been detected in BEEM attenuation length measurements. The contribution of these multiple passes has been shown to be the primary factor preventing previous BEEM observations of $k_\parallel$ conservation in thin metal layers. These results also indicate that any average diffuse component to interface transmission (interface scattering) must be small, since a substantial diffuse contribution would quickly alter the characteristic spectral shape observed at low temperature for thick Au layers.

TEM imaging by T. George is gratefully acknowledged. The research described in this Letter was performed by the Center for Space Microelectronics Technology, Jet Propulsion Laboratory, California Institute of Technology, and was jointly sponsored by the Office of Naval Research and the Ballistic Missile Defense Organization/Innovative Science and Technology Office through an agreement with the National Aeronautics and Space Administration (NASA). The Cray supercomputer used in this research was provided by funding from the NASA Offices of Mission to Planet Earth, Aeronautics, and Space Science.

[1] W. J. Kaiser and L. D. Bell, Phys. Rev. Lett. **60**, 140 (1988); L. D. Bell and W. J. Kaiser, *ibid.* **61**, 2368 (1988)
[2] G. Binnig, H. Rohrer, Ch. Gerber, and E. Weibel, Phys Rev. Lett. **49**, 57 (1982).
[3] L. J. Schowalter and E. Y. Lee, Phys. Rev. B **43**, 930 (1991).
[4] K. Oura and T. Hanawa, Surf. Sci. **82**, 202 (1979).
[5] A. K. Green and E. Bauer, J. Appl. Phys. **47**, 1284 (1976)
[6] F. J. Garcia-Vidal, P. L. de Andres, and F. Flores, Phys Rev. Lett. **76**, 807 (1996).
[7] R. H. Ritchie and J. C. Ashley, J. Phys. Chem. Solids **26** 1689 (1965).
[8] L. D. Bell *et al.*, Phys. Rev. B **50**, 8082 (1994).
[9] M. T. Cuberes, A. Bauer, H. J. Wen, M. Prietsch, an G. Kaindl, Appl. Phys. Lett. **64**, 2300 (1994).
[10] J. J. Quinn, Phys. Rev. **126**, 1453 (1962).
[11] M. H. Hecht, L. D. Bell, W. J. Kaiser, and F. J. Grunthane Appl. Phys. Lett. **55**, 780 (1989).
[12] H. Palm, M. Arbes, and M. Schulz, Appl. Phys. A **56**, (1993).
[13] C. A. Ventrice, V. P. LaBella, G. Ramaswamy, H.-P. Y and L. J. Schowalter, Phys. Rev. B **53**, 3952 (1996).
[14] R. Ludeke and A. Bauer, Phys. Rev. Lett. **71**, 1760 (199
[15] S. M. Sze, J. L. Moll, and T. Sugano, Solid State Electro **7**, 509 (1964).
[16] J. G. Simmons, J. Appl. Phys. **34**, 1793 (1963).
[17] J. Tersoff and D. R. Hamann, Phys. Rev. Lett. **50**, 19 (1983).
[18] N. D. Lang, A. Yacoby, and Y. Imry, Phys. Rev. Lett. **6** 1499 (1989).
[19] P. Niedermann, L. Quattropani, K. Solt, A. D. Kent, a O. Fischer, J. Vac. Sci. Technol. B **10**, 580 (1992).