Electron transport across complex oxide heterointerfaces
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Chapter 3

Metal-semiconductor interfaces and ballistic electron emission microscopy

This chapter is divided into two parts. In the first part the metal-semiconductor (M-S) interfaces are discussed - viz. the formation of the Schottky barrier (SB), followed by the models to determine the Schottky barrier height (SBH), possible barrier lowering mechanisms like image force lowering, lowering due tunneling and due to electrostatic screening. In the second part we discuss the basic concepts of hot electron transport, as used in ballistic electron emission microscopy (BEEM). The various modes of operation in BEEM are presented. This is then followed by discussions of the various possible scattering mechanisms for hot electrons. The most commonly used model to determine the local Schottky barrier height, called the Bell-Kaiser model is discussed.

3.1 Transport at metal-semiconductor interfaces

We discuss the different transport mechanisms that occur at biased and non biased Schottky interfaces between a metal and a semiconductor. First we discuss common transport models such as thermionic emission and tunneling across such interfaces [1], [2]. We explain the relevance of incorporating tunneling mechanisms to explain the observed current-voltage (I-V) characteristics in our devices (as presented in Chapter 5). Further, we also discuss in details the hot electron transport at similar Schottky interfaces using the technique of ballistic electron emission microscopy (BEEM). We explain the different contributions of hot electron scattering in metals, semiconductors and their interfaces to hot electron transport. We also discuss the factors that influence the hot electron attenuation length in metals. We finally discuss the Bell-Kaiser model that is commonly used to extract the local Schottky barrier height at metal-semiconductor (M-S) interfaces [3].

3.1.1 Schottky barrier formation

When an n-type semiconductor is brought in contact with a metal, electrons will flow from the semiconductor to the metal if the Fermi level of the semiconductor
(SC) is higher than that of the metal. Such flow of electrons causes the Fermi levels of the metal and the semiconductor to align. The electrons moving from the semiconductor to the metal leave depleted donors in a region close to the interface that create an electric field in the semiconductor. This field causes band bending in the semiconductor close to the interface, leading to the formation of a Schottky barrier as shown in Fig. 3.1. Such a barrier is a rectifying barrier for electronic transport across the metal semiconductor interface. In Fig. 3.1 (a) the conduction band, valence band and Fermi level of the semiconductor are given by $E_C$, $E_V$ and $E_{FS}$. $\phi_m$ is the work function of the metal, which corresponds to the energy difference be-

![Energy band diagram](image)

**Figure 3.1:** Energy band diagram of formation of a metal-semiconductor (n-type) (M-S) contact. (a) before contact, (b) after the contact; the formation of a Schottky junction for the case where $\phi_m > \phi_S$. The M-S interface shown in (b) is at equilibrium.
3.1. Transport at metal-semiconductor interfaces

between the vacuum level and the Fermi level of the metal. $\chi$ is the electron affinity of the semiconductor, which is measured from the bottom of the conduction band to the vacuum level. The obtained Schottky barrier allows electrons to flow from the semiconductor to the metal, but blocks it in the opposite direction, which makes it a rectifying junction. In this thesis, the two most important parameters that are to be considered are the depletion layer width ($W$) and the Schottky barrier height ($\phi_B$).

3.1.2 Depletion layer

As mentioned above, when a metal is brought in contact with a n-type semiconductor, electrons flow from the semiconductor to the metal. This leaves a region, close to
the interface, depleted of mobile electrons. This region is called the depletion layer. The depletion width ($W$) in a Schottky junction can be determined analytically using Poisson’s equation. The depletion layer width depends on the semiconductor permittivity ($\epsilon_s$), donor concentration ($N_D$), built-in potential ($V_{bi}$) and applied bias ($V$) [1], [2], following the equation:

$$W = \sqrt{\frac{2\epsilon_s}{qN_D}(V_{bi} - V)}$$

(3.1)

Because of the static charge in the depletion layer an electric field is present. The strength of this field depends on the charge carrier density ($N_D$), the depletion width ($W$), the permittivity of the semiconductor ($\epsilon_s$) and the distance from the interface ($x$). This dependence is given by [1], [2]:

$$|E(x)| = \frac{qN_d}{\epsilon_s}(W - x) \text{ for } 0 \leq x \leq W$$

(3.2)

The electric field is the largest at the interface, i.e. for $x = 0$

$$|E_{max}| = \frac{qN_d}{\epsilon_s}(W)$$

(3.3)

The presence of an internal electric field across the M-S interface results in a potential difference between the metal and the semiconductor bulk called the contact potential ($V$) which is given as:

$$V(x) = \frac{qN_d}{\epsilon_s}(Wx - \frac{1}{2}x^2) - \phi_B$$

(3.4)

