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Modeling of electron tunneling through a tilted potential barrier

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Tunnel junctions are interesting for both studying fundamental physical phenomena and providing new technological applications. Modeling of the tunneling current is important for understanding the tunneling processes and interpreting experimental data. In this work, the tunneling current is modeled using the Tsu-Esaki formulation with numerically calculated transmission. The feasibility of analytical formulae used for fitting experimental results is studied by comparing them with this model. The Tsu-Esaki method with numerically calculated transmission provides the possibility to calculate tunneling currents and fit experimental I - V curves for wide bias voltage and barrier width ranges as opposed to the more restricted analytical formulae. I - V curve features typical of tilted barrier structures are further analyzed to provide insight into the question, which of the phenomena can be explained with this simple barrier model. In particular, a small change in the effective barrier width is suggested as a possible explanation for experimental I - V curve features previously interpreted by a change in the tilt and height of the barrier. *Published by AIP Publishing.*
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I. INTRODUCTION

Quantum mechanical tunneling is a phenomenon where an electron is able to pass through a potential barrier exceeding its kinetic energy. Nowadays this process is frequently used in different kinds of devices from a tunnel diode to a scanning tunneling microscope, and it has been extensively studied both experimentally and theoretically for almost a hundred years.^{1,2} Still, new barrier nanostructures with different materials and tunneling related phenomena are constantly being invented and investigated.³ In this article, we present theoretical calculations of current density-voltage (J - V) curves of tunnel junctions in order to better understand experimental results and to further develop tunneling models.

A simple tunnel junction in a layered nanostructure consists of a thin insulating barrier between two conducting electrodes. Electron transport through a thin dielectric barrier can happen via different mechanisms, e.g., direct tunneling as a one-step process through the barrier, over the barrier emission of electrons having sufficient thermal energy, or trap-assisted tunneling (TAT) through defect states in the barrier as a two-step or as a multi-step process. Various models have been created to study both the direct tunneling processes (see, e.g., Refs. 1 and 4–6) and the defect related TAT processes that can be elastic or inelastic (see, e.g., Refs. 7–10). In this article, we focus on the modeling of three processes: direct tunneling (DT) through the whole barrier width, Fowler-Nordheim tunneling (FNT) in which the tunneling path is reduced by an electric field-induced barrier tilting, and thermionic emission (TE). Schematic presentations of these three mechanisms are given in Fig. 1.

The tunneling current can be calculated by taking the net difference between the currents flowing from one

electrode to the other and to the opposite direction, which is the basis of the Tsu-Esaki formula.^{1,11} We have used this approach in the present work. Examples of other tunneling formalisms are the transfer Hamiltonian,¹² Landauer-Büttiker, and the non-equilibrium Green's function methods.¹³ The Fermi-Dirac distribution is used in most schemes to model the electron supply from the electrodes. Commonly used methods for calculating the transmission probability, often called the transmission coefficient, as a function of energy through the potential barrier are the Wentzel-Kramers-Brillouin (WKB), the transfer matrix (TM),¹⁴ and the quantum transmitting boundary (QTB) methods.¹⁵

Many analytical formulae have also been derived for fitting experimental current-voltage (I - V) curves. These formulae can be used to extract values of physical parameters like the width and height of the barrier, which can be further correlated with microscopic materials properties.¹⁶ Fits of experimental results have also been used for identifying

FIG. 1. Schematic presentations of the direct tunneling (DT), Fowler-Nordheim tunneling (FNT), and thermionic emission (TE) processes for positive bias voltages V of different magnitudes.

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which type of tunneling, DT, FNT, or TE, is occurring in the junction (see, e.g., Refs. 17–19). The analytical formulae are always specific for a particular barrier shape, and they also have limitations regarding the bias voltage range and the barrier parameter values for which they are applicable.

In recent years, FTJs, i.e., tunnel junctions where the barrier is made of ferroelectric materials, have gained a lot of interest thanks to the multitude of physical phenomena they exhibit and the promising possibilities they provide for applications (for reviews on the topic, see, e.g., Refs. 3, 20, and 21). The simplest model for a FTJ is a tilted barrier, i.e., a rectangular barrier with a tilted top, where the tilt can be reversed by switching of the ferroelectric polarization in an applied electric field. Theoretical studies of the behavior of FTJs have focused on the electrostatic, interface, and strain effects on the conductance changes in the direct tunneling through the barrier (e.g., Refs. 22–24), and *ab initio* calculations have been performed for model systems (see, e.g., Refs. 25–29). Understanding the electronic structure and microscopic details of the junctions is very important, but on top of that, simplified models that can be used for fitting and analyzing experimental results are also needed. For fitting experimental curves, the analytical tunneling formulae for DT, FNT, and TE currents presented in the work by Pantel and Alexe¹⁶ are often used (see, e.g., Refs. 30–32).

