

The Development of BEEM Modeling for the Characterization of Si/Ge Self-Assembled Quantum Dot Heterostructures

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Abstract – In this paper we present a ballistic electron emission microscopy (BEEM) modeling for the Si/Ge quantum dots characterization. BEEM is a new characterization technique by using electrons ejected from the scanning tunneling microscopy (STM) tip to investigate the metal-semiconductor interfaces. Because of the high resolution of the STM system, BEEM is promising in the characterization of quantum dots as the charge transport on individual dot can be characterized compared to the multitude of dots necessitated in other techniques. This method requires three terminals: a connection to the STM tip to inject electrons, a connection to the sample to collect electrons that traverse the interface, and a third grounding terminal. The energy and angular distribution of the injected electrons can be controlled by varying the tip potential. By using the characteristic data of the injected and collected electrons, many useful transport-related properties of the sample can be obtained. The silicon quantum dots (Si QDs) may be fabricated by taking advantage of the Stranski-Krastanov growth model. Germanium layer has been chosen as a barrier layer due to the large lattice mismatch between Si and Ge. The n-type Si(100) was oxidized to grow ~10 nm thickness of SiO₂ layer. Hemispherical Si nanodot were self-assembled growth on an HF-treated SiO₂ layer by LPCVD technique. The Ge layer were deposited on the pregrow silicon dot. Thin gold (Au) films cap can be used to provide a conductive layer on top of the Si QDs for the BEEM measurement. When the STM tip is positioned on the dot, the injected electron would experience a band profile similar to a double-barrier heterostructure, wherein the quantum dot act as the potential well. However, when the tip is positioned away from the dot (off dot), the injected charge would rather experience a potential step (single barrier) with the band profile.

Index Term - Ballistic electron emission microscopy (BEEM), scanning tunneling microscopy (STM), silicon quantum dots (Si QDs), characterization.

I. INTRODUCTION

The ballistic electron emission microscopy (BEEM) technique is a three-terminal extension of conventional STM, and utilizes an STM tip to inject hot electrons into a semiconductor via a thin metallic layer. Hot electron is an electron with kinetic energy higher than thermal energy, $k_B T$. In BEEM, an atomically sharp STM tip (emitter) is brought

into close contact but not touching the thin conductive surface (base) on the top side of a semiconductor substrate (collector). If the electron injected energy is high enough, "ballistic" electrons can overcome the Schottky barrier height at the sample surface and are collected via a backside contact. The collector current as a function of tip bias is called BEEM current. These phenomenon can be explained by using a three-step model: (i) electrons are injected from the STM tip into the thin metallic layer (tunneling); (ii) electrons propagate through the layer suffering collisions with different quasiparticles (transport), and (iii) finally, electrons overcome the Schottky barrier and enter into the semiconductor (matching of metal and semiconductor wavefunctions across the interface). BEEM technique was introduced by Bell and Kaiser in 1988 [1], [2].

The collector current or BEEM current, is only a small fraction of the tunnelling current injected by the STM tip into metallic layer. At sufficiently small tunneling bias, only ballistic carriers are able to enter the collector, i.e. those carriers which have not been subject to any scattering event. In addition to the energy, the momentum component parallel to an interface is usually conserved to varying degrees. In fact, in the simplest theories capable to quantitatively describe the BEEM current as a function of the tunnelling bias, perfect conservation of the parallel momentum has been assumed [3]. Energy and parallel momentum conservation have the effect that the BEEM current, at a given tunnelling bias, is not only sensitive to lateral variations of the potential barriers, but also to any scattering processes taking place between the point of injection at the surface and the collector.

The properties of silicon quantum dots (Si QDs) have been studied intensively for nanoelectronic device applications. Their unique physical properties, such as size confinement effects and Coulomb blockade phenomena, make Si QDs suitable for use in new silicon-based devices like single electron transistors [4]. Because of electron mean free path in silicon at room temperature is about 10 nm [5], it is necessary to prepare Si QDs with size less than 10 nm to provides electron transport ballistically in the dots.

In the previous work [6], we have proposed a BEEM study for quantum dots characterization. The quantum dots under

testing can be Si quantum dots, InAs quantum dots, AlInP quantum dots, etc. In this paper, therefore, we present a BEEM modeling for the characterization of silicon/germanium self-assembled quantum dot heterostructures by using n-type silicon (100) substrate.

