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Role of elastic scattering in ballistic-electron-emission microscopy of Au/Si(001) and Au/Si(111) interfaces

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A ballistic-electron spectroscopy, based on the scanning tunneling microscope, was used to probe the conservation of transverse crystal momentum at the Schottky barrier between polycrystalline metal and semiconductor. The Au/Si(111) interface is of particular interest because, for this orientation, all of the Si conduction-band minima will require a large transverse-crystal-momentum component for transmission. Here we demonstrate, using Monte Carlo calculations of ballistic-electron-emission microscopy (BEEM) currents which are compared with experimental data, that transverse momentum appears to be conserved for most of the observed BEEM current but that elastic scattering must be taken into account. We show that this result implies that the spatial resolution of BEEM can vary greatly with substrate orientation and with the probability of elastic and inelastic scattering.

Ballistic-electron-emission microscopy (BEEM) is a new technique for measuring ballistic electron[1-3] and hole[4] transport across metal-semiconductor (M/S) Schottky barrier (SB) interfaces with high energy and spatial resolution. In BEEM, a scanning-tunneling microscope (STM) tip (emitter) is used to inject electrons into a thin metal layer (base) on a semiconductor substrate (collector). Both the base and collector are kept at ground potential and the initial energy and momentum distribution of the injected electrons is determined by the emitter-base bias. If scattering at the interface is neglected, simple kinematic considerations require that the injected electron can cross the SB and be detected as part of the BEEM current only if its (i) transverse momentum and (ii) total energy are conserved across the interface. For simple metals and semiconductors where the energy of the electron on both sides of the interface is proportional to the square of its momentum, these two conservation laws give rise to the familiar "escape" cone, which is centered about the normal to the interface, for an electron with energy greater than the SB height. For Au/Si(001) and Au/GaAs(001) this "free-electron" description would be expected to work well since two of silicon's conduction-band minima will have no transverse momentum component when projected onto the (001) interface, the GaAs conduction-band minimum is in the Brillouin-zone center, and Au is a noble metal with a nearly spherical Fermi surface. However, all six of the silicon conduction-band minima have large transverse momentum components when projected onto a (111) interface. Thus, the two kinematic conservation laws will result in six escape cones for electrons with energy greater than the SB height, all at large angles to the interface for the Au/Si(111) orientation.

In this Rapid Communication, our experimental study of BEEM spectra for Au/Si(111) is presented and we explain why elastic scattering of electrons in the base must be invoked to explain these results. A Monte Carlo (MC) approach to electron scattering (elastic and inelastic) is developed which successfully models the experimental spectra for both (001) and (111) orientations. This model suggests that the spatial resolution of BEEM is dependent on the crystallographic orientation of the interface, the ratio of the electron's elastic to inelastic mean free path, and type of scattering that occurs at the M/S interface and the metal surface.

A theory for BEEM has been developed[2] by Bell and Kaiser (the BK model) which approximates the initial energy and momentum distribution of the injected electrons from the STM tip as that due to tunneling between two planar electrodes.[5] It also assumed that the only effect of scattering, both in the metal base and at the interface, was to reduce the BEEM current. Thus, the BK model assumes that the energy and momentum distribution at the M/S interface is identical to the initial, injected distribution. The BK model has been very successful in explaining the experimental BEEM current dependence on emitter-base bias for both electrons and holes for Au on Si(001) and on GaAs(001) substrates. It also predicts lateral spatial resolution of BEEM to be on the order of a few nm for metal layers which are on the order of 10-nm thick due to the very large kinetic energy difference between electrons in the metal and the semiconductor. While spatial resolution of this order has been observed[6] for Au/GaAs(001), we found[7] that there were major discrepancies between the BK model and electron BEEM data taken for Au on Si(111) substrates.