In this work, we study the current density through a single tilted potential barrier in more detail using the Tsu-Esaki formulation with the transmission coefficient calculated numerically. We neglect atomistic details in the calculations and focus on the simple “particle tunneling through a barrier” picture. Our aim is to provide guidelines for using analytical formulae for fitting and show the key features in I - V curves of single barrier structures. First, we study the applicability and limitations of analytical formulae in the interpretation of experiments. By choosing a relatively simple barrier shape, we are able to study separately the effects of different approximations such as the finite temperature versus the zero-temperature limit and the change in the electron density in the electrodes. Second, we examine different I - V curve features of single barrier structures in order to give insight into the extent to which experimental results can be described with this kind of simple model potential. In an experimental setup, even if the junction has nominally just one tunnel barrier, an adjacent barrier might form unintentionally or on purpose at one or both of the electrode interfaces.^{24,33–36} Guidelines based on theoretical calculations are therefore useful for choosing the appropriate model potential. Our single barrier results also help in identifying phenomena that can only be explained by more complicated barrier profiles. Finally, based on our calculations, we suggest that small changes in the effective barrier width can be the cause of “leaf-like” patterns in experimental I - V curves that have been previously explained by differing barrier heights and tilts.¹⁹

II. MODELING OF TUNNELING

For calculating the tunneling current, we need to know the barrier parameters, such as the height and width in the

case of a simple rectangular barrier. In practice, however, the barrier parameters are not easily obtained. Often, they are determined indirectly by fitting the experimental I - V curves with analytical models and using the barrier parameters as fitting parameters.^{19,35,37} These analytical models are always based on a specific barrier shape, e.g., triangular or rectangular, and therefore fittings using different models can lead to different barrier parameters for the same I - V curve. In this work, we study the applicability of the indirect fitting methods with analytic solutions using the Tsu-Esaki approach for calculating the tunneling currents.

When modeling tunneling, the current density, J , is solved as a function of the bias, V . On the other hand, in experiments, the current, I , is measured as a function of the bias, V , and it is not always known what is the effective area through which the current flows. Therefore, it is practical to compare the shapes of the curves and assume that the area of current flow stays constant in the measured and calculated bias range.

A. Barrier parameters

The metal-insulator barrier height ϕ is often approximated using the Schottky-Mott rule for a metal-semiconductor interface: $\phi = W - X$, where W is the work function of the metal electrode and X is the electron affinity of the insulator.¹ Since the definition is based on homogeneous bulk parameter values of different constituents, it does not account for the interface effects that can have a significant influence on the height of the barrier as shown in a recent study on Al/Al₂O₃/Al systems.³⁸ Depending on the structure, metal states can penetrate into the insulator forming the so-called metal-induced gap states (MIGS), lowering the barrier height.³⁹ In addition, barrier properties such as ferroelectricity may cause accumulation of charge and induce screening effects, which alter the barrier height and shape.²³ Since measuring the barrier height experimentally is a difficult task, it is commonly included as one of the fitting parameters.

Different techniques (e.g., transmission electron microscopy (TEM), reflection high-energy electron diffraction (RHEED)) can be used both during and after growth to determine the dimensions of the structure. However, these methods do not always give correctly the effective barrier width since both the microscopic and electronic structures of the interface can have a significant effect on it.³⁸ Therefore, the width is also often used as a fitting parameter for experimental curves (e.g., Refs. 35 and 40).

In addition to the height and width, the image force effect causes the rounding of the potential barrier edges, and therefore, it lowers the barrier height and increases the tunneling current. There is still some controversy regarding the use of the image force correction in tunneling.^{41,42} It has been argued that the time scales connected to tunneling are not long enough for the effect to take place and that the effect is negligible for reasonable barrier heights.^{4,43,44} However, for very thin layers, the effect might be significant and different ways to correct the corresponding formulae have been suggested.^{41,45,46}

B. Tsu-Esaki formula

The most frequently used numerical method for calculating the tunneling current density is the so-called Tsu-Esaki formula that for a barrier potential varying only in the z -direction reads as^{1,14}

$$J_T(V) = \frac{em^*k_B T}{2\pi^2\hbar^3} \times \int_{eV}^{\infty} dE_z T_{tr}(E_z, V) \ln \left(\frac{1 + e^{(E_F + eV - E_z)/k_B T}}{1 + e^{(E_F - E_z)/k_B T}} \right). \quad (1)$$

