Ballistic Transport at Metal-Semiconductor Interfaces

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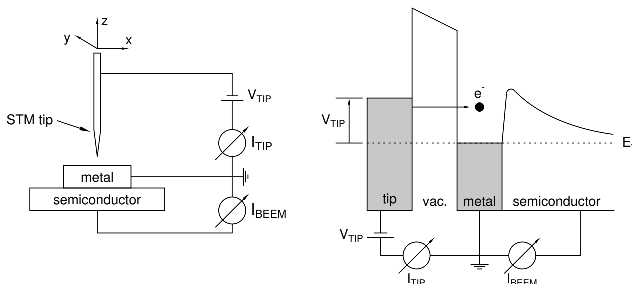
We propose a simple model to predict the effects of band structure and metal thickness on ballistic electron transport through metal-semiconductor interfaces. Using a Monte Carlo simulation, we study ballistic electron emission microscopy (BEEM) current through Au/Si and Au/GaAs as a function of Au thickness. Descriptions of the involved calculations can assist in modeling various electron transport phenomena of metal-semiconductor Schottky diodes.

I. INTRODUCTION

Ballistic electron emission microscopy (BEEM) is a three-terminal scanning-tunneling microscope (STM) technique. In this technique, electrons are injected from an STM tip into a grounded metal base of a Schottky diode. A fraction of these electrons travel ballistically through the metal to the metal-semiconductor interface; here, they encounter a Schottky barrier. Electrons with sufficient energy to surmount this barrier will be detected by a backside contact as BEEM current.

FIG. 1. two schematics describing BEEM (courtesy of A. J. Stollenwerk)



BEEM is an effective method for studying electron transport through thin metal films, metal-metal interfaces, and metal-semiconductor interfaces [1, 2]. BEEM takes advantage of the STM's atomic-scale positioning as well as the tip's narrow energy distribution, making it ideal for studying electron transport at metal-semiconductor interfaces [2–4]. BEEM can also be used to measure hot-electron attenuation lengths of metal-semiconductor contacts [5]. In this process, measurements of BEEM current at a tip bias above the Schottky height are taken as a function of metal thickness. The log slope of this data is known as the attenuation length.

There are two distinct variables which are thought to have significant impact upon the measured BEEM current of a sample. The first is the amount of ballistic electron scattering that occurs within the metal of a Schottky diode [6]. As the thickness of the metal increases, more electrons are scattered throughout, and fewer are compatible with the semiconductor's band structure. The second important variable is the availability of parallel momentum states within the semiconductor. As band structure varies significantly among different semiconductors, so do their available momentum states [7]. Both of these variables' importance have been confirmed in BEEM spectra acquired with Au/GaAs(001), Au/Si(001), and Au/Si(111) [6, 8]. Therefore, a simulation of ballistic electron transport through various metal-semiconductor interfaces would be useful in determining current transport properties of devices that make use of such interfaces.

We propose a simple model to predict the effects of interface band structure and metal thickness on ballistic transport through metal-semiconductor interfaces. We find that the scattering behavior in the metal can have a profound influence on the amount of current transmitted into the semiconductor. We also find that differences in semiconductors contribute little difference to BEEM current.

II. THEORY

When modeling BEEM, there are three separate regions of electron transport that must be accounted for. First, electrons must tunnel from the STM tip to the metal layer. The tunneling probability of electrons at this stage can be approximated by assuming a rectangular tunneling barrier:

$$T = |t|^2 = \frac{1}{1 + \frac{V_0^2 \sin^2(k_i a)}{4E(E-V_0)}} \tag{1}$$

where T is the electron's probability of tunneling, V_0 is the barrier height, E is the energy of the electron, a is the thickness of the barrier, $\hbar$ is the reduced Planck's constant, and k_i is

$$k_i = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \tag{2}$$

From these equations, a normalized tunneling probability distribution for a specific STM tip voltage can be created. These electrons are assumed to have entirely forward-directed momentum when they tunnel into the metallic layer.

As the electrons tunnel through the metallic barrier, they have a probability to be scattered after a certain

distance, assumed to be the width of an atomic layer. If the electron collides with an atomic nucleus, defect, or grain boundary, it is scattered at random θ (between 0 and π) and ϕ (between 0 and 2π) angles.

We assume each scattering event to be elastic in nature, i.e., scattered electrons retain the energy they start with at the tip. If the electron is backscattered (surpasses a θ of $\pi/2$), we assume it is not able to reach the interface. Both assumptions seem reasonable considering the small thickness of metals used in BEEM experiments [6].

