Effect of interface band structure on hot-electron attenuation lengths in Au thin films

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The hot-electron attenuation length in thin Au films has been determined by means of ballistic electron emission microscopy on Au/Si(111), Au/Si(001), and Au/GaAs(001) Schottky diodes. The attenuation length measured for Au/GaAs(001) was approximately ten times shorter than attenuation lengths measured on the Si substrates. In addition, the slope of the attenuation length vs tip bias decreases above the X conduction band minimum in GaAs. These observations are attributed to differences in the amount of allowed parallel momentum at the interfaces of both semiconductors. These results suggest that these apparent attenuation lengths are not an intrinsic property of the metal and can be utilized as a powerful method to probe the band structure at metal-semiconductor interfaces.

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I. INTRODUCTION

Ballistic or hot-electron transport is a relevant phenomenon to many different practical applications, ranging from hot-electron transistors to, more recently, spin injection into semiconductors.[1,2] One popular method for studying ballistic electron transport from a metal into a semiconductor is ballistic electron emission microscopy (BEEM), a three terminal scanning tunneling microscopy (STM) based technique with a high energetic ($\sim$0.02 eV) and spatial resolution.[3–6] In addition to measuring Schottky heights and band offsets, this technique can be utilized to measure hot-electron attenuation lengths in metals and silicides.[7–14] In this measurement, the attenuation lengths are extracted by measuring the BEEM current at a bias above the Schottky height as a function of metal thickness. However, these measurements result in attenuation lengths that are often shorter than found using internal photoemission.[9,15,16] This observation has not been convincingly reconciled and indicates that other overlooked effects are influencing these measurements.

It is well known that parallel momentum conservation and elastic scattering of the ballistic electrons at the metal-semiconductor interface has a significant influence on the measured BEEM current. Recent theoretical calculations by Smith *et al.* have shown that the BEEM spectra acquired on Au/GaAs(001) samples and similarities in the spectra obtained from Au/Si(001) and Au/Si(111) samples can only be explained when including the effects of elastic scattering at the interface and the distribution of available parallel momentum states within the semiconductor at the interface.[17] This distribution of states or interface band structure varies significantly between semiconductors and their various surface orientations. Because elastic scattering also occurs in the metal, one would expect that the interface transmission would also be dependent upon the amount of elastic scattering in the metal. This suggests that the measured attenuation length of a given metal is dependent on the interface band structure. However, an attenuation length study of Au(111)/Si(111) and Au(111)/Si(001) Schottky diodes measured only a 17% difference in the attenuation lengths, which was within the uncertainty of the measurement.[10] In contrast, a recent BEEM study of Fe/Si(001) diodes measured a drastic increase in the attenuation length above a second threshold voltage in the BEEM spectra. It was proposed that this increase was due to an increase in the amount of available parallel momentum in the second conduction band making the diode less sensitive to the elastic scattering in the metal.[12,18] This study suggests that the interface band structure of the semiconductor plays a prominent role in the magnitude of the measured attenuation length of the metal. However, to date, no thorough experiment has been performed to show this conclusively.

In this Brief Report, thickness dependent BEEM was performed on Au/Si(111), Au/Si(001), and Au/GaAs(001) Schottky diodes to measure the attenuation lengths in the thin Au films. It was found that the measured attenuation lengths in the Au/GaAs(001) samples was approximately ten times shorter than those in the Au/Si samples. In addition, changes in the slope of the attenuation length with tip bias are observed at the X conduction band minimum of GaAs. These observations can be attributed to differences in the parallel momentum distribution in the semiconductor at the interface and indicate that BEEM determined attenuation lengths are not an intrinsic property of the metal only but of the interface as well.

II. EXPERIMENT

To fabricate the GaAs Schottky diodes, commercially available Si doped ($N_a=10^{18}$) GaAs(001) wafers were introduced into a Veeco Gen II molecular beam epitaxy (MBE) chamber with base pressure of 8×10^{-11} mbar without any chemical cleaning. The native oxide layer was removed and a 2 μm thick Si doped ($N_a=5\times10^{16}$) GaAs layer was grown at 585 °C. These wafers were removed from the MBE chamber, diced into 5×5 mm^2 pieces, and introduced into a Varion 980 electron beam evaporator with a minimum base pressure of 3×10^{-6} mbar for Au deposition. Film thicknesses were monitored with a quartz microbalance calibrated by Rutherford backscattering spectrometry. The Au/Si diodes were fabricated from commercially available phosphorus doped Si(111) ($N_a=9.0\times10^{13}$) and Si(001) ($N_a=3.6\times10^{13}$) wafers. The oxide on the Si substrates was removed by a wet chemical etch and the Au was deposited as men-