Here, E_z is the kinetic energy of the electron in the z -direction, m^* is the electron effective mass, T is the temperature, V is the bias voltage, and $T_{tr}(E_z, V)$ is the transmission coefficient through the barrier. In the integration over the transversal kinetic energy E_t , parabolic bands ($E = E_z + E_t = \hbar^2 k_z^2 / (2m^*) + \hbar^2 k_t^2 / (2m^*)$) have been assumed and electron distributions on the left and right-hand sides of the barrier have been calculated using equilibrium Fermi-Dirac distributions characterized by the respective bulk Fermi levels. The zero-reference of the potential energy is at the conduction band minimum on the right-hand side, and the Fermi levels are $E_F + eV$ and E_F , on the left and right-hand sides of the barrier, respectively, as depicted in Fig. 1. At a low temperature, Equation (1) reduces to

$$J_{T=0K}(V) = \frac{em^*}{2\pi^2\hbar^3} \left[eV \int_{eV}^{E_F} dE_z T_{tr}(E_z, V) + \int_{E_F}^{E_F + eV} dE_z T_{tr}(E_z, V) (E_F + eV - E_z) \right]. \quad (2)$$

C. Transmission coefficient calculation

There are different methods for calculating the transmission coefficient $T_{tr}(E, V)$ in Equation (1). One of the most frequently used method is the WKB approximation. It gives an approximative solution to the Schrödinger equation by using an exponential function for the wavefunction, expanding the wavefunction semiclassically and assuming that the potential is slowly varying, i.e., the local de Broglie wavelength is much shorter than the length scale over which the potential varies. Because the WKB method does not take into account wavefunction reflection and interference effects, it cannot produce the oscillations observed in the transmission coefficient as a function of energy and barrier width.⁴⁷ The WKB approximation is valid in the region which is several wavelengths away from the classical turning point and where the potential varies slowly with z . Therefore, for very thin barriers, the WKB approximation breaks down.

Other commonly used approaches are the TM¹⁴ and the QTB methods.¹⁵ In the TM method, an arbitrary-shaped barrier is approximated by a series of rectangular or trapezoidal barriers and the wavefunctions for each barrier slice are matched at the discontinuities producing a transfer matrix from which the transmission coefficient can be calculated.^{48–50} In the QTB method, the problem is formulated by defining the boundary conditions for each lead, and then, for

example, the finite element method is used to solve the problem.

We use the Numerov method to solve the Schrödinger equation and calculate the transmission coefficients. It is a numerical method that can be used for solving second-order ordinary differential equations with no first-order term.^{51,52} The Numerov method is computationally efficient since a local error of $O(\hbar^6)$ is obtained with just one evaluation of the linear and constant terms of the differential equation compared to, e.g., the Runge-Kutta algorithm, requiring six function evaluations per step to achieve the same accuracy.⁵³

D. Analytical formulae

An early standard still in use in tunneling simulations is the Simmons model, which gives an analytical expression for the current density through a thin film with similar electrodes. In the model, the barrier is depicted using the average barrier height and width either as known or as fitting parameters.⁵ The Simmons model uses the WKB method for calculating the transmission through the barrier and the Fermi-Dirac distribution for the electrons in the electrodes. Different versions of the model have been derived also for a rectangular barrier including image force lowering, for various voltage ranges, and for the case of dissimilar electrodes.⁵⁴

For DT, FNT, and TE currents, three commonly used analytical formulae for modeling tunneling through tilted barriers are presented in the work by Pantel and Alexe¹⁶ on FTJs. Analytical formulae are typically used for fitting experimental data in order to obtain information about the barrier (e.g., the height and width).^{4,5,55,56} We compare our results to the curves obtained using these three formulae summarized below.

For DT through a tilted barrier, an analytical formula based on the model by Brinkman *et al.*⁵⁷ is presented in the work by Gruverman *et al.*⁵⁵

$$J_{DT} \cong C \frac{\exp \left\{ \alpha(V) \left[\left(\phi_2 - \frac{eV}{2} \right)^{3/2} - \left(\phi_1 + \frac{eV}{2} \right)^{3/2} \right] \right\}}{\alpha^2(V) \left[\left(\phi_2 - \frac{eV}{2} \right)^{1/2} - \left(\phi_1 + \frac{eV}{2} \right)^{1/2} \right]^2} \times \sinh \left\{ \frac{3}{2} \alpha(V) \left[\sqrt{\phi_2 - \frac{eV}{2}} - \sqrt{\phi_1 + \frac{eV}{2}} \right] \frac{eV}{2} \right\}. \quad (3)$$