3.1.3 Schottky barrier height

From Fig. 3.1 (b) it is seen that the Schottky barrier height depends on the work function of the metal ($\phi_m$) and the electron affinity of the semiconductor ($\chi$) as:

$$\phi_B = (\phi_m - \chi)$$

(3.5)

This relation is called the Schottky-Mott relation. This model of determining a Schottky barrier is based on a few assumptions: (a) The surface dipole contribution to $\phi_m$ and $\chi$ do not change when the metal and semiconductor are brought together. (b) There are no localized states present on the surface of the semiconductor, and it forms a perfect contact with the metal. In more complex approximations determining the Schottky barrier height, the influence of image potential, tunneling, and electrostatic screening should be taken into account. These three mechanisms are discussed as follows:
3.1. Transport at metal-semiconductor interfaces

Figure 3.3: (a) Left: field caused by an electron close to the metal-semiconductor interface and surface charges. Right: field caused by two opposite charges on either side of the interface. (b) Representation of a Schottky barrier showing the image force effect which lowers and pulls the SBH maximum inside the semiconductor, indicated by the shaded blue region.

1. Image force lowering.
2. Lowering due to tunneling.
3. Lowering due to electrostatic screening.

Schottky barrier lowering by image charge potential

When an electron approaches the metal-semiconductor interface, it attracts surface charges of opposite sign in the metal. These surface charges in the metal film exactly balance the field generated by the electron in the semiconductor, so that it does not penetrate into the metal as shown in the left side of Fig. 3.3 (a). The field produced by these surface charges and the electron in the semiconductor is the same as the field generated by an electron in the semiconductor and another particle of opposite charge in the metal as shown in the right side of Fig. 3.3 (a). This other particle is called the image charge. This image charge in the metal film creates an image charge
potential close to the barrier. This field is the highest at the barrier, because there the electron is very close to its image charge. At a large distance from the interface, the electron hardly feels the attraction of its image charge anymore and the attractive force goes to zero. The potential energy caused by this image charge as a function of distance from the interface is schematically depicted in Fig. 3.3 (b). When the image potential energy is added to the original potential in the depletion layer, we find the barrier shape that accounts for the image force. This resulting barrier height is lower by an amount $\Delta E_I$ given by [1], [2]:

$$\Delta E_I = \sqrt{\frac{qE_{\text{max}}}{4\pi\varepsilon_S}}$$  \hspace{1cm} (3.6)

In addition to lowering of the Schottky barrier, the image charge potential also pulls the potential maximum into the semiconductor as shown in Fig. 3.3 (b) over a distance of $\Delta z$ given as follows [1], [2]:

$$\Delta z = \frac{1}{4} \sqrt{\frac{q^2}{2\pi^2\varepsilon_S\varepsilon_0 N_D(\phi_B - V_N - k_BT)}}$$  \hspace{1cm} (3.7)

Because the maximum potential lies inside the semiconductor, the electrons first travel a short distance through the semiconductor before they reach the top of the barrier.
3.1. Transport at metal-semiconductor interfaces

Schottky barrier lowering by tunneling

The second mechanism that can cause lowering of the effective Schottky barrier height is tunneling, either direct or thermally assisted. Under forward bias, in heavily doped semiconductors at low temperatures, electrons can tunnel directly from the Fermi level of the semiconductor, through the Schottky barrier, to the metal. For reverse bias, tunneling from the metal to the semiconductor can happen under the same circumstances. The current that arises from these electrons is called field emission as shown in Fig. 3.4. When electrons have a certain thermal energy, they can also tunnel through the barrier with thermal assistance. Since the barrier is thinner at higher energies, electrons with higher energies have higher tunneling probability. On the other hand, the number of electrons with higher energies are few. This implies that the electrons with a certain amount of energy have maximum contribution to thermionic-field emission (denoted by \(E_m\)), as shown in Fig. 3.4. When the Schottky barrier is approximated as a triangular potential barrier, the tunneling probability (\(P\)) for an electron having an energy \(\Delta E\) less than the height of the barrier is given by following equation [2]:

\[
P = \exp\left[-\frac{2}{3} (\Delta E)^{3/2} / E_{00} V_{bi}^{1/2}\right]
\]

(3.8)

Here \(\Delta E\) is the energy of the electron below the top of the barrier and \(V_{bi}\) is the built-in potential. \(E_{00}\) is a parameter which plays an important role in tunneling theory. It is the diffusion potential of a Schottky barrier such that the transmission probability for an electron whose energy coincides with the bottom of the conduction band at the edge of the depletion region is equal to \(e^{-1}\) [2], and is given by:

\[
\Delta E_{00} = \frac{\hbar^2}{2} \sqrt{\frac{N_d}{m^* \varepsilon_S}}
\]

(3.9)

Here \(\hbar\) is the Planck constant, \(N_d\) the donor concentration and \(\varepsilon_s\) the permittivity of the semiconductor.

