Exactly solvable model for metal–insulator–metal stepped boundary
tunnel junctions


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Abstract

An exactly solvable model, which treats the effective barrier potential of the biased metal–insulator–metal tunnel junctions as a trapezoidal potential with an ideal stepped boundary, is presented. Thus, the exact analytic expressions for the electron wave functions and the tunneling probabilities were obtained by solving Schrödinger’s equation strictly. It is found that if the longitudinal kinetic energy of the electron, \( E \), is greater than the shorter side of the trapezoidal potential, in the barrier region Schrödinger’s equation has to be solved in the two subregions: where \( E \) is lower and higher than the barrier height, respectively. In order to compare the ideal stepped boundary model to Brinkman’s two approximation models (J. Appl. Phys. 89 (1970) 1915), the graded diffuse boundary and perfectly sharp boundary model, the trapezoidal barrier parameters were determined by fitting the calculated \( I–V \) curves to the experimental ones at 77 K. The results show that for three types of junctions (with Au, Ag, and Cu top electrodes), the variations in barrier parameters with the metal electrodes are in agreement with each other.

Keywords: Tunneling; Interfaces; Tunnel junctions; Trapezoidal barrier parameters

1. Introduction

Electron transport in metal–insulator–metal (MIM) tunnel junctions is one of the most important tunneling phenomena. The reason for this is that MIM tunnel junctions have been well modeled in studying the electron tunneling through a barrier experimentally and theoretically, and that have been applied in many aspects [1,2]. Recently, due to progress in the investigation of giant magnetoresistance (GMR), the research interests in spin-polarized tunneling magnetoresistance (TMR) of the ferromagnetic MIM tunnel junctions have been increasing rapidly [3,4]. The advantage in research on TMR is that it can be observed at room temperature even without a strong external magnetic field, thus it is a promising GMR device. A key problem in the characterization of the MIM tunnel junctions is to determine their \( I–V \) characteristics and so far many studies on the calculation of the \( I–V \) characteristics have been performed [3,4]. Of them, an important work, which was done by Brinkman et al., was to calculate the tunneling conductance of trapezoidal barrier potentials using two extreme models: the graded diffuse boundary model and the perfectly sharp boundary model [5]. For the graded diffuse boundary model, the tunneling probability was calculated by using the WKB approximation. For the perfectly sharp boundary model, the wave functions were exactly constructed based on the boundary conditions and then the tunneling current is calculated using Bardeen’s transfer Hamiltonian method. Brinkman’s work has shown that the inclusion of images does not radically alter the shape of the \( I–V \) characteristics of the junction. It should be emphasized that for the transfer Hamiltonian method the tunneling process is treated as a perturbing operator and then the tunneling matrix elements are calculated. So the transfer Hamiltonian method is a perturbation approximation method and it is effective only for the weak coupling between the wave functions on the two sides of the barrier [1]. In this paper, we will present an ideal stepped boundary
model, which treats the effective barrier potential of the biased MIM tunnel junctions as a trapezoidal potential and the resultant barrier potential is the trapezoidal potential plus an applied electric potential resulting from the bias voltage. It means that the applied electric field is located inside the insulator region of the junction and the junctions have the ideal stepped boundaries. Thus, to our knowledge for the first time, the exact analytic expressions for the electron wave functions and the tunneling probabilities in the biased MIM tunnel junctions were obtained by solving Schrödinger’s equation strictly, instead of using the WKB approximation or perturbation approximation method. In order to compare our model with Brinkman’s graded diffuse boundary model and perfectly sharp boundary model, three groups of the barrier parameters were determined by fitting the calculated $I-V$ curves to the experimental ones for three types of junctions (ones with Au, Ag and Cu top electrodes) at 77 K, respectively. For simplicity, the image force correction is not included because the effect of the image forces is only to round off the barrier corner and to make the average height of the barrier slightly lower [6].

