Theory of Ballistic-Electron-Emission Spectroscopy of $NiSi_2$/Si(111) Interfaces

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We discuss theoretical calculations of ballistic-electron-emission-microscopy spectra based in part on a first-principles computation of the transmission across the interfaces. We propose a way of presenting experimental data that highlights the transmission process with respect to contributions from the tunneling distribution. We present a specific application to A- and B-type $NiSi_2$/Si(111) interfaces showing a factor three difference between them at low voltages.

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Ballistic-electron-emission microscopy (BEEM) is an experimental technique based on scanning tunneling microscopy that can be used to investigate properties of buried interfaces. BEEM spectra are determined mainly by the tunneling process into a metal overlayer and the transmission process across a metal-semiconductor interface. In this paper we discuss the calculation of BEEM spectra, and propose a technique for analyzing experimental data that emphasizes the transmission process by canceling as much of the details of the tip-surface tunneling process as possible. Then we discuss a specific application of this technique to $NiSi_2$/Si(111) interfaces. While low transmission limits the technological potential of this interface,[1] characterization by our theoretical approach and by our proposed analysis of experimental data should be of value in assessing that of other systems.

In a BEEM experiment,[2] a scanning-tunneling-microscope (STM) tip is held over the thin (≈ 50 Å) metal overlayer, which is grown on the semiconductor substrate. A voltage is applied between the tip and the overlayer, with the overlayer and substrate held at the same voltage. Electrons are injected into the overlayer, some of which travel ballistically across the overlayer and are incident on the Schottky barrier at the buried interface. Those electrons that transmit across the interface are measured as a "collector" current between the tip and the substrate. The collector current as a function of tip voltage can be used to infer properties of the interface, like the Schottky-barrier height, and the behavior of the transmission across the interface.

Nickel disilicide, $NiSi_2$, grown on silicon (111) is an important test case for BEEM. The interfaces between these materials can be grown atomically abrupt and coherent, and can be grown with two interface structures depending on the growth conditions.[3] In the A-type interface, the $NiSi_2$ lattice has the same orientation as the Si substrate lattice; in the B-type interface, the orientation is reversed. The lattice constants are matched to better than 1%, and the interface quality is quite good.[4] In a recent calculation,[1] we showed that the transmission properties of these interfaces differed by about a factor of 3 for energies close to the Schottky-barrier threshold. Since BEEM can probe the transmission across interfaces, it should be possible to see this difference, given the ability to grow A-type and B-type interfaces on the same substrate, providing a test of our understanding of both BEEM and interface transmission.

The collector current in a BEEM experiment is equal to the integral of the flux distribution incident on the buried interface times the probability that an electron in each state will be transmitted across the interface. This integral can be written as a two-dimensional integral over wave vectors and an integral over energy,

$$I_c(V,d)=e\int_0^V dE\int_{\mathrm{IBZ}}\frac{d^2K}{(2\pi)^2}\sum_n \rho_I(n',E,\mathbf{K},V,d)\,T(n,E,\mathbf{K})\,. \tag{1}$$

Here, E is the electron energy relative to the metal Fermi level, IBZ is the interface Brillouin zone, $\mathbf{K}$ is a wave vector in the interface Brillouin zone, n refers to all states in the overlayer with a given E and $\mathbf{K}$, ρ_I is the distribution of electrons incident on the interface, V is the voltage applied between the tip and overlayer, d is the tip-sample separation, and T is the transmission probability across the interface.