II. THE PRINCIPLES OF BEEM TECHNIQUE

BEEM is a very useful technique to investigate various semiconductor material properties such as Schottky barrier height [7], [8], MOS structure [9]-[11], band offsets [12], size-quantized states [13], and local barrier height between quantum dots and substrate [14]. Ballistic transport, means electrons travel without scattering, occurs when device size is much smaller than the electron mean free path. The simplest structures of BEEM system are those consisting just of a thin conductive layer deposited on the semiconducting collector, as shown in Fig. 1(a). The electrons injected into conductive layer by the STM tip have an energy equal to eV_t , where V_t is the STM tip bias. The thickness of the layer must be comparable to or less than the electron mean free path, so that the electrons can transverse the layer ballistically (without scattering) [15].

If their energy higher than the potential step at the interface, the electron have a finite probability of being injected into conduction band, and after traversing the barrier, reaching the semiconductor substrate, where they emerge as a collector current I_c . The conduction band profile of a simple Schottky diode sample is shown in Fig. 1(b) [15]. Electron tunnel from the STM tip into the metal base. If $eV_t > eV_b$, electron from tip will be able to surmount the Schottky barrier and enter the semiconductor (collector). The applied tunnel voltage with the tip under negative voltage with respect to the base provides the electron potential lies much higher in the STM tip than in the base. Thus electrons entering the base by tunneling through the vacuum barrier have energies high above the Fermi level in the base metal, i.e. they are so-called hot electron.

Unlike other techniques (such as cathodoluminescence, transmission electron microscopy (TEM), and electron beam induced current (EBIC)), BEEM involves extremely low energy electrons, typically in the 1 - 2 V range versus the kilo-Volt range in other methods, and hence constitutes a unique tool to examine dislocation scattering (free of electron hole pair creation) and to study material buried well below the surface. This new form of microscopy could turn out to be a powerful tool for understanding the materials properties and the effects of defects/dislocations on important transport properties in the regime of interest for devices, i.e., few volts [16].

The BEEM technique has also been used to measure conduction band offsets, which are critical for the design of new heterostructure devices such as transistors, lasers, etc. Traditional methods based on current-voltage (I - V) and capacitance-voltage (C - V) measurements have long yielded highly varying results for the GaInP/GaAs system. Recent theoretical calculations have shown that the electronic band

structure depends markedly on the degree of ordering, i.e., the possible alternate stacking of Ga atoms and In atoms in an ordered- instead of a random- array. By careful control of the conditions of crystal growth, it is believed that the order parameter can be changed although the degree of order still varies spatially. Concurrent STM and BEEM measurements have been used to spatially map out simultaneously the ordered domains and the conduction band offsets as a function of ordering. These measurements once again show the power of BEEM to provide new information on electronic transport in semiconductors on a local scale, not possible by any other technique [17].

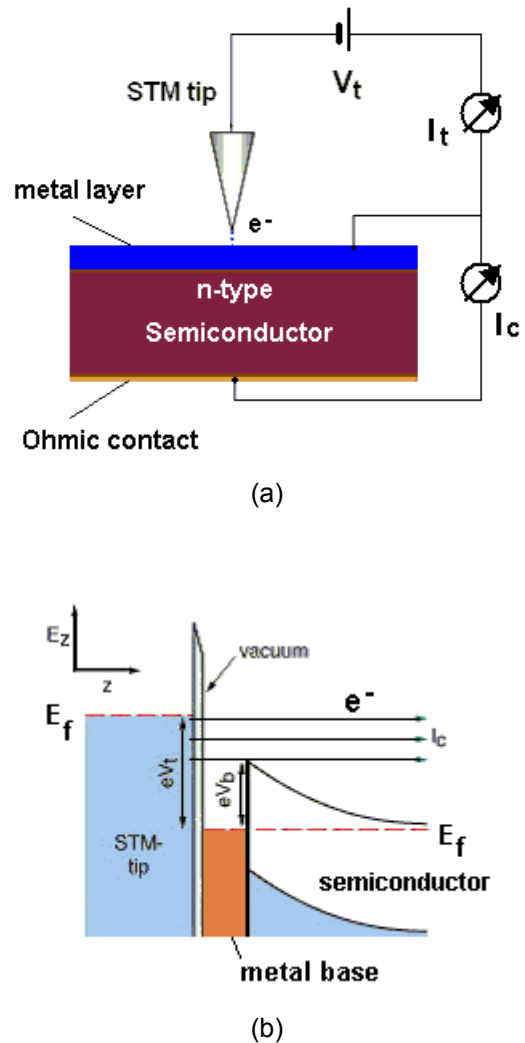


Fig. 1. (a) The simplest structures of BEEM system are consisting of a thin conductive layer on the semiconducting substrate, (b) a schematic of energy diagram of a BEEM model on a Schottky barrier diode.