Here, d is the width, ϕ_1 and ϕ_2 are the heights of the barriers at the left and right electrode, respectively, $C = -(4em_b^*) / (9\pi^2\hbar^3)$, and $\alpha(V) = [4d(2m_b^*)^{1/2}] / [3\hbar(\phi_1 + eV - \phi_2)]$ (m_b^* is the electron effective mass in the barrier). The WKB method has been used for evaluating the transmission coefficient when deriving Equation (3), and it has been assumed that the bias voltage is small ($eV < 2\phi_{1,2}$) and the barrier is not too thin ($d[(2m_b^*/\hbar^2)\phi_{1,2}]^{1/2} \gg 1$).

When the applied voltage is large enough, the barrier shape becomes effectively triangular (see Fig. 1). For a triangular barrier with the height of the vertical wall Φ_B , the FNT current is given by the Fowler-Nordheim equation⁴

$$J_{FN} = \frac{e^3 m^*}{16\pi^2 m_b^* \hbar \Phi_B} E^2 \exp\left(-\frac{4\sqrt{2m_b^* \Phi_B^3}}{3\hbar e E}\right). \quad (4)$$

Here, m^* and m_b^* are the electron effective masses in the electrodes and in the barrier, respectively, and E is the electric field in the barrier, i.e., due to the applied voltage, band alignment, and, e.g., in the case of ferroelectric barrier, the depolarization field in the barrier.¹⁶

The TE current can be calculated using⁶

$$J_{TE} = A^{**} T^2 \exp\left[-\frac{1}{k_B T} \left(\Phi_B - \sqrt{\frac{e^3 E}{4\pi\epsilon_0 \epsilon}}\right)\right], \quad (5)$$

where Φ_B is the height of the potential barrier, E is the electric field as in Eq. (4), A^{**} is the effective Richardson's constant, and ϵ is the permittivity of the barrier material. The effective Richardson's constant A^{**} is a material constant depending on the electron effective mass and the atomic structure at the interface, and it is typically obtained experimentally (see, e.g., Ref. 58). Equation (5) has been obtained by calculating the current due to electrons that have a higher energy than the barrier. For TE, the barrier height Φ_B is lowered by the combined effect of image force and electric field E . At low voltages ($V < 3k_B T/e$), the above formula is not valid and Pantel and Alexe approximated the current using an ohmic relation extrapolating linearly to $J_{TE} = 0$ at $V = 0$.

In Eq. (3), the barrier heights ϕ_1 and ϕ_2 are measured from the quasi-Fermi levels of the corresponding electrodes, and in Eqs. (4) and (5), the barrier height Φ_B is measured from the quasi-Fermi level of the emitting electrode. Note that the barrier height Φ_B in the FNT and TE Equations (4) and (5), respectively, refers to the barrier that electrons have to overcome, and therefore, it may depend on the bias polarity when the electrodes are dissimilar. In the DT Equation (3), $\Phi_B = \phi_1$ for $V > 0$ and $\Phi_B = \phi_2$ for $V < 0$. Contrary to the Tsu-Esaki equations (Eqs. (1) and (2)), the finite energy range of the occupied states with their thermal distribution in the conduction band is not taken into account when deriving the analytical equations (3), (4), and (5).

III. RESULTS

A. Accuracy of the Numerov method

We tested the accuracy of the Numerov method by solving numerically the transmission through rectangular barriers of different heights (0.2...1.0 eV) and widths (0...20 nm) and with different energies of the incoming electron and compared the result against the analytical solution. As an example, the results for the case of a rectangular barrier with a height of 0.7 eV for an incoming electron energy of 0.5 eV are presented for different barrier thicknesses in Fig. 2. The discretization step used was 0.02 a_0 ($= 0.0011$ nm), and the floating-point numbers were presented in the double precision. Figure 2 shows that the numerically calculated transmission coefficient matches the analytical solution over a wide range of barrier widths and coefficient values. The relative error of the numerical solution stays below 1% for

FIG. 2. Transmission coefficient T of a rectangular barrier of a height of 0.7 eV for a particle with an energy of 0.5 eV and for barrier widths 0...20 nm plotted in logarithmic and linear (inset) scales.

transmission coefficient values relevant in this work, i.e., for those greater than 10^{-15} .