For transmission through coherent interfaces, those with a common interface lattice net for both materials, an electron's crystal momentum parallel to the interface, as well as its energy, are conserved. These two conservation principles constrain the transmission probability T such that if there is no state in the substrate with the same E and $\mathbf{K}$, the transmission probability will be zero. These kinematic constraints depend only upon the band structures of the two materials and the Schottky-barrier height of the interface and they indicate which states might possibily transmit across the interface. The kinematic constraints for $CoSi_2$/Si(111) interfaces indicate that there is a projected gap in the $CoSi_2$ at the wave vectors equal to the projection of the Si conduction-band minimum.[5,6] This gap leads to a delay in the onset of transmission of about 0.2 V in calculated BEEM spectra, and has been observed experimentally.[7]

The kinematic constraints are not sufficient to calculate the detailed shape and size of BEEM spectra which depend on the transmission probabilities across the interface. These transmission probabilities must be found from a calculation which takes into account the atomic-scale details of the wave functions in each material and of the potential at the interface. We calculate them using an *ab initio* method[8] developed to treat complicated interfaces like $NiSi_2$/Si(111).[1]

Previous calculations of BEEM spectra have used approximate models for the band structures and the transmission probabilities.[2,9–11] While these models contain some of the qualitative physics that is necessary to interpret BEEM spectra, they contain approximations that are not valid. They have been successfully compared with experiments in part because they are adjusted with an arbitrary scale factor which is included to account for uncertainties in the tunneling distribution and scattering.

Following earlier models of BEEM spectroscopy, we use a modified planar-barrier tunneling model to describe the current distribution injected into the overlayer from the tunneling tip,

$$I_t(V,d)=e\int_0^V dE\int_{\mathrm{IBZ}}\frac{d^2K}{(2\pi)^2}\times\sum_n t(E-K^2/2m,V,d)\,, \qquad (2)$$

where t is a WKB approximation to the tunneling probability. This approximation for the tunneling distribution captures the essential physics of the tunneling process, but ignores the atomic-scale details of the overlayer surface electronic structure, image-potential effects, the detailed shape of the tunneling tip, and tip densities of states. Much of the uncertainty caused by these ignored details can be removed by measuring the spectra in constant-height mode and analyzing the data in a way discussed below. In a constant-height measurement, the tip and the collector currents vary as a function of voltage for fixed tip-sample separation. Such measurements are more difficult to do, but easier to interpret than constant-current measurements in which the tip-sample separation and the collector current vary for fixed tip current. They are more difficult because the current varies over a wider range, but easier to interpret because the tip-sample separation is not a function of voltage.

When scattering in the overlayer and substrate is not important, the tunneling and interface distributions are the same. In this case much of the uncertainty due to the unknown tunneling distribution can be removed from constant-height measurements by taking the ratio of the voltage derivative of the collector current to that of the tip current. The currents depend on the voltage both through the upper cutoff of the energy integration and because the barrier is skewed by the voltage. Differentiating the tip current with respect to voltage gives a contribution from both dependences. The contribution from the upper cutoff removes the energy integral from Eq. (2) and sets the energy E equal to the voltage eV in the first term. The other term is roughly half of the first term, because the tunneling probability to a good approximation depends on the energy and voltage in the combination $E+eV/2$. On the other hand, differentiating the collector current with respect to voltage gives a result that is dominated by the contribution from the upper cutoff. Taking the ratio of the leading contributions to these two derivatives leaves an approximate expression that is an average of the transmission probability over the interface Brillouin zone at the energy of the applied voltage eV,

$$\frac{dI_c/dV}{dI_t/dV}\approx\frac{2}{3}\int_{\mathrm{IBZ}}\frac{d^2K}{(2\pi)^2}\sum_n W(\mathbf{K},V,d)\,T(n,eV,\mathbf{K})\,, \qquad (3)$$

where W is a normalized weighting function that depends on the tip-sample separation, but only weakly on the voltage for low voltages,

$$W(\mathbf{K},V,d)=t(eV-K^2/2m,V,d)\Big/\int_{\mathrm{IBZ}}\frac{d^2K'}{(2\pi)^2}\sum_{n'}t(eV-K'^2/2m,V,d)\,. \qquad (4)$$

Any unknown scale factors in the tunneling distribution cancel out in this expression, leaving a weighting factor that is roughly Gaussian in the parallel wave vector and dependent on the tip-sample separation.