As electrons become scattered throughout multiple layers of the metal, the momentum associated with each electron changes direction. The momentum wave vector for each electron can be calculated as:

$$\vec{k} = \langle (k_i \sin\theta\cos\phi)\hat{\imath}, (k_i \sin\theta\sin\phi)\hat{\jmath}, (k_i\cos\theta)\hat{k}\rangle \quad (3)$$

The two components we are interested in, k_x and k_y, can therefore be calculated as

$$k_x = k_i \sin\theta\cos\phi \quad (4)$$

$$k_y = k_i \sin\theta\sin\phi \quad (5)$$

Electrons that successfully tunnel through the metal have the potential to be transmitted through the second region, known as the Schottky barrier. If the electron has an energy less than the Schottky barrier, it will be reflected. If the electron has an energy greater than the Schottky barrier, it can be transmitted into the semiconductor if there is an available momentum state. For Si and GaAs, the Schottky barriers have heights of .79 and .88 eV, respectively.

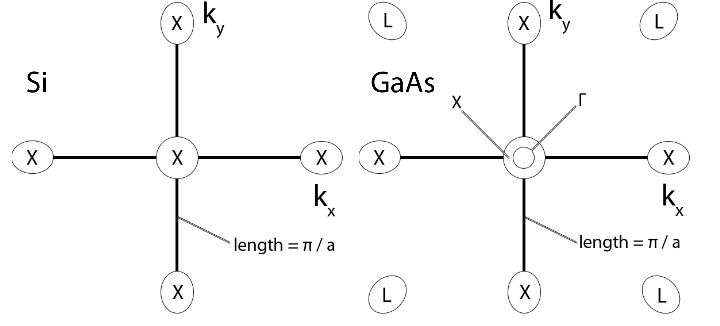
The third region of electron transport occurs within the semiconductor and is dependent on its band structure. In our model, the band structure of each semiconductor is approximated using the interface Brillouin zone (IBZ) [9]. The IBZ can be described as a three-dimensional projection of the semiconductor's band structure onto a two-dimensional plane. For Si and GaAs, this projection creates a plane containing a number of ellipses, which represent the available parallel momentum states within the semiconductor. Our model approximates these ellipses as circles.

The band structure of silicon is formulated such that there are five available conduction band minima (CBM). These minima exist within what is called the X-valley of silicon's band structure. Four of these states are at a distance π/a from the center of the IBZ, with a being silicon's lattice constant. One state lies directly in the center of the zone. Silicon and gallium arsenide's IBZs are visually represented in figure 2.

Consequently, an electron in Si which surmounts the Schottky height has five CBM into which it can possibly enter. Whether an electron transmits through the X-valley is dependent on its parallel momentum; therefore, we assume it must fulfill one of the following equations, with $m^* = 0.33m$ and $a = 5.4$ Å:

$$\sqrt{(k_x + (\pi/a))^2 + k_y^2} \leq \sqrt{\frac{2Em^*}{\hbar^2}} \quad (6)$$

FIG. 2. simplified IBZs of Si and GaAs



$$\sqrt{(k_x - (\pi/a))^2 + k_y^2} \leq \sqrt{\frac{2Em^*}{\hbar^2}} \quad (7)$$

$$\sqrt{(k_x^2 + (k_y + (\pi/a))^2} \leq \sqrt{\frac{2Em^*}{\hbar^2}} \quad (8)$$

$$\sqrt{(k_x^2 + (k_y - (\pi/a))^2} \leq \sqrt{\frac{2Em^*}{\hbar^2}} \quad (9)$$

$$\sqrt{k_x^2 + k_y^2} \leq \sqrt{\frac{2Em^*}{\hbar^2}} \quad (10)$$

The band structure of gallium arsenide is formulated such that there are three separate valleys: the Γ, X, and L-valleys. In the IBZ, the Γ-valley of GaAs consists of one CBM. The X-valley of GaAs, like the X-valley of Si, consists of five CBM in a similar arrangement. The L-valley of GaAs consists of four CBM, each in a separate corner of the IBZ.

To transmit through GaAs's Γ-valley, an electron must have an energy greater than the Schottky height and also satisfy equation 10 with $m^* = 0.067m$.

To transmit through gallium arsenide's X-valley, an electron must have an energy greater than 1.2 eV and satisfy any one of equations 6 through 10, with $m^* = 0.41m$ and $a = 5.6533$ Å.