B. Analytical vs numerical results

To study the validity and usability of the analytical formulae (3), (4), and (5) as a function of the barrier width, we calculated J - V curves for the same tilted barriers as Pantel and Alexe¹⁶ did. They approximated ferroelectric tunnel junctions by tilted barriers and followed the model proposed by Zhuravlev *et al.*²³ for the polarization dependence of the potential barriers. Pantel and Alexe show J - V curves for three different barrier widths, 1.2 nm, 3.2 nm, and 4.8 nm, and for each barrier width, two J - V curves are presented corresponding to two different polarizations of the FTJ barrier. For the sake of clarity, we present only one J - V curve for each barrier width with barrier heights corresponding to the positive polarization ($P > 0$) of the barrier in the notation by Pantel and Alexe.

The barrier heights ϕ_1 and ϕ_2 for each tilted barrier are defined as in Ref. 16 and given in Table I. The other parameter values used in calculating the DT (Eq. (3)), FNT (Eq. (4)), and TE (Eq. (5)) currents, $\epsilon = 10$, $m^* = m_b^* = m_e$, $A^{**} = 10^6$ A m⁻² K⁻², and $T = 300$ K, are taken from Ref. 16.

1. Finite electron density of electrodes

In the analytic formulae (3) (DT) and (4) (FNT), the Fermi energies in the leads are not taken into account. Using the low temperature Tsu-Esaki formula with exact transmission (3), we calculated the tunneling current densities for two different electrode Fermi energies, 0.1 and 1.0 eV, with respect to the bottom of the conduction electron band in the electrodes. We set $T = 0$ K in order to eliminate the effect of TE.

TABLE I. Barrier heights ϕ_1 and ϕ_2 for different barrier widths defined as in Ref. [16] and used in the present work to produce the results in Figs. 3 and 4.

	Barrier width		
	1.2 nm	3.2 nm	4.8 nm
ϕ_1	1.012 eV	1.020 eV	1.023 eV
ϕ_2	0.968 eV	0.945 eV	0.937 eV

FIG. 3. Comparison of the J - V curves calculated for three different barrier widths using the formula (3) for DT (blue curves) and formula (4) for FNT (red curves) (these results are adapted from Ref. [16]) with the curves obtained using the $T = 0$ K Tsu-Esaki formula (2) and the Numerov method for two different electrode Fermi energies, $E_F = 0.1$ eV (solid black curves) and $E_F = 1.0$ eV (dotted black curves).

The J - V curves in Fig. 3 are calculated with the analytical formulae (3) (blue curves) and (4) (red curves) compared with the curves calculated using the low temperature Tsu-Esaki formula with exact transmission coefficient (2) (black curves) for the three different barrier widths.

As can be seen from Fig. 3, the curves practically coincide for the two thicker barriers for $E_F = 0.1$ eV. The only difference here is that the Tsu-Esaki approach with the exact transmission coefficient shows oscillations at higher voltages that are not reproduced when using the WKB approximation. These oscillations result from the partial reflection and interference of electron waves due to the large potential gradients

at the vertical barrier walls.⁴⁷ For the higher Fermi energy of 1.0 eV, the Tsu-Esaki formula gives slightly higher current densities, but the forms of the curves are maintained. For a larger Fermi energy, the density of states at the Fermi level is higher and the conduction band is broadened. Both of these effects increase the current density.

For the 1.2 nm barrier, the results from the analytical formulae differ notably from those of our Tsu-Esaki approach. As already discussed in Section II C, the WKB approximation used in deriving the analytical formulae breaks down for very thin barriers, and this is the case here (see also the discussion in Ref. 41). The WKB gives too high transmission coefficients resulting in overestimated currents. This has been reported also for thin and low barriers when comparing $T(E)$ values calculated with WKB, TM, and QTB methods.⁵⁹

2. Thermionic emission and image lowering effect

Image force lowering is considered by Pantel and Alexe¹⁶ only for TE. In the case of DT, they pointed out that the analytical formula (3) rather underestimates the tunneling current because of this. For FNT, they argued that the image force lowering will not affect the tunneling current considerably at room temperature or below, i.e., much below the Fermi temperature. As there is still some controversy whether or not image force lowering should be taken into account in FNT (see, e.g., Refs. 44, 60, and 61), we performed the $T = 300$ K calculations both with and without image force lowering of the potential in order to study differences in the corresponding J - V curves.

We calculated the effect of image force lowering on the tunnel barrier using the simple approximation developed by Simmons:⁵ $V_i = -1.15\lambda d^2/x(d-x)$, for $0 < x < d$, where $\lambda = e^2 \ln 2 / (8\pi\epsilon_0\epsilon d)$ and ϵ is the dielectric constant of the barrier material. We used the same $\epsilon = 10$ as in Ref. [16].