Figure 1 compares our full calculation of the derivative ratio with the approximate expression given in Eq. (3) for the two $NiSi_2$/Si(111) interfaces. For a series of tip-sample separations, and for both interfaces, the agreement is quite good. This figure also shows the main results of our calculation for $NiSi_2$/Si(111) interfaces: a large difference in transmission for the two interface structures, a strong dependence on the tip-sample separation, and much more structure than is seen in published BEEM spectra.

The large difference in the BEEM spectra for the two interfaces is due to the large difference in the transmission between them, illustrated in Fig. 2. Below the

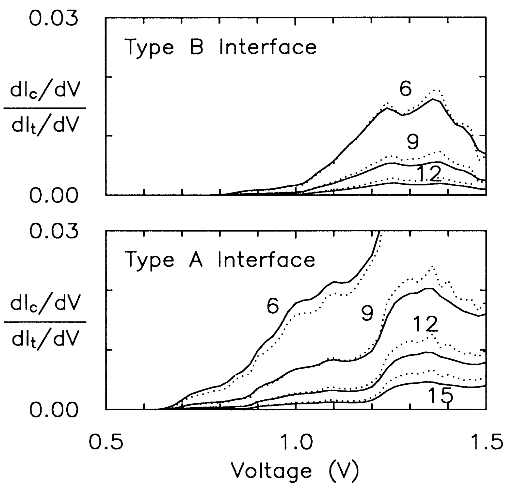

FIG. 1. BEEM spectra for $NiSi_2$/Si(111) interfaces. For a series of tip-sample separations (in Å), the solid lines show the ratio of the derivative of the collector current to the derivative of the tip current and the dotted lines show the transmission probability averaged over parallel wave vector (and multiplied by $\frac{2}{3}$) as discussed in the text.

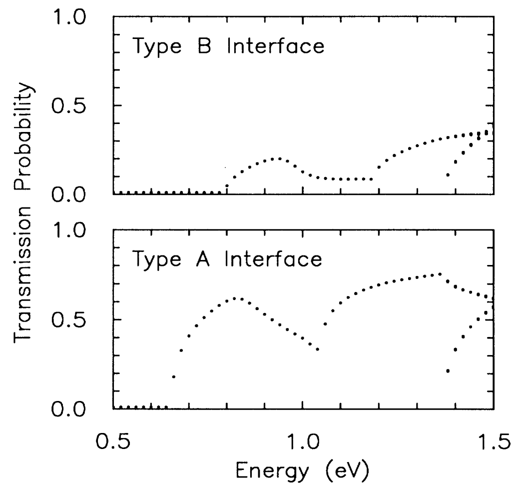

FIG. 2. Transmission probability summed over final states for electron states in $NiSi_2$ incident on a $NiSi_2$/Si(111) interface. The electrons have the same parallel wave vector as the Si conduction-band minimum.

Schottky barrier, 0.65 and 0.79 eV for the A-type and B-type interfaces, respectively,[3] there are no states in the Si so the transmission probability is zero. Above the barrier there is one state in both the Si and the $NiSi_2$ and the transmission probability increases from zero as the square root of the energy above the threshold, as expected, but differs by about a factor of 3 between the two interfaces. At higher energies there are multiple states in the $NiSi_2$; each has a different transmission probability. For energies higher than those shown here the difference between the behavior of the two interfaces becomes more complicated.

Figure 3 illustrates how the constraints of energy and parallel momentum conservation contribute to the BEEM current. It shows how many states there are in both materials at the thirty independent parallel wave vectors used for the integrations in these calculations. States at each energy in the $NiSi_2$ can only transmit into the Si if there is a state in the Si with the same parallel momentum. The middle panels show the net transmission based on these constraints and the calculated probabilities. At the lowest energy there are states at all parallel wave vectors in the $NiSi_2$, but only near the conduction-band minimum in the Si. At these energies the average transmission probability is quite small, both because there are only a few available states in the Si, and also because the weighting function W, which multiplies these net probabilities, is peaked in states near the zone center $\bar{\Gamma}$. The peaking of the distribution near the zone center arises because the tunneling probability from the tip depends on the combination $E-K^2/2m$. The peaking becomes more pronounced as the tip-sample separation is increased, leading to the strong dependence of the BEEM spectra on the tip-sample separation. As the energy increases, the area of allowed states in the Si continues to increase while the area in the $NiSi_2$ tends to de-