From Eqn. 3.8 it can be deduced that an \(E_{00}\) value of 0 leads to a tunnel probability of zero and a higher value leads to a higher tunnel probability. Also, a lower \(\Delta E\) value, which means a higher electron energy, leads to a higher tunnel probability. When \(\Delta E\) becomes zero, i.e. the electron has an energy equal to that of the Schottky barrier, the tunnel probability goes to 1, which we would expect, since the electron has enough energy to overcome the barrier. Because the tunneling electrons can cross the barrier at an energy lower than the maximum of the Schottky barrier, direct and thermally assisted tunneling lower the effective Schottky barrier height as shown in Fig. 2.8. The amount of Schottky barrier height lowering due to these
Figure 3.5: Schottky barrier lowering due to electrostatic screening. $\phi$ and $\phi_{eff}$ represent the original and effective Schottky barrier height and $\Delta E_{ES}$ is the Schottky barrier lowering due to electrostatic screening. Adapted from [4].

Schottky barrier lowering due to electrostatic screening

The third mechanism that can cause Schottky barrier lowering is electrostatic screening. In ideal Schottky theory, the potential distribution in the metal is assumed to be constant. However, this condition may be violated in the metal close to the interface with the semiconductor, when the magnitude of the free charge carriers induced at the surface of the metal becomes large [5]. This is the case at an interface with a large permittivity semiconductor, such as Nb:SrTiO$_3$. This large permittivity causes a voltage drop on the metal side of the junction due to the conservation of electric displacement, as shown in Fig 3.5 [6]. The barrier potential corresponds to the energy that is needed to excite an electron from the bulk of the metal to the semiconductor. From Fig. 3.5 we can see that this barrier is lowered by the amount of the voltage drop in the metal. For zero applied bias, this value can be calculated as:

$$\Delta E_{ES} = \sqrt{2\phi_B q N_D \varepsilon_S / \varepsilon_0 \varepsilon_M^2 \lambda^2}$$  \hspace{1cm} (3.11)
3.2. Electronic transport across a Schottky barrier

In contrast to barrier lowering by image force and tunneling, the barrier lowering due to electrostatic screening is proportional to the square root of the semiconductor permittivity. Thus for higher values of the relative permittivity the Schottky barrier is reduced by a larger amount.

3.2 Electronic transport across a Schottky barrier

For macroscopic characterization of Schottky junctions, current-voltage measurements (I-V measurements) are most commonly used. In such measurements, a varying voltage is applied across the interface and the current through the interface is measured as shown in Fig. 3.6. In this circuit, electrons cross the barrier at the interface between the semiconductor and the metal. Following are the various mechanisms by which electronic transport across the barrier can take place (Fig 3.6) [1], [2].

1. Thermionic emission over the top of the barrier.
2. Thermally assisted tunneling through the barrier.
3. Direct tunneling through the barrier.
3. Metal-semiconductor interfaces and ballistic electron emission microscopy

3.2.1 Thermionic emission

The electrical transport across an ideal Schottky barrier is described by thermionic emission [1]. By subtracting the current which flows from the metal to the semiconductor \(J_{M\rightarrow S}\) from the current flowing from the semiconductor to the metal \(J_{S\rightarrow M}\) the following expression for the total current \(I\) is obtained [1], [2]:

\[
I = A^* AT^2 \exp\left(-\frac{q\phi_B}{k_BT}\right) \left[ \exp\left(\frac{qV}{nk_BT}\right) - 1 \right]
\]

where \(q\) is the charge of the electron, \(k_B\) the Boltzmann constant, \(T\) the temperature, \(A^*\) the Richardson constant, \(\phi_B\) the barrier height and \(n\) the ideality factor (unity for purely thermionic emission dominated transport), and \(A^*\) is given by:

\[
A^* = \frac{4\pi em_e^* k_B^2}{h^3}
\]