FIG. 4. J - V curves for a tilted barrier without image force lowering (solid black curves) and with image force lowering (dashed black curves). The results are for $T = 300$ K and for barrier widths of (a) 1.2 nm, (b) 3.2 nm, and (c) 4.8 nm. In the Tsu-Esaki calculations (black curves), the Fermi energy was 0.1 eV. Blue, red, and green curves are the DT, FNT, and TE results calculated with the analytical equations (3), (4), and (5), respectively (the DT, FNT, and TE results are adapted from Ref. [16]). (d) The zero bias potential profile for the 4.8 nm barrier without (solid curve) and with (dashed curve) image force lowering.

The resulting potential barrier shape for a 4.8 nm wide barrier and $E_F = 0.1$ eV is compared in Fig. 4(d) with the corresponding shape without the image force lowering. In this context, we tested also the precision needed for integrating the Fermi-Dirac distribution in Equation (1), and it turned out that for thicker barriers, quadruple precision had to be used for floating-point numbers in order to avoid numerical errors. The J - V curves at $T = 300$ K for the two barriers are shown in Fig. 4 for the three barrier widths.

Comparing Figs. 3 and 4, it is clearly visible that for $d = 1.2$ nm and $d = 3.2$ nm, raising the temperature does not affect the Tsu-Esaki J - V curves. Thus, for the two thinner barriers, the TE current due to increasing temperature does not affect the total current. For $d = 4.8$ nm, the $T = 300$ K Tsu-Esaki approach gives larger current densities for small bias values than FNT and DT formulae and a fair match with the TE curve including the asymmetry at low biases. Thus, our results are in agreement with those of Ref. 16 in that the thermionic emission is visible only for the thickest barrier ($d = 4.8$ nm). Image force lowering increases currents in all cases and throughout the whole bias range, while the shape of the J - V curve is modified only for the thickest barrier.

The total currents as a sum of the DT, FNT, and TE contributions shown in Fig. 4 give similar results as the Tsu-Esaki curves we have calculated. However, our model provides the possibility to fit the whole I - V curve in order to obtain the parameters of the barrier structure. When using the analytical formulae, care has to be taken to first identify the dominant tunneling process (DT/FNT/TE) and second, if different processes need to be considered to produce the whole I - V curve, to check whether different fits produce compatible barrier parameters. The approximations used when deriving the analytical formulae impose additional constraints to their use. These extra steps can be avoided when using the Tsu-Esaki model for fitting.

C. Experimentally observed features in tunnel junctions

It is often difficult to identify from experimental I - V curves the origin of different features and, more specifically, what kind of a potential profile could be used to model the experimental setup. The DT formula (3) is commonly used for fitting low-bias results and getting estimates for the physical parameters, such as the barrier heights ϕ_1 and ϕ_2 , the barrier width d , and the effective mass m^* (e.g., Refs. 19, 35, and 37). The FNT formula (4) is used in the same way for high-bias results by fitting a line in a $\ln(I/V^2)$ vs. $\ln(1/V)$ plot to get the barrier height Φ_B . Usually, only one of these two formulae is used, and the compatibility of the obtained physical parameters is not checked outside the bias region used for fitting. This can lead to unphysical barrier parameters when considering the whole I - V curve.

To get a handle on how different I - V curve features can be seen from the perspective of the single-barrier model, we present here how current varies due to variations in three different parameters, i.e., in the barrier width, in the tilt of the barrier, and in the electron effective mass. What kind of features can or cannot be produced by varying these quantities

is discussed using example cases. These general trends can be used in analysing experimental curves and assessing whether or not the measured structures can be modeled by a single-barrier structure or should a more complicated barrier profile such as a step barrier be considered.^{16,22,55,59,62}

1. Barrier width

The width of the tunnel barrier does not always equal the width of the barrier layer material. In recent papers, a change in the width of the tunnel barrier under different experimental circumstances has been used to explain the shape and asymmetries of the I - V curves.^{34,35,40} The changes in the barrier width due to switching the FTJ's polarization direction in the barrier material have been studied also theoretically.^{23,63}

To show what kind of changes barrier width variations can produce in the measurements, we calculated J - V curves for barriers of different widths ($d = 1 \dots 5$ nm) but with the same tilt angle representing a constant electric field within the barrier. The barrier height at the right electrode was fixed to $\phi_2 = 1.1$ eV and the tilt to $\Delta\phi = -0.1$ eV/nm so that for $d = 1$ nm, the barrier height at the left electrode is $\phi_1 = 1.0$ eV and for $d = 5$ nm, $\phi_1 = 0.6$ eV. Calculations were performed for both $T = 0$ K and $T = 300$ K and also with and without image force lowering. The calculated J - V curves and some of the corresponding potential barriers with and without image force lowering are shown in Fig. 5. We choose to present J - V curves as these are directly obtained from the calculations, and no assumptions are required on the effective device area ($J = I/A_{\text{device}}$).