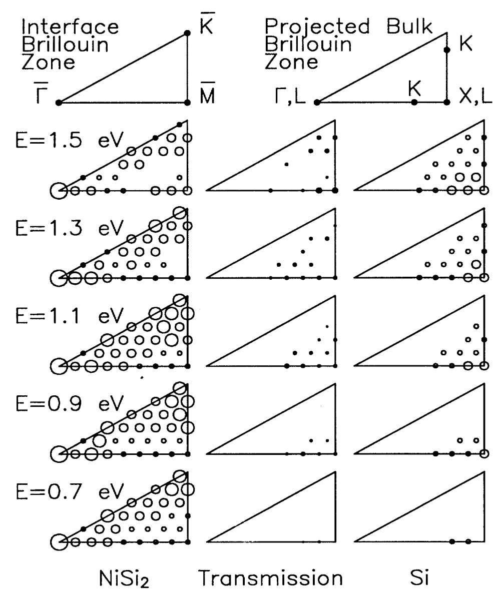

FIG. 3. Phase space for electron transmission through a $NiSi_2$/Si(111) type-A interface. The panels on the left (right) show the irreducible wedge of the interface Brillouin zone of the $NiSi_2$ (Si). At each parallel wave vector used in the calculation the radii of the open circles are proportional to the number of states in each material at the energy given to the left. In the middle panels the solid circles show the amount of transmission through the interface summed over the states at each parallel wave vector in the $NiSi_2$.

crease. Thus, the average transmission probability initially increases, but then decreases as the overlap between the states in the two materials decreases. Strong features in the spectra arise when bands in the two materials start or cease overlapping each other; these changes need not occur at band extrema.

The BEEM spectra will be changed by scattering in the metal overlayer which changes the distribution of electrons incident on the interface, ρ_I, from that tunneling from the tip, ρ_t. Elastic scattering, due to defects in the overlayer, will not change the electron energy, but will just redistribute the electrons between different n's and $\mathbf{K}$'s. This will effectively change the weighting function W in Eq. (3). For systems with the conduction-band minima away from the zone center, like those considered here, strong elastic scattering will increase the average transmission close to threshold and reduce the sensitivity on the tip-sample separation. Inelastic scattering, whether due to phonons or electron-hole pairs, is likely to decrease the collector current because some of the electrons will be scattered into states below the Schottky barrier. The effect of these scattering mechanisms on ρ_I should increase in proportion to the overlayer thickness. Measuring the thickness dependence of the BEEM spectra could test the magnitude of these effects.

An additional factor that can complicate the comparison between the experimental data and the calculated transmission probabilities is scattering in the semiconductor substrate.[11] It is possible for electrons to scatter back into the overlayer after they have successfully transmitted over the interface into the substrate. It should be possible by changing the doping of the substrate and the temperature to minimize this effect.

We find qualitative agreement between our calculations and some preliminary constant-height measurements of the BEEM spectra,[12] but these spectra have not factored out the tunneling distribution so detailed comparisons cannot be made. Calculations can be made to quantitatively agree with constant-current measurements[9] by adjusting the tip-sample separation at threshold. However, without knowing the height as a function of voltage it is impossible to say whether this agreement is significant or not. It is also impossible to say whether scattering in the overlayer is important or not in any of these experiments.

We have shown that detailed calculations of the BEEM spectra can be carried out for atomically abrupt, coherent interfaces like $NiSi_2$/Si(111), based on a first-principles calculation of the band structures and the transmission probabilities across the interface. We have also shown that there is a large difference in the transmission probability between the A-type and B-type interfaces. Observation of this difference would increase our confidence in our ability both to understand the process of transmission across interfaces and to interpret BEEM investigations of buried interfaces. Analyzing the experimental data in a way that eliminates much of the dependence on the tunneling distribution should facilitate comparisons between theory and experiment.

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