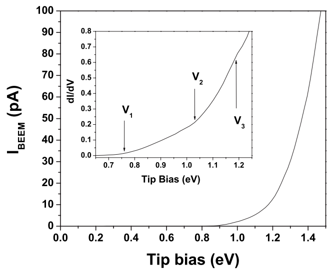

FIG. 1. Typical BEEM spectra obtained from a 19 nm thick Au/GaAs(001) Schottky diode with a tunneling current of 5.0 nA. The three threshold voltages were found to occur at $V_1=0.76$, $V_2=1.03$, and $V_3=1.18\pm0.04$ eV. The inset shows the derivative of the BEEM spectra.

tioned above. Samples were mounted to the sample holder *ex situ* using indium solder, which served as an ohmic contact, while a BeCu clip served as the top side contact. The sample holder was introduced into an ultrahigh vacuum (UHV) chamber with a base pressure of 4×10^{-11} mbar and loaded onto the STM stage that had been cooled to 80 K for all BEEM measurements. A modified low temperature (4–300 K) UHV STM system (Omicron) was utilized to perform the BEEM measurements and has been described elsewhere.[19] BEEM spectroscopy was performed using Au tips fabricated by cutting 10 mil diameter wire at a sharp angle. For each sample, spectroscopy was performed at about 75 locations over an area of about 5×5 μm^2. The spectra were averaged together in order to reduce the effects of surface roughness on the BEEM current. STM images determined the rms roughness to be approximately 1.3 nm.

Auger electron spectroscopy depth profiling was performed to investigate the composition of the films using a Perkin-Elmer PHI 600 scanning Auger microprobe with a base pressure of 7×10^{-9} mbar. Compositional sputter depth profiling was accomplished by focusing a 2 keV argon ion beam on the surface while recording the elemental peaks for the film species and silicon as a function of sputter time. The depth profiling showed no noticeable difference in the intermixing on the three types of samples. The crystallographic texture of the gold films was measured using x-ray pole figures acquired on beamline X-20A of the National Synchrotron Light Source.

III. RESULTS

An example of a typical BEEM spectrum obtained from a 19 nm thick Au/GaAs(001) Schottky diode is shown in Fig. 1. Fits to the modified Bell-Kaiser model ($n=5/2$) found three threshold voltages occurring at $V_1=0.76$, $V_2=1.03$, and $V_3=1.18\pm0.04$ eV.[20] The inset in Fig. 1 shows the derivative of the BEEM spectra. The kinks in the slope indicate better the three threshold voltages. Schottky heights of 0.84 and 0.80 ± 0.02 eV were obtained from the Au/Si(111) and Au/Si(001) samples, respectively.

The (200) x-ray pole figures for 26 nm thick Au films on all three substrates, as well as a pole figure for bare GaAs(001), are shown in Fig. 2. The Au/Si(111) pole figure

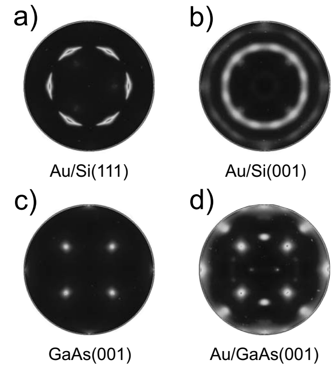

FIG. 2. (200) x-ray pole figures for 26 nm thick Au: (a) Au/Si(111), (b) Au/Si(001), (c) GaAs(001) (substrate only), and (d) Au/GaAs(001).

shows a ring of elongated spots with sixfold symmetry, as displayed in Fig. 2(a). The Au/Si(001) pole figure shows a diffuse intensity ring with a trace of 12-fold symmetric spots, as displayed in Fig. 2(b). The bare GaAs(001) pole figure shows four sharp spots, as displayed in Fig. 2(c). The Au/GaAs(001) pole figure shows the four sharp spots of the substrate, as well as additional spots attributed to the Au film, as displayed in Fig. 2(d).

The logarithm of the percentage transmission of the BEEM current acquired at 1.2 eV is plotted versus metal film thickness in Fig. 3 for the Au/GaAs(001), Au/Si(111), and Au/Si(001) samples. The line through each set of data is the least squares fit to

$$\frac{I_{BEEM}}{I_{tip}} = C(E,T)\exp[-d/\lambda(E,T)], \qquad (1)$$

where I_{BEEM} and I_{tip} are the respective currents, $C(E,T)$ is a proportionality constant that accounts for scattering due to interfaces or within the semiconductor, d is the thickness of the metal, $\lambda(E,T)$ is the hot-electron attenuation length, E is the electron energy, and T is the temperature. From this fit, the attenuation lengths at a tip bias of 1.2 eV are determined to be 11.9 ± 2.4, 13.4 ± 2.7, and 1.6 ± 0.1 nm for the Au/Si(111), Au/Si(001), and Au/GaAs(001) samples, respectively.