where \(m_e^*\) is the effective mass of the electron in the semiconductor. The value of \(A^*\), the Richardson constant, used in this thesis for Nb doped SrTiO\(_3\) semiconductor is 156 Acm\(^{-2}\)K\(^{-2}\) [8]. When temperature is kept constant during a measurement, the only variables are the ideality factor and Schottky barrier height for zero applied voltage, so these parameters can be determined by fitting the experimental data. However in practice, resistances appear in the semiconductor and the rest of the circuit as well, and contribute to the series resistance causing the current-voltage characteristics to deviate from thermionic emission theory at high voltages. Because of the series resistances in the circuit, the applied voltage does not drop completely at the Schottky barrier, but also drops partially in the rest of the circuit and in the semiconductor. To reckon for the voltage loss due to these resistances we can adjust Eqn. 3.12. The voltage drop over the interface is then given by \(V - IR\) instead of \(V\), where \(R\) is the total resistance of all elements in the circuit. This results in following equation for current:

\[
I = A^* AT^2 \exp\left(-\frac{q\phi_B}{k_BT}\right) \left[ \exp\left(\frac{q(V - IR_s)}{nk_BT}\right) - 1 \right]
\]

3.2.2 Electron transport by tunneling

Thermally assisted tunneling and direct tunneling

Since electrons have a higher thermal energy at higher temperatures, thermal emission (represented by (a) in Fig. 3.6) is more dominant in that case. For lower temperatures, electrons lose their thermal energy and direct tunneling becomes dominant. In between these two regimes lies the thermally assisted tunneling regime. While
3.3. Ballistic electron emission microscopy (BEEM)

at very low temperatures electrons tunnel directly through the barrier (direct tunneling, represented by (c) in Fig. 3.6), at intermediate temperatures electrons first get thermally excited and then tunnel at a higher energy corresponding to a thinner part of the barrier (thermally assisted tunneling, represented by (b) in Fig. 3.6). In the direct tunneling regime the current is given by [7]:

\[ I = I_s \left[ \exp\left(\frac{qV}{E_{00}}\right) - 1 \right] \quad (3.15) \]

Where \( E_{00} \) is given by Eqn. 3.9 and the saturation current density \( I_s \) depends weakly on temperature as \( cT/sin(cT) \), where \( c \) is a constant. In the thermally assisted tunneling regime, the current density is given by [9]:

\[ I = I_s \left[ \exp\left(\frac{qV}{E_0}\right) - 1 \right] \quad (3.16) \]

and

\[ E_0 = E_{00}coth\left[\frac{qE_{00}}{kT}\right] \quad (3.17) \]

where, \( E_{00} \) is a tunneling parameter (also called as characteristic energy). \( E_{00} \) (T = 0 K) is 1, (Eqn. 3.9.) hence \( E_0 \) (T = 0 K) equals \( E_{00} \). It also implies that for this case Eqn. 3.16 approaches to Eqn. 3.15 at very low temperatures.

3.3 Ballistic electron emission microscopy (BEEM)

Introduction

The technique of ballistic electron emission microscopy (BEEM) was developed by Kaiser and Bell in late 1980’s [3]. BEEM is a non destructive technique and is based on a scanning tunneling microscope (STM) [10]. It is a modified form of STM, with an additional contact at the bottom of the semiconducting substrate, which can collect the electrons traveling through the metal overlayer and across a Schottky interface. Here, the STM tip is used to inject a distribution of hot electrons into the metal overlayer to be investigated. The hot electrons travel through the metal overlayer and get scattered. A fraction of these electrons are able to cross the Schottky interface when they have the necessary energy and momentum to do so.

BEEM has been used for studying hot electron transport in thin films and multi-layers using conventional semiconductors like Si, GaAs [11], [12], [13], [14]. Energy and spatial dependence of carrier transport, at the nanoscale and across buried layers and interfaces using current perpendicular to the plane of the device can be
investigated using BEEM. The basic schematic of BEEM with its circuit diagram is shown in Fig. 3.6. A negative bias, $V_T$, is applied to the tip to inject electrons into the metal film, as tunnel current, $I_T$. The electrons travel through the film, across the interface and are collected in the semiconductor as a BEEM current, $I_B$. The BEEM current constitutes a fraction of electrons which have the proper energy and momentum to overcome the Schottky barrier height. Such an energy and momentum filter is represented by an acceptance cone at the Schottky interface as shown in Fig. 3.8. The energy schematic of the BEEM is shown in Fig. 3.9.