2. Ideal stepped boundary model

Consider a MIM junction consisting of two metal electrodes and separated by a thin barrier insulator layer (10–20 Å). The effective trapezoidal barrier potential of the junction is modeled in one dimension with width $d$, as shown in Fig. 1a. As the junction is biased, since the applied electric field is located in the insulator region, the resulting barrier potential, $U(x)$, for the biased junction is the barrier potential plus the applied electric potential, as shown in Fig. 1b or c. Based on the free-electron and effective mass approximation, the tunneling electron wavefunctions $\psi(x)$ must satisfy the Schrödinger’s equation

$$\frac{-\hbar^2}{2m^*}\frac{d^2}{dx^2}\psi(x) + U(x)\psi(x) = E\psi(x)$$  \hspace{1cm} (1)

where

$$U(x) = \begin{cases} 0 & x < 0 \\ \phi_1 + E_{IL} - (\phi_1 - \phi_2 + eV)x/d & 0 \leq x \leq d \\ -eV & x > d \end{cases}$$ \hspace{1cm} (2)

$m^*$ is the tunneling electron effective mass; $E_x$ is the longitudinal kinetic energy in the $x$-axis direction (perpendicular to the junction interface). Note that for tunneling problems, there should be $E_x < E_{IL} + \phi_1$. As seen in Fig. 1a, if the bottom of the conductance band is taken as the zero point of potential, $E_{IL}$ and $E_{IR}$ is the Fermi energy of the left and right electrode, $\phi_1$ and $\phi_2$ is the trapezoidal barrier height on the left and right, respectively; $V$ is the bias voltage and the electrode on the right is biased positive.
In the region $x<0$ and $x>d$, the solutions for Eq. (1) has, respectively, the form of $\psi_1(x)$ and $\psi_2(x)$

$$\psi_1(x) = e^{ikx} + Re^{-ikx}, \quad x < 0$$

$$\psi_2(x) = Se^{ikx}, \quad x > d$$

(3)

(4)

where $R$ and $S$ is the reflection and transmission coefficient, respectively; $k_1 = (2m^*E_x)^{1/2}/h$, $k_2 = [2m^*(E_x + eV)]^{1/2}/h$.

In the barrier region $0 \leq x \leq d$, by introducing

$$l = \left[ \frac{d^2 \psi}{dx^2} + \frac{x}{l} - \frac{\lambda}{l^2} \right] \psi = 0$$

Eq. (1) becomes

$$\frac{d^2 \psi}{dx^2} + \frac{x}{l} - \frac{\lambda}{l^2} \psi = 0$$

(6)

Both $l$ and $\lambda$ are positive, $l$ has a length dimension and $\lambda$ is dimensionless. Note that because the tunneling electrons with the different $E_x$ face different parts of the trapezoidal barrier, in solving Eq. (6) there are two cases to be considered separately: $l \gg \lambda$, i.e. $E_x \geq (E_R + \phi_2 - eV)$ and $l \ll \lambda$, i.e. $E_x \leq (E_R + \phi_2 - eV)$.

As shown in Fig. 1b, in the case of $d \gg \lambda$, for the tunneling electron there are the two different subregions inside the trapezoidal barrier region: $0 \leq x < \lambda$ ($E_x$ is lower than the barrier potential) and $\lambda \leq x \leq d$ ($E_x$ is higher than the barrier potential).

In the barrier subregion $0 \leq x < \lambda$ ($E_x$ is lower than the barrier potential), introducing the dimensionless parameter $\xi = -l/(x/l)$, Eq. (6) becomes

$$\frac{d^2 \psi}{d\xi^2} + \xi \psi = 0$$

(7)

In terms of the transformations and $z = (2/3)\xi^{3/2}$, Eq. (7) can be rewritten as

$$\frac{d^2 \varphi}{dz^2} + \frac{1}{z} \frac{d\varphi}{dz} - \left[ 1 + \frac{(1/3)^2}{z^2} \right] \varphi = 0, \quad 0 \leq x \leq \lambda$$

(8a)

This is a modified Bessel equation, a general solution of which is

$$\varphi(x) = C_1 I_{1/3}(z) + C_2 K_{1/3}(z)$$

(8b)

where $I_{1/3}$ and $K_{1/3}$ are modified Bessel functions [7].