The Schottky barrier height formed at the metal-semiconductor interface is then one of the quantities of interest, determining the potential barrier to be surmounted by the hot charge carriers. The barrier height, Φ_B , can be obtained

by measuring the collector current, I_c , or BEEM current as a function of the tunnelling bias V_t , and by fitting the resulting spectra to a power law of the form:

$$I_c(V_t) = R(eV_t - \Phi_B)^\alpha \quad (1)$$

The exponent α has a value of 2 when quantum mechanical reflection at the interface is neglected, or 5/2 if it is taken into account within an effective mass approximation. Schottky barrier height inhomogeneities are responsible for many anomalies in the behaviour of macroscopic Schottky diodes. Schottky barrier height fluctuations on a nanometer scale have been observed by several groups [1], [18].

Kaiser and Bell [1] is one of the first to use this technique in the characterization of semiconductor structures. In their work, they described a ballistic electron spectroscopy technique to characterize the spatially resolved charge transport properties of the interfaces as well as the theoretical treatment in order to understand the spectroscopic features they were observing. Since then, many researchers have utilized BEEM in their research on semiconductor structures and several extensive reviews [18]-[20] have been published about the applications of BEEM. Among the many of material systems were investigated using BEEM include InAs/GaAs, Si p-n junction, and SiGe strained layers [21], [22]. The Bell-Kaiser [2] and the Ludeke-Prietsch model [23] uses a planar tunneling formalism and transverse momentum conservation at the metal-semiconductor interface to determine Schottky barrier height. The Bell-Kaiser model has been found to fit the BEEM current spectra for Au/Si system [2] by using a $I_c \approx (V_t - V_s)^2$ approximation, see Eq. (1). However, Ludeke and Prietsch [23] found that a $I_c \approx (V_t - V_s)^{5/2}$ model more closely approximated conditions in a metal/GaP system and an Au/GaAs system [24]. The difference in the Ludeke-Prietsch model takes into account the electron mean free paths in the base metal layers and quantum mechanical transmission at the metal-semiconductor interface. However, at near threshold conditions the difference between both models is very small [19], [25] and within experimental error. Higher deviations might be expected with voltages far from the threshold values. These deviations might be caused by the voltage dependent energetic distribution of the tunneling current, carrier scattering in the metal overlayer as well as carrier scattering and impact ionization in the semiconductor substrate.

III. PHYSICAL MODEL AND MEASUREMENT DESIGN

The first BEEM study of quantum dots were done by Rubin et.al. [26] in their research on single InAs self assembled quantum dots buried beneath a Au/GaAs interface. InAs dots were grown on top of undoped GaAs buffer layer and covered with GaAs cap layer. BEEM images show shifted current thresholds when comparing spectra taken with the tip over the quantum dot with off dot spectra. The off dot spectra showed structure for Au on bulk GaAs. A slight dip in the center of each dot was believed to be caused by strain induced

preferential buildup of the cap GaAs layer away from the center of the dot during growth. They have been observed an enhancement of the BEEM current when the tip was over the buried quantum dots. The fine structure was consistent with resonant tunnelling through two different quantum states of the dot with an energy separation of ~ 0.1 eV.

When introducing BEEM, Bell and Kaiser [2] presented a formula for the modelling of the ballistic current, which has been widely utilized in BEEM since then. Their first step in developing their model was to use the well-known formalism for tunnelling between planar electrodes as an approximation. For simplicity, the STM tip and the base layer are assumed to be identical metals.

The silicon quantum dots (Si QDs) to be studied in this work can be fabricated by taking advantage of the Stranski-Krastanov growth model [27]. Germanium layer has been used as a barrier layer due to the large lattice mismatch of Si and Ge. Chemically cleaned by HF of n-type Si(100) wafer was oxidized in O_2 ambient to grow ~ 10 nm thick SiO_2 layer. Hemispherical Si nanodots were first self-assembled on an HF-treated SiO_2 layer by using LPCVD technique. The Ge layer may be deposited on the pregrow silicon dots via same deposition processes. Thin gold (Au) films cap can be used to provide a conductive layer on top of the Si QDs for the BEEM measurement as shown in Fig. 2. There is no intralayer required at the Au/Si QDs system. The STM tip will be used to inject electrons in thin Au films. Electrons can travel through these structures and be collected in the back contact of semiconductor if two conditions are fulfilled: the Au film thickness should be comparable or less than electron mean free path (typically 10 nm for electron of 2 eV) and the electron energy should be above the Schottky barrier height at the interface.