**Hot electrons and their scattering mechanisms**

When the injected electrons have an energy a few tenths of an electron volt above the Fermi level of the system they are referred to as "hot" electrons. By applying a bias of a few eV to the STM tip with respect to the Fermi level of the metal layer we inject a distribution of electrons into the metal overlayer. As $k_B T$ is 25 meV at room temperature, a similar analysis yields an equivalent temperature of $\approx 12000$ K for 1 eV [14]. Such an analogy leads to the term "hot" electrons when the energy of the injected electron is few eV above the Fermi level of the metallic film. Scattering
mechanisms for hot electrons and for electrons at the Fermi level are very different. Hot electrons injected at an energy $eV_T$ can scatter into all unoccupied states between $eV_T$ and $E_F$, according to Fermi’s golden rule. Such an electron-electron (e-e) scattering for hot electrons results in inelastic scattering (loss of energy) and is a dominant scattering mechanism. In contrast, at the Fermi level elastic or quasi-elastic scatterings are the dominant scattering mechanism. When the hot electrons reach the interface without being scattered inelastically or elastically, they are called "ballistic" electrons.

The hot electron transport in BEEM can be divided in different steps:

1. Injection of the hot electrons from the tip into the metal base.
2. Transport of hot electrons through the metal base.
3. Transmission of hot electrons across the metal-semiconductor interface.
4. Collection at the conduction band of the semiconductor.

Charge carriers are injected from the tip by tunneling into unoccupied states of the thin metal base. This results in momentum and energy distribution of the injected carriers at the metal surface. After injection, the hot electrons travel through

Figure 3.8: Energy schematics of the BEEM technique. It shows the hot electron distribution injected into the metal overlayer. Subsequently, a fraction of them get collected in the conduction band of the semiconductor.
3. Metal-semiconductor interfaces and ballistic electron emission microscopy

the metal film and are scattered by cold electrons (lying close to Fermi level) by inelastic scattering. However, an energy independent elastic [15] or quasi-elastic scattering by with either defects, grain boundaries, phonons, magnons etc. can also occur. When the electrons reach the interface and satisfy the energy and momentum criteria at the interface, they can be transmitted through and enter the conduction band of the semiconductor and constitute the BEEM current. Due to the local nature of injecting electrons and the requirement of lateral momentum conservation at the Schottky interface, this technique results in a very high spatial resolution [16].

3.4 BEEM Theory

In order to extract the Schottky barrier height from spectroscopy measurements, a theoretical model is needed to fit the data. The first theoretical description dealing with the transport of hot charge carriers through a metal-semiconductor system in a BEEM setup was proposed by L.D. Bell and W.J. Kaiser [3]. For all the work presented in this thesis, electrons are the charge carriers responsible for the BEEM current, due to the use of n-type semiconducting substrates (Nb doped SrTiO$_3$).

3.4.1 Tunnel injection of non-equilibrium charge carriers

The applied potential between the tip and the metal base, called the tip voltage $V_T$, will determine the energy of the injected electrons. Tunneling across the potential barrier between the tip and the metal will always result in a distribution of the energy and momentum of the electrons. In common BEEM theory [3], the tunnel injection of non-equilibrium electrons from the tip into the base is assumed to behave according to the planar tunneling theory [17]. Although it has been shown that it is not always valid to use planar tunneling theory, the voltage spectroscopy measurements with BEEM are found to agree well with planar tunneling based theory [18]. At tip voltages close to the threshold this results in a sharply peaked distribution of the injected electrons perpendicular to the M-S interface. Therefore the injected electrons will have little momentum parallel to the metal base ($k_\parallel \ll k_\perp$).

3.4.2 Transport across the metal base

Due to scattering the spatial and energetic distribution of the electrons will broaden when traversing the metal base. When assuming a free electron like behavior the attenuation of the electrons can be described by a single parameter called the attenuation length, $\lambda(E)$, which in principle is energy dependent. The attenuation can
3.4. BEEM Theory

Figure 3.9: Four different scattering mechanisms in a forward biased BEEM, where the solid spheres represent electrons and hollow spheres represent holes. (1) is a purely ballistic transport (red), (2) is inelastic scattering of hot electrons in the metal overlayer (pink) can also lead to secondary electrons, (3) elastic scattering in the metal over layer and (4) impact ionization where an electron-hole pair is created (green).

then be described by an exponentially decaying function depending on the injection angle $\theta$ away from the surface and metal film thickness $d$:

$$\frac{I_B}{I_T} \propto e^{(-d/\lambda(E)\cos(\theta))}$$  \hspace{1cm} (3.18)

Since the electrons are injected with almost zero parallel momentum $k_\parallel = 0$ we can assume $\cos(\theta) \approx 1$, simplifying the equation.

### 3.4.3 Scattering mechanisms

All of the different scattering processes which are relevant in this thesis occur in the metal base and interface. In Fig. 3.9, the most prominent scattering mechanisms are depicted, which are:

**Ballistic charge carriers** Ballistic transport is the unscattered propagation of electrons through the metal base. These electrons do not lose energy or undergo a change in momentum and form an important contribution to the BEEM current.
If the electrons travel ballistically through the metal base they might have enough energy, depending on $V_T$, to surmount the Schottky barrier at the M-S interface.