The attenuation lengths were measured on all three types of Schottky diodes for tip biases ranging from 1.0 to 1.3 eV

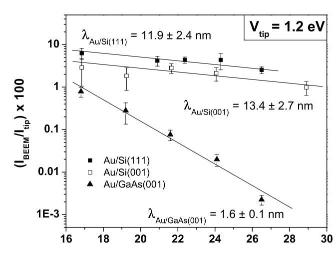

FIG. 3. Normalized BEEM current as a function of Au thickness for a tip bias of 1.2 eV obtained using Au/Si(111), Au/Si(001), and Au/GaAs(001) samples. The solid lines represent the fits to Eq. (1).

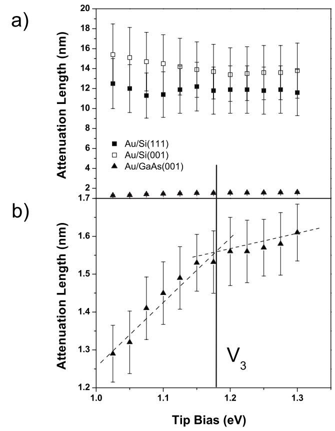

FIG. 4. (a) Energetic dependence of the attenuation length measured using Au/GaAs(001), Au/Si(001), and Au/Si(111) Schottky diodes. (b) Enlarged plot of the attenuation lengths measured on the Au/GaAs(001) samples.

and are displayed in Fig. 4(a). The attenuation lengths show little dependence on tip bias at this scale. However, when magnified, the attenuation length for the Au/GaAs(001) shows an increase with tip bias and a change of slope at the third threshold voltage at 1.18 eV, as seen in Fig. 4(b).

IV. DISCUSSION

The observation of three threshold voltages in BEEM spectra obtained from the Au/GaAs(001) Schottky diodes, as displayed in Fig. 1, has been previously documented and is attributed to the multiple conduction band minima in the band structure of GaAs.[21–23] These threshold voltages correspond to ballistic injection into the Γ, L, and X minima, respectively. The relative difference between the two upper threshold voltages to the lowest, 0.27 and 0.42 eV, agrees well with the relative difference between the L and X minima to the Γ minima, 0.29 and 0.48 eV.[24] The Schottky heights measured on the Au/Si samples are in good agreement with values obtained in previous studies.[7,25,26] The BEEM spectra, measured Schottky heights, and secondary thresholds are similar to other studies which utilized both high vacuum (HV) and UHV depositions of the gold, indicating that the deposition of gold under HV conditions in this study has little effect on the interface influence upon the BEEM measurements.[9,10,21]

Most striking is the approximately ten times shorter attenuation length measured in the Au on the GaAs(001) substrates. Since the attenuation length is a property of a metal, it is insightful to first look at the structure of the Au films to understand this difference. The (200) x-ray pole figures indicate that the Au films are (111) oriented on both Si substrates and (011) oriented on GaAs(001). The Au films on Si(111) have a highly oriented fiber texture with a sixfold symmetry about the Si[111] direction. The Au films on Si(001) surface show a [111] fiber texture [Au(111) parallel to Si(001)] with an apparent 12-fold pattern arising from fourfold twinning about the Au[111] direction. Deposition of Au on GaAs(001) shows an epitaxial relationship that is emphasized by comparing the pole figure from the bare GaAs substrate in Fig. 2(c) with that of the substrate with the Au film in Fig. 2(d). In agreement with earlier studies, the Au/GaAs(001) pole figure indicates that the crystallographic relationship is Au(011) parallel to GaAs(001) and Au$[0\bar{1}1]$ parallel to GaAs [110].[27] The lattice mismatch in the [001] direction of fcc Au(011) (surface lattice constant of 0.408 nm) with the Si(001) (surface lattice constant of 0.384 nm) substrate is 6% and only 2% for the GaAs(001) (surface lattice constant of 0.400 nm) substrate, which may help explain the difference in orientation of the films between the substrates. In addition, the Au overlayer on the GaAs(001) substrate must be forming a two-domain epitaxial layer due to the rectangular Au(110) surface net.