Similarly, in the barrier subregion $\lambda \leq x \leq d$ ($E_x$ is higher than the barrier potential), introducing $\xi = (x/l) - \lambda$, Eq. (6) is rewritten as $d^2\psi/d\xi^2 + \xi \psi = 0$, which can be transformed, by using $\psi = \xi^{1/2} \varphi$ and $z = (2/3)\xi^{3/2}$, as a Bessel equation of one third order

$$\frac{d^2 \varphi}{dz^2} + \frac{1}{z} \frac{d\varphi}{dz} - \left[ 1 - \left( \frac{1/3}{z^2} \right) \right] \varphi = 0, \quad \lambda \leq x \leq d$$

(9a)

a general solution of which is

$$\varphi(x) = D_1 J_{1/3}(z) + D_2 N_{1/3}(z)$$

(9b)

where $J_{1/3}$ is Bessel function, $N_{1/3}$ is Neumann function [7].

Thus, for the case of $d \gg \lambda$, returning to the variable $x$ in Eq. (8b) and Eq. (9b), we obtained the solutions of Eq. (6), $\psi_2$ and $\psi_3$ as follows:

$$\psi_2(x) = \left[ \frac{\lambda - x}{l} \right]^{1/2} \{ C_1 I_{1/3} \left( \frac{2}{3} \left( \frac{\lambda - x}{l} \right)^{3/2} \right) \}
+ C_2 K_{1/3} \left( \frac{2}{3} \left( \frac{\lambda - x}{l} \right)^{3/2} \right), \quad 0 \leq x \leq \lambda$$

$$\psi_3(x) = \left[ \frac{\lambda - x}{l} \right]^{1/2} \{ D_1 J_{1/3} \left( \frac{2}{3} \left( \frac{\lambda - x}{l} \right)^{3/2} \right) \}
+ D_2 N_{1/3} \left( \frac{2}{3} \left( \frac{\lambda - x}{l} \right)^{3/2} \right), \quad \lambda \leq x \leq d$$

(10)

(11)

where $C_1$, $C_2$, $D_1$, and $D_2$ are unknown constants. Using (i) the recurrence relations of Bessel, Neumann and modified Bessel functions [7], and (ii) the boundary conditions at $x=0$, $\lambda$, and $d$: $\psi_1(0) = \psi_3(0)$ and $\psi'_1(0) = \psi'_3(0)$; $\psi_1(\lambda) = \psi_3(\lambda)$ and $\psi'_1(\lambda) = \psi'_3(\lambda)$; $\psi_1(d) = \psi_3(d)$ and $\psi'_1(d) = \psi'_3(d)$, the constant $C_1$, $C_2$, $C_1$ and $D_2$, along with $R$ and $S$ in Eq. (3) and Eq. (4), were determined as follows:

$$C_1 = \frac{2ik_1 - b_{23}C_2 \pi / 2 \sin(\pi/3)}{b_{13}}$$

$$C_2 = \frac{4ik_1 \sin(\pi/3)}{b_{24} \pi + b_{15} \pi \left[ -(b_{68} / b_{23}) + 1 + \cos(\pi/3) \right]}$$

$$D_1 = \frac{b_{68} C_2 \pi}{2b_{23} \sin(\pi/3)}$$

$$D_2 = -C_2 \pi / 2$$

$$R = C_1 a_1 + \frac{a_2 C_2 \pi}{2 \sin(\pi/3)} - 1$$

$$S = -e^{-ik_2a} [a_1 D_1 + a_2 D_2 / \sin(\pi/3)]$$

(12)

where $b_{13} = ik_1 a_1 - a_3 / 2$, $b_{24} = ik_1 a_2 - a_4 / 2$, $b_{57} = ik_2 a_5 - a_7 / 2$, $b_{68} = ik_2 a_6 - a_8 / 2$ and

$$a_1 = \lambda^{1/2} e^{-i\pi/6} J_{1/3}(\lambda t_0)$$

$$a_2 = \lambda^{1/2} \left[ e^{i\pi/6} J_{-1/3}(\lambda t_0) \right.$$

$$\left. - e^{-i\pi/6} J_{1/3}(\lambda t_0) \right]$$

$$a_3 = \frac{1}{l} \lambda^{1/2} e^{-i\pi/6} J_{1/3}(\lambda t_0) + \frac{\lambda}{l} e^{i\pi/3} [J_{-2/3}(\lambda t_0) - J_{1/3}(\lambda t_0)]$$