**Inelastic scattering**  If the electrons are scattered inelastically their energy will be reduced. The processes dominating this form of scattering, at the energies relevant for this thesis is electron-electron (e-e) scattering [3] and will typically result in a reduction of half the electron energy. At low tip voltage this effectively means that any inelastically scattered electron will not have enough energy to surmount the Schottky barrier. However at higher tip voltages, at least twice that of the Schottky barrier, the collision might result in a secondary electron with enough energy to surmount the Schottky barrier, while the primary electron still has energy above the Schottky barrier, thereby increasing the BEEM current. Although phonon scattering can also result in energy loss, they are not taken into account since the change in energy is negligibly small (in the order of $k_B T$) in comparison with e-e scattering. Although plasmon excitations also cause inelastic scattering they are not relevant since the electron energies relevant for this thesis are too low for plasmon excitations to occur.

**Elastic scattering**  This form of scattering will change the momentum but conserves the total, kinetic, energy of the electrons. Therefore any elastic scattering will result in a broadening of the distribution of angular momentum. Since transmission across the M-S interface depends sensitively on the momentum, as shown in section 3.4.4, elastic scattering will also have an effect on the BEEM current. Grain boundaries, defects and any inhomogeneities in general are the main elastic scattering sites.

**Impact ionization**  When an electron with high enough energy enters the semiconductor, it could transfer a part of this energy to an electron in the valence band. If enough energy is transferred, it could excite the electron to the conduction band creating an electron-hole pair. This electron could then contribute to the BEEM current. However, for this to occur the impacting electron should have an excess energy nearly more than twice the semiconductor band gap. Since all experiments performed in this thesis are below this limit, impact ionization is absent.

**Transport across the metal base**

Scattering causes broadening of the spatial and energetic distribution of the injected electrons while traveling through the metal overlayer. Scattering in the metal overlayer can be quantified by hot electron attenuation length When assuming a free
electron like behavior the attenuation of the electrons can be described by a single parameter called the attenuation length, $\lambda(E)$, which is usually an energy dependent parameter (Eqn. 3.18).

### 3.4.4 Transmission across the M-S interface

The transmission across the barrier is dependent on the energy and the momentum of the incoming electrons. Assuming the electrons satisfy the 2-d free electron model, their energy would be given as:

$$E = \frac{\hbar^2}{2m} (k_{\perp}^2 + k_{\parallel}^2) = E_{\perp} + E_{\parallel}$$  \hspace{1cm} (3.19)

where $m$ is the rest mass of the electron and $k_{\perp}$ and $k_{\parallel}$ are the momentum of the electron perpendicular and parallel to the M-S interface, respectively. Here, $k_{\parallel}$ is assumed to have both $K_x$ and $k_y$ components. The energy of the electron just at the maximum of the Schottky barrier height can now be expressed as:

$$E = \frac{\hbar^2}{2m^*} (k_{\perp S}^2 + k_{\parallel S}^2) + E_f - eV + \phi_B$$  \hspace{1cm} (3.20)

where $m^*$ is the effective mass of the electron inside the semiconductor and the subscript of $k_S$ denotes the momentum in the semiconductor. If we now assume conservation of parallel momentum we can obtain an analytical expression for the maximum allowed parallel moment $k_{\parallel S}$. This argument would only be fully convincing for a fully epitaxial system without defects, any deviations from such a system would break the symmetry and therefore conservation of parallel momentum could be lost to a certain degree. Despite this, experimental evidence for non-epitaxial Au/Si systems showing momentum conservation has been observed [19]. We can equate Eqns. 3.20 and 3.21 which will give us an expression for $E_{\parallel}$:

$$E_{\parallel} = \frac{m^*}{m - m^*} (E_{\perp} - E_{\perp S} - E_f + eV - \phi_B)$$  \hspace{1cm} (3.21)

The maximum amount of parallel energy $E_{\parallel}^{\text{max}}$ would be obtained if the electron would have exactly zero perpendicular energy left after crossing the Schottky barrier i.e. $E_{\perp S} = 0$. This shows that due to the effective mass there is a restriction on the amount of parallel momentum:

$$E_{\parallel}^{\text{max}} = \frac{m^*}{m - m^*} (E_{\perp} - E_f + eV - \phi_B)$$  \hspace{1cm} (3.22)