The attenuation lengths measured using the Au/Si samples are similar to those previously reported in this energy and thickness range using Au/Si samples.[9,11,28,29] About two times longer attenuation lengths were measured for Au/Si samples by Weilmeier *et al.* for Au thicknesses up to 60 nm, twice as thick as reported here.[10] This difference can be attributed to the thicker films used, since for thinner films, electrons can make multiple attempts to enter the semiconductor from reflections between the metal-semiconductor and vacuum-metal interfaces, which decreases the measured attenuation length.[11] The attenuation lengths measured on the Au/Si(001) and Au/Si(111) diodes are nearly identical and within the uncertainty of each other despite the significant differences in texture observed in the x-ray measurements, consistent with previous findings.[10] The lower amount of BEEM current for the Si(001) oriented substrate is due to the smaller effective mass of the electrons in the (001) direction relative to the (111) direction, which lowers the transmissivity of the interface, as defined in the Ludeke-Bauer model.[13]

The x-ray data demonstrate that the Au films are epitaxial on GaAs(001), i.e., more ordered than the Au films on Si. This is in direct contrast to the shorter attenuation length measured for Au on GaAs(001). This indicates that the differences in texture cannot explain the large difference in attenuation lengths. The smaller effective mass of GaAs(001) does result in less BEEM current when compared to Si due to the reduced transmissivity, as mentioned above; however, this effect does not change with metal thickness and cannot account for the large difference in the attenuation lengths.[13]

The large difference in attenuation lengths can be understood when considering the differences in the available parallel momentum states at the interface. An interface that has a large amount of available parallel momentum states (broad interface band structure) will be less sensitive to the elastic scattering in the metal film when compared to an interface with a small amount of available parallel momentum states (narrow interface band structure). Consequently, a broad interface band structure will measure a larger attenuation length than a narrow interface band structure. This is a natural consequence of the theoretical treatment of Smith *et al.* when including elastic scattering within the metal and the differences in available parallel momentum states between GaAs and Si.[17,30,31]

This understanding can be further confirmed by observing the change in the slope of the attenuation length as a function of tip bias in the Au/GaAs(001) samples, as seen in Fig. 4(b). The rate of change is quicker for tip biases below the X conduction band minimum. This indicates that the interface is quickly becoming less sensitive to the elastic scattering in the metal. These electrons are accessing the L band, which has a large amount of parallel momentum states and is thus less sensitive to elastic scattering in the metal, causing the attenuation length to increase quickly. The rate of change is slower for tip biases above the X conduction band minimum because this band has a smaller amount of parallel momentum states compared to the L band.[17] This increases the interface sensitivity to elastic scattering in the metal at these high energies, causing a slower rate of change. A similar change in slope was observed for both unpolarized and spin-polarized transport above a second threshold voltage for Fe/Si(001) samples.[12,18] Furthermore, these tip-bias-dependent plots of the attenuation length contain detailed information not only of the transport through the metal but also of the parallel momentum distribution of the interface band structure of the semiconductor. One could use these measurements to theoretically extract these momentum distributions for these and other more complex interfaces such as those between transition metals and semiconductors.

Extrapolating the plots in Fig. 3 in the limit of zero Au thickness results in transmissivity values of 29%, 14%, and 363% for Si(111), Si(100), and GaAs(100), respectively. The low values for the Si substrates indicate that the interface has a significant impact on scattering of the electrons. However, the greater than 100% value for GaAs is nonphysical and indicates that the attenuation length must *increase* for thinner films. Such effects have been observed previously for Pd films thinner than 2 nm on Si, since the probability of elastic scattering decreases exponentially with film thickness, resulting in the longer length inelastic scattering dominating the transport in the thinner films.[13] The effect of the GaAs(001) interface band structure on the attenuation length will decrease with decreasing elastic scattering in the Au, allowing the measured attenuation length to increase for thinner films.

V. CONCLUSIONS

These results demonstrate that the attenuation lengths measured with BEEM are not an intrinsic property of the metal. Rather, they are dependent on the interface band structure of the semiconductor as well. In order to accurately measure the true attenuation length of the metal, the proportionality constant in Eq. (1) must be modified to be thickness dependent, $C(E,T,d)$. With this understanding, the attenuation lengths reported in this Brief Report, and most likely, all BEEM attenuation length measurements, underestimate the true attenuation length. This finding helps reconcile BEEM results with those from internal photoemission. Furthermore, this insight indicates that attenuation length measurements can be utilized to study the momentum distributions of the interface band structures of a wide range of metal-semiconductor interfaces.

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