As can be seen in Fig. 5(a), for the thinnest barrier, the J - V curve is almost linear in the logarithmic scale as a function of bias voltage, but for the thicker barriers, a curved shape appears for low biases. This agrees well with what was shown in Ref. 16 and in Fig. 3. Namely, as the width of the barrier increases, the change from DT to FNT current becomes more visible and produces the curved shape.

There is not much change in the J - V curves if image force lowering is included, but the temperature is kept at $T = 0$ K (Fig. 5(b)) because the DT and FNT currents increase only slightly due to the lower barrier height without changing the shapes of the J - V curves. When the temperature is raised to $T = 300$ K, there is a clear change due to emergence of the TE current, which can be seen in Fig. 5(c).

According to Fig. 5(d), it is clear that the effect of the image force lowering on the potential is the strongest for the thinnest barrier. For increasing barrier thicknesses, the current first decreases, but for the thickest barriers, the current actually starts to increase again for the positive bias and becomes even higher than for the thinner barriers. Since we have kept the barrier height ϕ_2 at the right electrode (see Fig. 5(d)) constant, with increasing barrier thickness, the barrier height ϕ_1 at the left electrode decreases. For positive bias voltages, the potential is raised on the left electrode, and with increasing barrier thickness, the barrier height at the left electrode, ϕ_1 , becomes lower (see Fig. 5(d)). Because of this, the current for positive bias increases for increasing barrier thickness. This is due to the TE current, which depends strongly on the barrier height at the emitting electrode, and is

FIG. 5. J - V curves for tilted barriers with widths on the range 1.0...5.0 nm. (a) $T=0$ K, trapezoidal barrier (no image force lowering). (b) $T=0$ K, image force lowering included in the potential. (c) $T=300$ K, image force lowering included in the potential. (d) Barrier shapes for widths $d = 1.0, 3.0$, and 5.0 nm, the bare tilted (solid line), and image force lowered (dashed line) potentials. Moreover, $\epsilon = 10$, $E_F = 0.1$ eV, and $m^* = m_e$.

practically independent of the barrier thickness, (see Fig. 1 and Eq. (5)). As a consequence, for tunnel junctions operating at higher temperatures, the increase in the barrier thickness could possibly be used to increase the asymmetry of the I - V curves. This requires that the electric field is constant within the barrier. In FTJs, this is realized when polarization charges are effectively screened by charge carriers inside the electrodes (i.e., when the electrodes are good conductors).

2. Leaf-like patterns in J - V curves

We studied in more detail two closely spaced barriers of thicknesses $d = 4.0$ nm and $d = 4.5$ nm, for which the barrier

heights were defined in the same way as in the preceding calculations, i.e., $\phi_1 = 0.65$ eV and $\phi_2 = 1.1$ eV for $d = 4.5$ nm and $\phi_1 = 0.7$ eV and $\phi_2 = 1.1$ eV for $d = 4.0$ nm. The J - V curves for both barriers are shown in Fig. 6.

A “leaf-like” shape, with two loops (“leaves”) on each bias voltage direction, can be seen in the J - V curves in Figs. 6(a) and 6(b) in the bias range -1.0 V... $+1.3$ V. At small voltages, the curves are further apart, but as the bias is increased, the curves start to overlap. This could model resistive switching where the lower curve corresponds to the high resistance state (HRS) and the upper curve to the low resistance state (LRS). This kind of hysteretic behaviour and the “leaf-like” shape has also been seen in experimental I - V

FIG. 6. J - V curves for tilted barriers with widths $d = 4.0$ and 4.5 nm. (a) $T=0$ K, trapezoidal barrier (no image force lowering). (b) $T=0$ K, image force lowering included in the potential. (c) $T=300$ K, image force lowering included in the potential. In addition, $\epsilon = 10$, $E_F = 0.1$ eV, and $m^* = m_e$. Parts of the curves are highlighted to illustrate the leaf-like shapes.