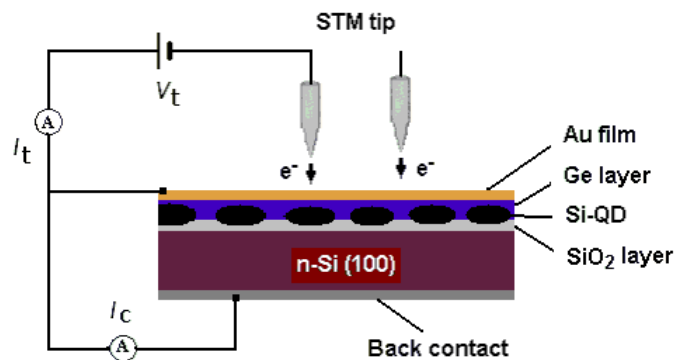
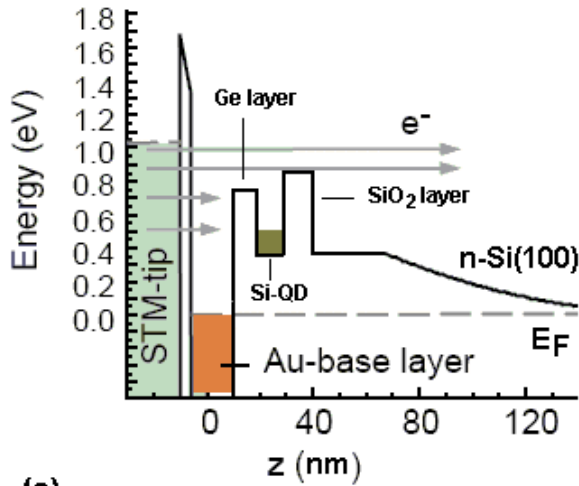


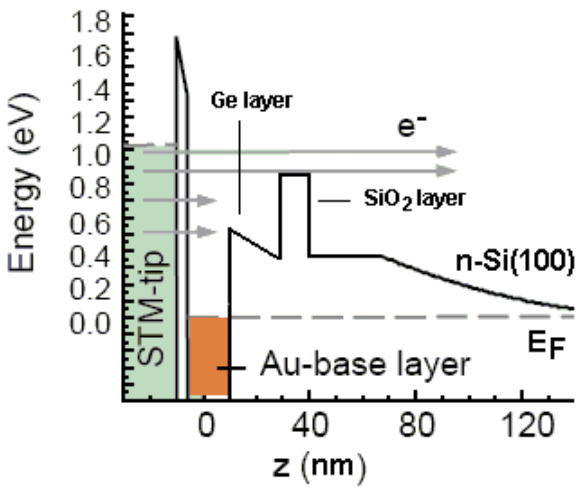
Fig. 2. Schematic of a BEEM set-up for Si/Ge quantum dot heterostructures. STM tip may be positioned on the dot or away from the dot (off dot).

When the STM tip is positioned on the dot, the injected electron would experience a band profile similar to a double-barrier heterostructures of Ge/Si-QDs/ SiO_2 /n-Si, wherein the silicon quantum dot act as the potential well, as shown in Fig. 3(a). However, when the tip is positioned away from the dot (off dot), the injected charge would rather experience a

potential step (single barrier) with the band profile of Ge/SiO₂/n-Si, see Fig. 3(b). In the both case, if the injected electron has enough energy will travel through the barrier to reach the semiconductor back contact (collector) and thus contribute to the BEEM current (I_C), see Fig. 2. These phenomena are similar to reported by Reddy et al. [28] for InP self-assembled quantum dots on GaAs substrate. The Bell-Kaiser or Ludeke-Prietsch model may be used for the electron transport analysis purpose on the Ge/Si QDs heterostructures which is expected that the both models will be produced result with almost same or a very little different only.



(a)



(b)

Fig. 3. Typical conduction band profile that an injected electron would experience when the STM tip is positioned on the dot (a) and off the dot (away from the dot) (b).

Analysis based on the thermionic emission theory gives a barrier height of Au/Ge contact of 0.4 eV at temperature of 130 K and 0.5 eV at room temperature [29], [30]. The BEEM

and internal photoemission (IPE) measurements in Au/Si structures gives Schottky barrier of 0.79-0.83 eV [31]. Redy et al. [28] obtained Au/GaAs barrier height of 0.92 ± 0.02 eV by performing the BEEM spectroscopy on a reference GaAs epilayer sample. The threshold of the off dot curve is determined to be 1.24 ± 0.02 eV, the band offset between GaAs/InAlGaP is 0.32 ± 0.02 eV. However, on dot spectrum look quite different with appearance of an inflection point with threshold of 1.17 ± 0.02 eV.

IV. CONCLUSION

The BEEM provides an alternative method for study of electron transport properties on nanoscale devices as a replacement for conventional $I-V$ and $C-V$ measurement techniques. The main advantage of the BEEM technique is its very high resolution and promising in the characterization of quantum dots as the charge transport on individual dot can be characterized. As the beam of injected electrons is very narrow, its diameter at the interface is estimated to be less than 10 nm. The expected energy resolution is typically 50 meV

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