If the electron has more parallel momentum than $E_{\parallel}^{\text{max}}$ it cannot be transmitted across the M-S interface and will bounce back into the metal base. This effect is
much like the total refraction of light at an interface of two media having different refractive indices. Since we have found the maximum parallel momentum that electrons can have and we know that the maximum total energy is the Fermi energy, the minimum perpendicular energy $E_{\perp}^{\min}$ is equal to:

$$E_{\perp}^{\min} = E_F - (eV - \phi_B) \quad (3.23)$$

We can now express this momentum requirement in the form of an acceptance cone at the M-S interface:

$$\theta = \frac{k_{\parallel}^{\max}}{k_{\parallel} + k_{\perp}} = \sqrt{ \frac{m^* eV - \phi_B}{m E_f - eV}} \quad (3.24)$$

### 3.4.5 BEEM transport models

In order to extract the Schottky barrier height from spectroscopy measurements a theoretical model is used. The first theoretical description dealing with the transport of hot-charge carriers through a metal-semiconductor system in a BEEM setup was proposed by L.D. Bell and W.J. Kaiser [3]. The tunnel current between tip and top metal based on planar tunneling theory can be written as:

$$I_T = A \int_0^\infty dE_{\perp} T(E_{\perp}) \int_0^\infty dE_{||}[f(E) - f(E + eV_T)] \quad (3.25)$$

$T(E_{\perp})$ is the tunnel probability for an electron to tunnel through the vacuum barrier over the transverse and parallel (to the interface) energies, $E_{\perp}$ and $E_{||}$. $A$ is the constant related to effective tunneling area, $f(E)$ is the Fermi distribution function, and $V_T$ is the applied tip voltage.

According to the widely used Bell-Kaiser (BK) model [3], BEEM transmission is the fraction of the ballistically transmitted tunnel current:

$$I_B = AR \int_{E_{\perp}^{\min}}^{E_{\perp}^{\max}} dE_{\perp} T(E_{\perp}) \int_0^\infty dE_{||}[f(E) - f(E + eV_T)] \quad (3.26)$$

where $R$ is an attenuation factor due to scattering in the metal base and the M-S interface. According to the BK model, $R$ is considered to be energy independent but it can also be weakly dependent on energy (other parameters are: $E_{\perp}^{\min} = E_F - e(V_T - \phi_B)$ and $E_{||}^{\max} = [m_t/(m-m_t)] \times [E_{\perp} - E_F + e(V_T - \phi_B)]$).

For $V_T$ just above $\phi_B$, close to threshold, above Eqns. 3.26 and 3.27 predict:

$$I_B \propto I_T (V_T - \phi_B)^2 \quad (3.27)$$
Such a quadratic onset considers classical transmission across the M-S interface with parabolic conduction band minimum in the semiconductor. Considering quantum mechanical transmission across the M-S interface another model was given by Ludeke-Prietsch (LP model) according to which $I_B \propto I_T (V_T - \phi_B)^2.5$ [12]. It was found that near the threshold regime, no significant difference between the BK and LP models can be resolved beyond experimental error. For the Schottky barrier extraction in our experimental measurement we have considered the BK model instead of the LP model and we have seen a better match of SBH with the macroscopic $I - V$ measurements.

3.4.6 **BEEM spectroscopy**

**Direct and Reverse BEEM spectroscopy**

In direct BEEM spectroscopy, which is one of the most commonly used modes in BEEM, a negative bias, $V_T$, is applied to the tip with respect to the metal forming a Schottky barrier contact with a n-type semiconductor. When the sample-tip bias is below the Schottky barrier height, no BEEM transmission is observed. However, $I_B$ increases after a certain onset that corresponds to the local SBH. A typical direct BEEM spectra thus can be obtained by recording the BEEM current with respect to the sample-tip bias at a fixed tip position (shown in fig. 3.8). Usually, to improve
the signal to noise ratio, several BEEM spectra are recorded to obtain a single averaged spectrum. The final BEEM spectrum provides valuable information on energy dependence of hot electron transport in the metal film as well as the M-S interface. The onset of the BEEM spectra determines the local Schottky barrier height with high accuracy (of ±0.02 eV) whereas the spectral shape carries information about scattering in the metal film, across the M-S interface and in the semiconductor.

In Reverse BEEM spectroscopy, a positive bias is applied to the STM tip with respect to the metal layer and a distribution of electrons is extracted from the metal overlayer (grown on a n-type SC) to the STM tip. Reverse BEEM is based on the collection of only secondary electrons in the conduction band of the semiconductor. These secondary electrons are produced by electron-electron scattering which is similar to Auger like scattering.