Figure 1 shows a typical BEEM spectrum (open circles) from a sample with an approximately 5-nm-thick gold layer on a Si(111) substrate measured in our laboratory using a Au STM tip. The sample preparation procedure was similar to one discussed in Ref. 1. The experimental spectrum represents an average of 50 scans. The BEEM spectra for Au/Si(111) are remarkably similar to spectra published[1,2] by the group at the Jet Propulsion Laboratory (JPL) for Au/Si(001) which we have also reproduced in our laboratory.[8] As shown in Ref. 2, the BK theory fits the Au/Si(001) data extremely well. However, when this theory is applied to the Au/Si(111) case, a qualitatively different spectrum is generated. This is be-

cause k parallel and energy conservation across the Au/Si(111) interface will allow only those electrons injected from the STM tip into one of the six escape cones, corresponding to the projections of the six conduction-band minima onto the (111) interface, to cross the SB. All of these escape cones will be along directions which are at an angle of 39° from the (111) surface normal (calculated using the Au Fermi energy of 5.4 eV and the appropriate X-point conduction-band minima[9] for Si). In the case of Au/Si(001), ballistic electrons which travel in the metal base at angles close to the (001) surface normal can be collected as BEEM current since two of the X-point conduction minima will be aligned with the (001) surface normal. However, planar tunneling theory[5] gives a tunneling current distribution which is sharply peaked in the forward direction. Thus, the probability that an electron will tunnel into the Au layer with the appropriate momentum to cross the Au/Si(111) interface (which needs to be at an angle of 39° to the surface normal) is much smaller than in the Au/Si(001) case resulting in a significantly smaller BEEM current. Even the shape of the predicted spectra will be different (as shown by the triangles in Fig. 1). Both of these predictions are in marked contrast to experimental observations which find the magnitude and shape of the BEEM spectra to be approximately the same for the two crystal orientations. We should note that, in these calculations, the band structure of the gold in the STM tip and in the gold metal base is assumed to be that of a simple metal. The actual Fermi surface[10] of Au is nearly spherical with necks along (111), and it seems unlikely that the deviation from sphericity would have a significant impact on the fit to the data especially since the Au layer is polycrystalline.

It might be argued that these results are simply due to the fact that the gold layer is polycrystalline and that the Au/Si interfaces will have many imperfections which will scatter electrons crossing the interface. These scattering centers could cause the transverse crystal momentum to not be conserved so that the only criterion for an electron crossing the SB would then be whether it had sufficient energy to make it into one of the Si conduction-band minima. Certainly this hypothesis is consistent with the observation that BEEM spectra from Au/Si(001) and Au/Si(111) are nearly identical. However, a calculation of the BEEM spectra without conservation of transverse crystal momenta (shown as solid circles in Fig. 1), is inconsistent with BEEM spectra for both orientations of Si since it results in a turn-on of the BEEM current which is much more abrupt than that which is actually observed. While some more complex mechanism of scattering could exist, it seems difficult to derive a model which would result in transverse momentum not being conserved across the SB and yet is consistent with the excellent agreement of the BEEM spectra for Au/Si(001) and Au/GaAs(001) when transverse momentum conservation is assumed.

On the other hand, a successful approach is suggested by the fact that, if we arbitrarily make the spatial momentum distribution of the injected electrons uniform (in contrast to the sharply peaked forward distribution predicted by Simmons planar tunneling theory) while keeping all other elements of the BK theory, the calculated shape of the BEEM spectra for Au/Si(111) will become identical to that calculated for Au/Si(001) (Ref. 7) and both fit the measured data very well. However, the magnitude of the calculated BEEM current for both orientations is sharply reduced since many more electrons will now be traveling in directions which will not be able to cross the Schottky barrier. This last observation points out the key problem for any proposed solution which simply broadens the injected electron momentum distribution sufficiently to explain the Au/Si(111) since the observed BEEM currents for Au/Si(001) are very close to their theoretical maximum in the BK theory after quantum-mechanical reflection and optical-phonon scattering is taken into account.[11] Broadening the momentum distribution reduces the theoretical BEEM current below what is observed experimentally.

However, we have also considered the effect of elastic scattering in the metal base which, it turns out, provides a plausible explanation of BEEM spectra for both Au/Si(111) and Au/Si(001). It seems intuitive that this approach will help solve the problems discussed above since elastic scattering will broaden the momentum distribution of the injected electrons in agreement with the observed BEEM spectra but, at the same time, it will increase the BEEM current since electrons which are not initially in an escape cone can be elastically scattered into one. Elastic scattering is also suggested by photoresponse measurements[12] having indicated that the elastic mean free path of electrons in gold, for energies $\lesssim 1$ eV above their Fermi sea, is much shorter than their inelastic mean free path (which is approximately 120 nm for this energy). Several sources for elastic scattering have been suggested[13] including surface contamination, bulk impurities, and defects. Optical phonons are another source of quasielastic scattering.[14] While not strictly elastic, in the range of electron kinetic energies of interest to us here, typical optical-phonon energies are small enough that the change in energy during the optical-phonon scattering event can be neglected.