$$a_4 = \frac{1}{l} \lambda^{1/2} \left[ e^{i\pi/6} J_{-1/3}(\lambda t_0) - e^{-i\pi/6} J_{1/3}(\lambda t_0) \right.$$

$$\left. \times \left( e^{i\pi/3} J_{-2/3}(\lambda t_0) - J_{1/3}(\lambda t_0) \right) \right.$$
\[ a_6 = (d/l - \lambda)^{1/2} [J_{1/3}(t_1) \cos(\pi/3) - J_{-1/3}(t_1)], \]
\[ a_7 = \frac{1}{l} \frac{(d/l - \lambda)^{1/2}}{J_{1/3}(t_1)} \left[ \frac{d/l - \lambda}{l} J_{-1/3}(t_1) - J_{-1/3}(t_1) \right], \]
\[ a_8 = \frac{1}{l} \frac{(d/l - \lambda)^{1/2}}{J_{1/3}(t_1)} \left[ J_{1/3}(t_1) \cos(\pi/3) - J_{-1/3}(t_1) \right] \]
\[ + \frac{(d/l - \lambda)}{l} \left\{ [J_{-2/3}(t_1) - J_{4/3}(t_1)] \cos(\pi/3) - [J_{-4/3}(t_1) - J_{2/3}(t_1)] \right\} \]
and \( t_0 = \frac{2}{3} \lambda^{3/2} e^{i\pi/2} \) and \( t_1 = \frac{2}{3} (d/l - \lambda)^{3/2} \).

As shown in Fig. 1c, in the case of \( d < \lambda \), over all the barrier region \( E_s \) is lower than the barrier potential and thus the wave functions of the tunneling electron must only satisfy Eq. (8a) and there are the constant \( R, S, C_1, C_2 \) to be determined. In this case, the solutions of Eq. (8a) has the form of Eq. (10) in the region \( 0 \leq x < d \) instead of the region \( 0 \leq x < \lambda \). Using the boundary conditions at \( x = 0 \) and \( x = d \): \( \psi_3(0) = \psi_2(0) \) and \( \psi' \left( 0 \right) = \psi'_2(0); \psi_3(d) = \psi_2(d) \) and \( \psi'(d) = \psi'_2(d) \), the constant \( C_1, C_2, R \) and \( S \) were determined as follows:

\[ C_1 = \frac{2ib_0 b_1 k_1}{b_{13} b_{68} - b_{57} b_{24}}, \]
\[ C_2 = \frac{2b_2 C_3 \sin(\pi/3)}{b_{60} \pi}, \]
\[ R = C_4 a_1 + \frac{a_2 C_2 \pi}{2 \sin(\pi/3)} - 1, \]
\[ S = e^{-ik_0 d} \left[ C_1 + a_0 C_2 \pi / 2 \sin(\pi/3) \right], \]

where \( b_{57} = ik_2 a_5 + a_7/2 \), \( b_{68} = ik_2 a_6 + a_8/2 \), and

\[ a_5 = (\lambda - d/l)^{1/2} e^{-i\pi/6} J_{1/3}(t_1), \]
\[ a_6 = (\lambda - d/l)^{1/2} e^{-i\pi/6} J_{1/3}(t_1), \]
\[ a_7 = \frac{1}{l} \frac{(d/l - \lambda)^{1/2}}{J_{1/3}(t_1)} \left[ \frac{d/l - \lambda}{l} e^{i\pi/3} J_{-2/3}(t_1) - J_{4/3}(t_1) \right], \]
\[ a_8 = \frac{1}{l} \frac{(d/l - \lambda)^{1/2}}{J_{1/3}(t_1)} \left[ e^{i\pi/6} J_{-1/3}(t_1) - e^{-i\pi/6} J_{1/3}(t_1) \right] \]
\[ + \frac{(\lambda - d/l)}{l} \left\{ e^{i\pi/3} J_{-2/3}(t_1) - J_{4/3}(t_1) \right\} \]
\[ + e^{-i\pi/3} J_{-2/3}(t_1) - J_{4/3}(t_1) \]
and \( t_1 = \frac{2}{3} (\lambda - d/l)^{3/2} \).