In the case of R-BEEM [20], hot holes injected by the tip (corresponding to hot electron extraction from the metal overlayer) lose energy by creating a secondary electron-hole (e-h) pair. The energy of the injected holes is transferred to the excited electrons up to a maximum of $E_{F,m} + eV_T$. If the secondary electrons have enough energy and momentum to surmount the barrier, they can be collected as collector current with the same sign as direct BEEM. Considering free electrons and

Figure 3.11: Energy schematic of the reverse BEEM spectroscopy.
zero temperature, R-BEEM transmission can be written as:

$$I_{RB} = AR \int_{E_{F,m} - eV_T}^{E_{F,b}} dE \int_0^E dE_\perp P(E, E_\perp)T(E_\perp)$$  \hspace{1cm} (3.28)

where $E_{F,m}$ is the base Fermi energy, $P(E, E_\perp)$ is the probability of creation of excited electrons from the injected hot holes. The excited electrons are then collected above $\phi_B$ with proper momentum. Near threshold, the above expression of R-BEEM transmission can be simplified as:

$$I_{RB} \propto I_T(V_T - \phi_B)^4.$$  \hspace{1cm} (3.29)

3.4.7 Hot electron attenuation length

With increasing metal base thickness the BEEM current is attenuated. The total attenuation length, $\lambda$, is related to the inelastic attenuation length, $\lambda_i$, and the elastic attenuation length, $\lambda_e$, as described by Matthiessen’s rule:

$$\frac{1}{\lambda} = \frac{1}{\lambda_i} + \frac{1}{\lambda_e}$$  \hspace{1cm} (3.30)

$\lambda_e$ corresponds to scattering due to different factors viz. defects, grain boundaries, phonons, magnons, polarons etc. From equation 3.18 it is clear that the transmission is exponentially dependent on the thickness of the metal base. Therefore, by varying the metal base layer thickness and measuring the BEEM transmission at a particular energy, a plot can be obtained of the transmission versus metal base thickness and energy. The slope of the plot (semi-log) gives the electron attenuation length at a particular energy. The energy dependence of the attenuation length can now be obtained by repeating this process at different energies. Although there are possibilities of extracting the two different attenuation lengths $\lambda_i$ and $\lambda_e$ from $\lambda$, this is generally not straight forward.

3.4.8 BEEM sample requirements

In BEEM, the measured signals are often very low (tenths of pA) and it is thus important to reduce noise in the system to measure such tiny currents. The most important source of noise in the BEEM signal arises from the feedback resistors of the operational amplifier (op-amp) circuits, which amplify the BEEM current, and from the Schottky interface. The feedback resistors of the op-amp circuits (BEEM current is monitored by a two-stage-op-amp) add noise to the BEEM channel. Although this is hard to avoid, the other noise source related to the sample can be reduced. The
Figure 3.12: As the electrons pass through the metal over layer they are inelastically scattered resulting in an exponential decay of the transmission.

Voltage fluctuation across a resistor at finite temperature is known as Johnson noise and is given by

\[ \Delta V = \sqrt{4k_B TBR} \]  

(3.31)

where \( \Delta V \) is the root mean square of the voltage fluctuations, \( k_B \) is the Boltzmann constant, \( T \) the measurement temperature, \( B \) the measurement bandwidth and \( R \) the value of the resistor.

The current passing through a Schottky diode, described by thermionic emission theory is given by Eqn. 3.14. In BEEM we are interested in the zero bias resistance of the diode which is given as

\[ R_0 = \left( \frac{dI}{dV} \right)_{V=0}^{-1} = \frac{k_B}{qA^*A} e^{\frac{q\phi_B}{k_BT}} \]  

(3.32)

From the above equation it is clear that the sample resistance can be increased by reducing the area or by lowering the measurement temperature. The current noise measured by the op-amp can be expressed as

\[ \Delta I = \sqrt{\frac{4k_BTBR}{R}} \]  

(3.33)

Thus, by increasing the zero bias resistance \( R_0 \) of the diode, its contribution to noise can be decreased. To make sure the diode is not dominating the noise, its resistance should be higher than the resistance of the op-amp. For common M-S interfaces such
as Au/Si the SBH is $\approx 0.8$ V, the junction resistance is of the order of $1$ G$\Omega$ at room temperature for a diode area with a diameter of 150 $\mu$m and thus is high enough to make sure the sample is not dominating the noise. This is thus an important sample requirement for BEEM studies [11].

### 3.5 Conclusions

In this chapter we discussed the different transport mechanisms across a metal-semiconductor (M-S) interfaces along with the different models that are essential to the determination of the Schottky barrier height. We also discussed the different modes of ballistic electron emission microscopy that are used in this thesis and the commonly used model to interpret hot electron transmission in metal layers and across their interfaces with a semiconductor.

### Bibliography