If an electron has an energy greater than 1.4 eV, transmission through GaAs's L-valley depends on satisfying one of the following equations:

$$\sqrt{(k_x + (\pi/a))^2 + (k_y + (\pi/a))^2} \leq \sqrt{\frac{2Em^*}{\hbar^2}} \quad (11)$$

$$\sqrt{(k_x - (\pi/a))^2 + (k_y + (\pi/a))^2} \leq \sqrt{\frac{2Em^*}{\hbar^2}} \quad (12)$$

$$\sqrt{(k_x + (\pi/a))^2 + (k_y - (\pi/a))^2} \leq \sqrt{\frac{2Em^*}{\hbar^2}} \quad (13)$$

$$\sqrt{(k_x - (\pi/a))^2 + (k_y - (\pi/a))^2} \leq \sqrt{\frac{2Em^*}{\hbar^2}} \quad (14)$$

The total number of electrons which successfully transmit into a semiconductor can be calculated as BEEM current.

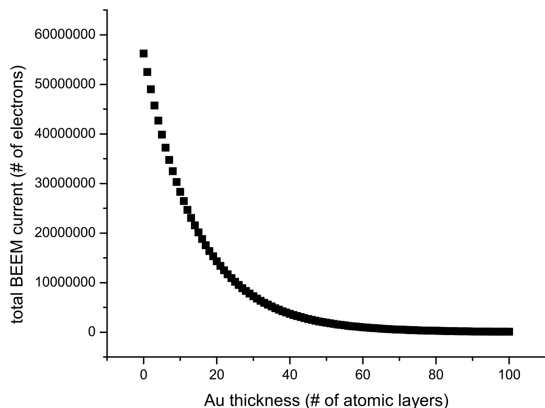
III. RESULTS

When simulating BEEM current, a few variables can greatly affect the end result. These include the number of atomic layers the electron must travel through, the maximum scattering angle of θ, the voltage bias of the tip, and the scattering probability per atomic layer of metal. Less effective than anticipated is the difference in band structure between Si and GaAs.

For most instances of the simulation, we altered certain variables while leaving our tip bias at a constant 1 eV. Although this doesn't take advantage of our X and L-valley conditions for GaAs, it is a common tip voltage used in metal-semiconductor BEEM spectroscopy and therefore most applicable [9]. Each simulation included sample sizes ranging from one million to one hundred million electrons. For all simulations, we take all energies relative to gold's CBM. This requires us to add 5.3 eV to our distribution of electrons out of the tip, the Schottky heights, and our Γ, X, and L-valley heights.

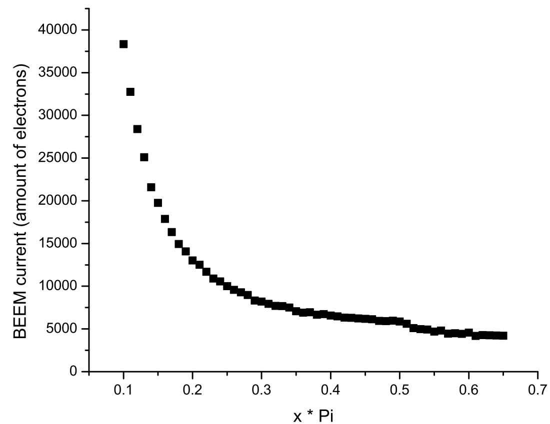
In our results, as the number of atomic layers of Au increased, fewer electrons were transmitted through the semiconductor. We propose this is mainly due to backscattering of electrons in increased amounts. However, the current is also somewhat dependent on the band structure. The greater the amount of scattering, the less likely it is for electrons to transmit through an available parallel momentum state. The result of increasing Au thickness is demonstrated in figure 3.

FIG. 3. BEEM current of silicon at various gold thicknesses; n = 1×10^8 electrons



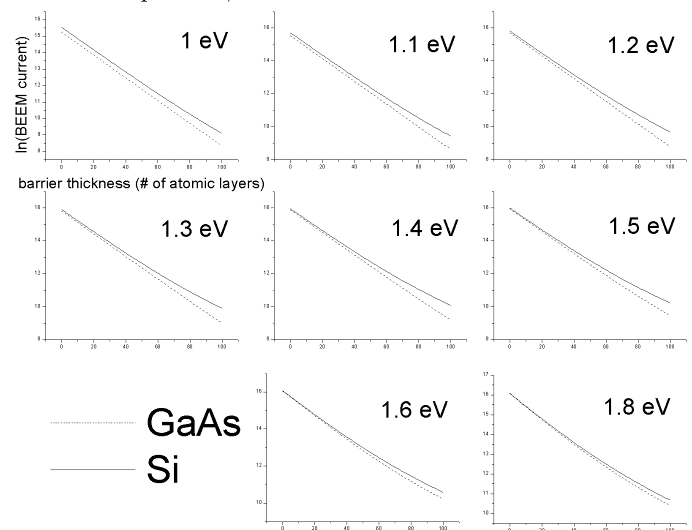
In varying the maximum scattering angle for θ, we also see a noticeable change in BEEM current. As the possible θ is decreased, more electrons can enter parallel momentum states. As we increase the possible θ, electrons are deflected at wider angles. If more electrons scatter, fewer can enter a parallel momentum state and more are backscattered. The effect of variable maximum scattering angles is displayed in figure 4, in which the barrier thickness of Au was kept constant.