To confirm this intuitive suggestion, we have performed detailed calculations of the effect of elastic scattering on BEEM spectra using the Monte Carlo (MC) technique[15] which is briefly summarized below; a more detailed account will be published elsewhere. The phase space at a single point on the Au base surface, representing states accessible to tunneling electrons from the Au tip (at $T=0$), was divided into 30000 elements. Each of these pulse space elements is weighted with a probability determined by Simmons planar tunneling theory[5] (a tip separation of 0.5 nm was assumed for those calculations). As described earlier, this results in an initial momentum distribution of injected ballistic electrons which is sharply peaked in the forward direction. The MC simulation for a particular phase-space element was terminated if its kinetic energy was less than that of the SB. Otherwise, elastic and inelastic scattering were modeled by tracking one electron from each phase-space element and assigning it an elastic x_{el} and an inelastic x_{inel} path length. These lengths are chosen randomly so as to satisfy a probability density $P(\lambda_i,x_i)=(1/\lambda_i)\exp(-x_i/\lambda_i)$ where the subscript i stands for either elastic or inelastic scattering and λ_{el} and

λ_{inel} are the elastic and inelastic mean free paths, respectively. In all subsequent motion of the electron, the MC simulation continues until either the electron makes it across the SB and becomes part of the collector current or the total distance d traveled by the electron exceeds x_{inel}, in which case the electron is assumed to have undergone an inelastic scattering event of sufficient energy loss to render the electron incapable of crossing the SB. When d exceeds x_{el}, the electron is assumed to have undergone an elastic scattering event. At the elastic scattering point, a different direction (all directions are considered equally likely) and x_{el} are generated (which determines the distance to the next elastic scattering event if the MC calculation continues that far). If the path of the electron intersects the metal surface, diffuse elastic scattering is assumed to occur which is modeled by randomly selecting a direction among the π steradians back into the metal base.

If the path of the electron intersects the M/S interface, its transverse momentum and its total energy are compared with possible final states in the Si collector. We modeled the six conduction-band minima in Si as ellipsoids with the longitudinal mass, $m_l = 0.92$, and the transverse mass, $m_t = 0.19$ with the centers of the ellipsoids located at $(2\pi/a)$ [0.86, 0, 0] along the ⟨100⟩ directions. If the electron has appropriate energy and transverse momentum to match a final state, it was accepted into the BEEM (collector) current 20% of the time. The other 80% of the time, it is reflected back into the metal base. The 20% transmission coefficient was chosen to match our calculations[9] for the expected effect of quantum-mechanical reflection and optical-phonon scattering at the M/S interface. The electron was also reflected back into the Au if there was no final state in the Si which matched the energy and transverse momentum of the electron. When the electron was reflected back into the semiconductor, it was again assumed to be a diffuse reflection and all possible directions back into the metal layer were considered equally likely.

In Fig. 1, the average of 10 MC runs of the BEEM current (crosses) for Au/Si(111) is compared with the measured BEEM currents as a function of STM tip bias. Although not shown, almost identical MC spectra were generated for Au/Si(001).[16] For these MC calculations, the Schottky barrier height was chosen to be 0.80 eV in agreement with previous measurements[1,2] (the theory is insensitive to a variation of $\sim \pm 20$ meV in the SB height), λ_{el} to be 10 nm and λ_{inel} to be 120 nm for ballistic electrons 1 eV above the Fermi sea.[17] In addition, the magnitude of the BEEM current was scaled by an arbitrary, but reasonable (near unity) factor. The MC spectra for both Au/Si(001) and Au/Si(111) were very insensitive to the choice of λ_{el} and λ_{inel} over a wide range of values. These particular values are representative. However, with them, the BEEM current in the MC simulation was found to decrease approximately exponentially with Au thickness[18] with characteristic lengths of 14 and 16 nm, respectively, for the Au/Si(001) and Au/Si(111) orientations. The value for λ_{el} was chosen to give good agreement between the calculated Au/Si(001) attenuation length and that measured[4] for this orientation.