We have obtained the exact analytic solutions (for the electron wave functions) of Eq. (1) in the two cases: (i) \( d \gg \lambda \), the solutions consist of Eq. (3), Eq. (4), Eq. (10), Eq. (11) and Eq. (12); (ii) \( d \ll \lambda \), the solutions consist of Eq. (3), Eq. (4), Eq. (10) and Eq. (13). The electron tunneling probability, \( P \), is given by

\[ P = |S|^2 \] (14)

where \( S \) is the transmission coefficient appearing in Eq. (4). The tunneling current density is [8]

\[ J = \frac{4\pi e \tau^*}{h} \int_0^{E_{\text{MAX}}} |S|^2 dE_x \int_0^\infty \left[ \ln \left( 1 + e^{E_x/k_B T} \right) - \ln \left( 1 + e^{E_x/k_B T} \right) \right] dE_x \]

\[ = \frac{4\pi e \tau^*}{h} \int_0^{E_{\text{MAX}}} |S|^2 k_B T \left[ \ln \left( 1 + e^{E_x/k_B T} \right) - \ln \left( 1 + e^{E_x/k_B T} \right) \right] dE_x \]

\[ = \frac{4\pi e \tau^*}{h} \int_0^{E_{\text{MAX}}} |S|^2 k_B T \left[ \left( e^{E_x/k_B T} - 1 \right) \ln \left( 1 + e^{E_x/k_B T} \right) \right] dE_x \] (15)

where \( E_x = E - E_s \) is the transverse kinetic energy of the electron in the direction perpendicular to the x-axis (parallel to the junction interface), \( k_B \) is Boltzmann’s constant and \( T \) is temperature.

3. Experiment

In order to compare Brinkman’s two extreme models to the ideal stepped boundary model presented in this paper, we determined the parameters (width and height) of the trapezoidal effective barrier by fitting the calculated \( I-V \) curves based on the above the three models to the experimental ones. The preparation of the junctions used to obtain the experimental \( I-V \) curves was described in detail elsewhere [9]. First, Al film strips were evaporated on glass slides in a vacuum chamber of typically \( 2 \times 10^{-5} \) Torr. Then, to grow a thin Al₂O₃ barrier layer on the Al film surface, the Al films were exposed to an oxygen glow discharge at the pressure of \( 1 \times 10^{-1} \) Torr for 10 min. This was followed by baking the samples in air at 200 °C for 30 min and then cooling the heated samples in air to room temperature slowly. Next MgF₂ film strips were evaporated over the edges of the oxidized Al film strips to increase the insulator thickness at the edges. Finally, the top metal electrode film strips (Au, Ag, or Cu) were deposited and the tunnel junctions of 2.5×2.5 mm² were obtained. Baking the samples in air made the Al₂O₃ barrier layer denser and the increase in the insulator thickness at the edges eliminated the problem of leakage current at the junction edges, thus the applied bias to the junctions can be up to 5.12 V at room temperature. The experimental \( I-V \) curves of the junctions are shown in Fig. 2 and were measured in a liquid nitrogen Dewar (77 K) and the top metal electrodes on the right were biased positively. The bare Al₂O₃ barrier layer thickness was measured with an ellipsometer (Rudolph 2436) before the top metal electrode deposition. The incident angle of the
the trapezoidal barrier potential model [6]. The effective mass of electron in the $Al_2O_3$ barrier layer, $m^*$, was chosen to be $0.2 m_e$, where $m_e$ is the free-electron mass [9]. Thus, the barrier parameters obtained by fitting the calculated $I$–$V$ curves to the experimental ones are shown in Table 1.

The bare $Al_2O_3$ barrier layer thickness was determined to be $34.2 \pm 2.5$ Å by the ellipsometric measurement and it is greater than the barrier width $d$, as shown in Table 1. This difference can be understood as follows: (i) because grown $Al_2O_3$ barrier layer is not uniform and has the surface roughness, and the tunneling probability increases exponentially with decrease in the barrier width, the tunneling electrons prefer to go through the thinner area. Since the ellipsometric values are the geometric average ones, the tunneling values are the physical effective ones; (ii) the diffusion of the metal electrode atoms into the barrier layer leads to a decrease in the average barrier thickness.