FIG. 4. varying of the maximum scattering angle, θ, in Au-GaAs; n = 1×10^7 electrons; thickness = 100 atomic layers



In varying the voltage bias of the tip, at lower biases, we see larger differences between Si and GaAs's BEEM current. The behavior of these differences is accentuated by taking the log of BEEM current. These instances of the simulations display, importantly, that band structure is, indeed, a somewhat important variable in the calculation of BEEM current. As the tip bias increases, the attenuation lengths of both semiconductors become more alike.

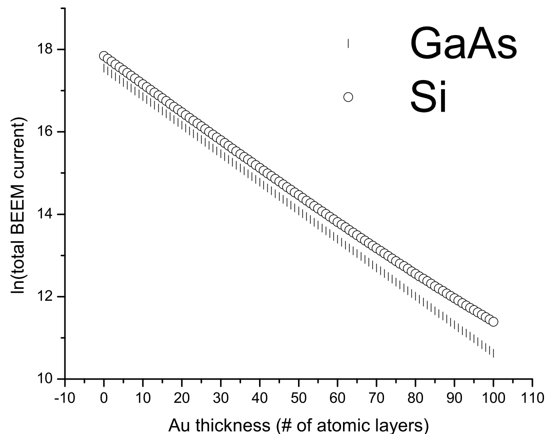
FIG. 5. a comparison of BEEM current between Si and GaAs at various tip biases; n = 1×10^7 electrons



At a tip bias of 1 eV, we found unexpected results in the log scale of BEEM current. Experimentally, the attenuation lengths of Si and GaAs differ substantially

[7]. In our simulation, at reasonable tip biases, they were remarkably similar. This feature of the simulation is demonstrated by figure 6, in which the two semiconductors share almost an identical attenuation length.

FIG. 6. a comparison of BEEM current between Si and GaAs at $V_{tip} = 1$ eV; $1{\times}10^8$ electrons



IV. DISCUSSION

In our model as well as our simulation, we found success in mimicking the general behavior of BEEM current as a function of gold thickness. This implies that our model for the distribution of energies at the tip and our model for electron scattering throughout the metallic region are both generally correct. More importantly, however, we found difficulty in mimicking the difference in BEEM current due to variability in semiconductor band structure. This is apparent when comparing the log scales of Si BEEM current versus GaAs BEEM current, as in figure 6.

This difficulty leaves us open to many opportunities for improvement. First, our assumption of elastic-only scattering in the metal may be too inaccurate to utilize. Another inaccuracy may stem from the assumption that high and low-energy electrons scatter at equal probabilities. The implementation of models which account for these two potential problems would benefit the overall accuracy of the simulation [9]. However, it is unclear if these alterations would significantly impact the effect of band structure.

Within the metal, we assumed a purely random orientation of gold atoms. Although our use of the Monte Carlo method to approximate scattering within the metal seems reasonable, it may be beneficial to implement an iterative structural, physical description for gold within the program. This would allow us to better characterize electrons' collisions with gold nuclei. We also did not take into account Coulombic interactions which may occur between electrons and gold nuclei at relevant distances.

There is also room for improvement in our model of available states within the semiconductor. Our current model assumes a zero temperature, but at nonzero temperatures, each state in the semiconductor has a possibility of being partially filled [9]. Also, as mentioned, the implementation of inelastic scattering may have noticeable effects on transmission through the semiconductor. As E has significant weight in our conditions for an electron's entrance into a state, the alteration of such an E value may change final results considerably.

V. CONCLUSIONS

We have presented a detailed description of the calculations involved in our model of ballistic electron transport through metal-semiconductor interfaces. Although the model is simple, it is capable of producing good approximations of behaviors exhibited in BEEM. The accompanying simulation of our model is robust, quick, and allows for variability of metal, metal thickness, tip voltage, semiconductor band structure, and various scattering variables.

Any improvements to the model would mainly concern the transmission of electrons through the semiconductor. As semiconductor band structure varies, our current model shows little difference in final BEEM current. This result is contrary to experimental data. Modeling scattering as inelastic and altering our semiconductor model may rectify this problem.

VI. ACKNOWLEDGMENTS

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"three-dimensional projection of a semiconductor's band structure onto a two-dimensional plane" is). Finally, I'd like to tip my hat to those that have researched this subject prior to the advent of the Internet.

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