In Fig. 2, we show MC calculations of the spatial resolution for Au/Si(001) and Au/Si(111) as a function of gold thickness. Each data point represents the average of 10 runs and the error bars represent the deviation observed between MC runs. It should be noted that the predicted resolution of BEEM will be a sensitive function of the probability of inelastic scattering at the M/S interface. Our results here should be treated as a worst case analysis of spatial resolution since inelastic scattering at the M/S interface will improve the spatial resolution. Inelastic scattering at the Au/GaAs interface may explain the very high spatial resolution observed by the JPL group for this structure.[4]

In conclusion, we measured BEEM spectra for Au on

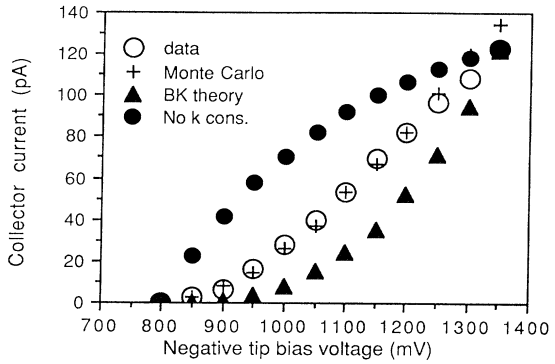

FIG. 1. A typical experimental BEEM spectrum for Au/Si(111) is plotted along with theoretical spectra for three different models. The BEEM spectrum (shown as open circles) was measured on a 5-nm-thick Au film with an STM tunneling current of 2 nA. The Bell-Kaiser (BK) theory (triangles) neglects scattering as explained in the text, while the solid circles show the spectrum that would result if scattering completely eliminated transverse momentum conservation at the interface. The crosses represent our Monte Carlo calculations which allow elastic scattering to redirect some ballistic electrons back into the exit cone. All calculated spectra assume a SB height of 0.80 eV.

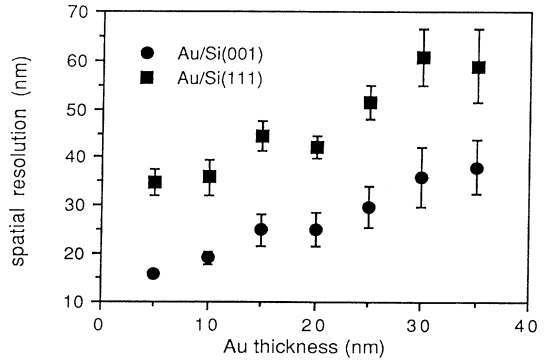

FIG. 2. The spatial resolution of BEEM, at an emitter-base bias of −1.2 V, is shown as a function of the thickness of the base. As detailed in the text, these results were determined by Monte Carlo calculations assuming: (i) a mean free path 10 nm for elastic scattering of electrons, (ii) diffuse elastic scattering at the surface and interface of the metal layer, and an energy dependent, inelastic mean free path.

Si(001) and Si(111) substrates and found that they were almost identical for the two substrate orientations, in disagreement with conventional (BK) BEEM theory which predicts a substantially different spectra for the two orientations. We have also demonstrated that this discrepancy cannot be resolved simply by arguing that defects along the Au/Si interface will destroy the need for conservation of transverse crystal momentum across the Schottky barrier. An approach which is consistent with all the BEEM data taken on Au/Si structures takes the elastic mean-free-path length of the electrons in the gold metal base to be much smaller than the inelastic mean-free-path length. The observation of small ratios of $\lambda_{el}/\lambda_{inel}$ is consistent with photoresponse data[15] on M/S interfaces. The spatial resolution of BEEM can be significantly broadened by these elastic collisions, but if inelastic scattering dominates at the M/S interface the spatial resolution will not be degraded as much which may explain the BEEM observation of 1 nm features at the Au/GaAs interface. The use of BEEM to determine the ratio of elastic to inelastic scattering will have significant impact on the development of devices which depend on ballistic transport of electrons across M/S interfaces such as SB infrared detectors and metal-base transistors.[19]

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