As seen in Table 1, for the ideal stepped boundary model the barrier height $\phi_1$ in the Au- (Ag-, Cu-) junctions are approximately equal to each other because they characterizes the same Al–$Al_2O_3$ interface. The results for the ideal stepped boundary model are what they should be and are in agreement with ones for both graded diffuse boundary and perfectly sharp boundary models. In contrast, for all the three models the barrier height $\phi_2$ at the $Al_2O_3$–Au (–Ag, –Cu) interface are quite different, in particular, $\phi_2$ at the $Al_2O_3$–Cu interface much higher than that at the $Al_2O_3$–Au (–Ag) interface.

For both graded diffuse boundary and perfectly sharp boundary models, the difference in the barrier height $\phi_2$ between the $Al_2O_3$–Au (–Ag) and –Cu interfaces can be understood by considering that at the interfaces oxygen atoms with dangling bonds can combine with Cu atoms but inactive Au and Ag atoms, thus copper oxide of one or two monolayer thickness is grown at the interface and an additional barrier must be considered [10]. On the other hand, the top electrode atoms have the different atom radii: $1.442$ Å (Au), $1.442$ Å (Ag), $1.280$ Å (Cu) and the Cu atoms with the smaller raddium are easier to diffuse into the $Al_2O_3$ barrier. As shown in Table 1, this means that the barrier width of

Table 1
The effective trapezoidal barrier parameters determines by fitting the calculated $I$–$V$ curves to the experimental ones

<table>
<thead>
<tr>
<th>Parameters Models</th>
<th>$d$ (Å)</th>
<th>$\phi_1$ (eV)</th>
<th>$\phi_2$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>GDB</td>
<td>PSB</td>
<td>ISB</td>
</tr>
<tr>
<td>Al–$Al_2O_3$–Au</td>
<td>24.4</td>
<td>27.3</td>
<td>21.0</td>
</tr>
<tr>
<td>Al–$Al_2O_3$–Ag</td>
<td>25.3</td>
<td>28.0</td>
<td>23.1</td>
</tr>
<tr>
<td>Al–$Al_2O_3$–Cu</td>
<td>12.0</td>
<td>10.7</td>
<td>15.2</td>
</tr>
</tbody>
</table>

The calculated $I$–$V$ curves were in the basis of Brinkmann’s graded diffuse boundary (GDB) model and perfectly sharp boundary (PSB) model, and the ideal stepped boundary (ISB) model presented in this paper.
the Cu-junction is much shorter than that of the Au- and Ag-junctions. However, for inelastic electron tunneling spectroscopy (IETS) the case is different. It is found that some top metal electrodes of junctions (e.g. Al and Cr) will destroy the layer of molecules that were doped into the junction and others (e.g. Pb and Ti) will not [11]. For Pb top electrode, tunneling spectra are obtained that closely resemble infrared spectra or Raman spectra of the dopant molecules without a top electrode. Therefore, Pb top electrode is widely used in junctions of IETS.

Based on the same explanations as above, for the ideal stepped boundary model the $\phi_2$ at the Al$_2$O$_3$–Cu interface much higher than that at the Al$_2$O$_3$–Au (–Ag) interface and the barrier width of the Cu-junction is much shorter than that of the Au- and Ag-junctions. It should be noted that, as seen in Table 1, in the Cu-junction there is $\phi_1 < \phi_2$ for both graded diffuse boundary and perfectly sharp boundary models and, in contrast, there is $\phi_1 > \phi_2$ for the ideal stepped boundary model. This difference between the ideal stepped boundary model and the graded diffuse (or the perfectly sharp) boundary model can be explained as follows: as seen in Eq. (5a), $I$ (with a length dimension) should be positive for any given bias voltage $V$, in other words, for the ideal stepped boundary model the assumption of $\phi_1 > \phi_2$ has been made (of course, the another assumption of $\phi_1 < \phi_2$ can be chosen to make). In contrast, for the graded diffuse (or the perfectly sharp) boundary model there is not such a pre-assumption of $\phi_1 > \phi_2$ (or $\phi_1 < \phi_2$). It should be emphasized that the assumption of $\phi_1 > \phi_2$ makes no difference to characterizing the junction interfaces. For example, as shown in Table 1, for the ideal stepped boundary model the barrier height $\phi_2 = 1.82, 1.77$ and $2.97$ eV at the Al$_2$O$_3$–Au, –Ag and –Cu interface, respectively, and the $\phi_2$ at the Al$_2$O$_3$–Cu interface are much higher than that at the Al$_2$O$_3$–Au (–Ag) interface. Obviously, for ideal stepped boundary model the variation in the $\phi_2$ values with the top electrodes is in agreement with that for the graded diffuse boundary model and the perfectly sharp boundary model.

The experimental $I$–$V$ curves were measured at in liquid nitrogen (77 K), which is easy to get. The temperature dependence of the current density in a MIM tunnel junction can be described by

$$J(V,T) = J(V,0)[1 + (\pi c_1 k_B T)^2(1/6) + (\pi c_1 k_B T)^4(7/360) + \cdots],$$

where $V$ is the bias voltage, $T$ is temperature, $k_B$ is Boltzmann constant and the coefficient $c_1$ for small bias voltages ($\leq 1.0$ V) is approximately 20 (eV)$^{-1}$ [12]. Since $k_B T (77 K) = 6.4 \times 10^{-3}$ eV, the increase in the current density is less 3% as the temperature goes from 0 to 77 K. This shows that the $I$–$V$ characteristics at 77 K differs only slightly from that at 4.2 K. Recently, temperature dependence of the (spin-independent) conductance $G(T, V=0)$ for a zero-biased Co–insulator–Py tunnel junction with the insulator composed of 4 Å Al and 10 Å Dy oxidized was measured, but the temperature dependence of the $I$–$V$ characteristics is absent from this type of tunnel junction [13]. In general, a small influence of temperature on the $I$–$V$ characteristics is typical for tunneling. Nevertheless, there is still a requirement for measuring the temperature dependence of the $I$–$V$ characteristics, in particular, for determining the temperature dependence of the tunneling barrier parameters. It would be good to perform the measurements of the $I$–$V$ characteristics at a temperature as low as possible to eliminate thermionic emission, which will results in a nontunneling current component in the junctions. However, for IETS the tunneling spectra are taken always at 4.2 K (or lower temperature). The reason for this is that vibrational modes of surface species have characteristic width of order 1 meV (or greater) and a contribution to the spectrum width is made by the thermal broadening, which comes from the thermal smearing of the electron distribution around the Fermi energy [11]. Hence, the tunneling spectra must be run at cryogenic temperature to obtain resolutions sufficient for the vibrational spectroscopy.

5. Summary

We presented an ideal stepped boundary model, which treats the effective barrier potential of the biased MIM tunnel junctions as a trapezoidal potential plus an applied electric potential (from the biased voltage). Thus, to our knowledge for the first time, the exact analytic expressions for the electron wave functions and the tunneling probabilities were obtained by solving Schrödinger’s equation strictly. For comparison to Brinkman’s two extreme models: the graded diffuse boundary model (based on WKB approximation) and the perfectly sharp boundary model (based on perturbation approximation), the three groups of barrier parameters were determined by fitting the calculated $I$–$V$ curves to the experimental ones for three different junctions with the Au, Ag and Cu top electrodes at 77 K. The results show that: (i) according to the ideal stepped boundary model the tunneling electron behavior in the trapezoidal barrier region is dependent on whether the electron energy $E_x$ is lower or higher than the barrier height; (ii) the variations in the barrier parameters obtained from the above three models are in qualitative agreement with each other. Also the results suggest that though a barrier layer of tunnel junctions is a real existence, it can be modeled in many ways to different effective barrier potentials, for example, to rectangular or trapezoidal ones with diffuse or sharp boundaries. Thus, a group of the barrier parameters for each effective barrier potential model can be obtained by fitting the calculated $I$–$V$ curves based on the barrier model to the experimental
ones. In addition, since the ferromagnetic MIM tunnel junctions with TMR is a promising GMR device, the effect of an applied external magnetic field on the calculated barrier parameters on the basis of our model should be a forthcoming subject for study.

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