curves, and it was explained to originate from differences in barrier heights and tilts.¹⁹ According to our results in Figs. 6(a) and 6(b), the switching could also be caused by a change in the effective thickness of the barrier. Starting at zero bias in the LRS (upper curve), a large positive bias voltage (in Figs. 6(a) and 6(b) $\sim +1.3$ V) would induce an increase in the effective width of the barrier and switch the tunnel junction to the HRS (lower curve). After the bias voltage is decreased and reversed, at a large negative bias voltage (in Figs. 6(a) and 6(b) ~ -1.0 V), the original barrier width is restored and the junction switches back to the LRS (this corresponds to the direction of bias switching in Ref. 19). Since the FNT current does not tunnel through the whole barrier, the thickness change has a relatively small effect on it, whereas even a small change in the effective barrier thickness affects greatly the DT current. Therefore, single barriers with slightly different widths would have a big difference in currents for small bias values, but in the FNT regime, the currents could coincide if the change in the barrier height, Φ_B , stays relatively small.

In closer detail, the $d = 4.0$ nm and $d = 4.5$ nm curves in Fig. 6(a) show a very similar behavior to the experimental curves in the work by Tian *et al.*¹⁹ In their experiments, the currents for both the LRS and HRS are larger at small negative bias voltages than the LRS and HRS currents at small positive bias voltages, similar to our results. When bias is then further increased, the currents for both the LRS and HRS at the large positive bias exceed those at large negative bias, similar to our results (see also supplementary material for Ref. 19). This might indicate that a change in the effective barrier thickness could be a plausible explanation, since, e.g., a change in the direction of the tilt should result in the opposite behavior for small bias voltages.

The leaf-like shape disappears at higher temperatures for the chosen barrier parameters as can be seen in Fig. 6(c). This is due to TE that starts to dominate the transport at low bias as was discussed earlier. By choosing suitable barrier parameters, the contribution of TE can be suppressed for higher temperatures also, as shown in Fig. 4.

3. Changing the barrier tilt magnitude and direction

Often the I - V curves for tunnel junctions are asymmetrical depending on the direction of the bias drop, and this has been interpreted using both the tilted barrier and step barrier models.^{19,36,64} In a standard FTJ model, the direction of the tilt changes when the polarization in the barrier switches and the average height of the barrier changes as well.²³ To see how large an asymmetry can be produced with a single tilted barrier, we studied a $d = 3.2$ nm barrier and varied the tilt across the barrier. We calculated the current densities for barriers where the barrier height at the right electrode, $\phi_2 = 1.0$ eV, stays fixed and the barrier height at the left electrode, ϕ_1 , varies from 0.4...1.6 eV. This is the limiting case where the change in the average barrier height is maximal. Typically, in FTJ models, in addition to the change in the tilt direction, for the barrier at one electrode, ϕ_1 (LRS) $< \phi_1$ (HRS), and for the barrier at the other electrode, ϕ_2 (HRS) $< \phi_2$ (LRS). Therefore, the change in the average

barrier height is often relatively small. The J - V curves and the potential profiles are shown in Fig. 7.

The difference between the currents at -2 V and $+2$ V bias voltages is maximally about two orders of magnitude, which is the case for the barrier with the lowest average height. As the average barrier height increases, the asymmetry actually decreases. It seems that very large asymmetries, i.e., differences of several orders of magnitude, between positive and negative bias voltages cannot be explained with a single barrier structure and more complicated structures such as a step barrier (i.e., two adjacent barriers, sometimes called also a double barrier) should be considered.^{59,62,63}

4. Effective mass

The effective mass is often used as a fitting parameter for DT results.^{19,40} Since the fitting is performed within the low bias regime, its consequences are not taken into account within the high bias region. To see the overall effect of the effective mass on different bias regions, we calculated the J - V curves for a tilted barrier of a width $d = 3$ nm and barrier heights $\phi_1 = 0.95$ eV and $\phi_2 = 1.05$ eV for effective masses in the range $m^* = 0.1 \dots 5.0 m_e$. The results are shown in Fig. 8.

From the results, we see that the smaller the effective mass, the flatter the current density profile. Therefore, if the I - V curve shows steep current rises, which is often the case, a small effective mass of the carriers is not applicable when a single barrier model is assumed. Since it does not seem

FIG. 7. (a) J - V curves for different tilts of a barrier with the width $d = 3.2$ nm. The barrier height $\phi_2 = 1.0$ eV was kept constant, and the barrier height ϕ_1 was varied in the range of 0.4...1.6 eV. (b) The corresponding potential profiles used in the calculations. Other parameters used were $T = 0$ K, $E_F = 0.1$ eV, and $m^* = m_e$.

FIG. 8. J - V curves for different effective electron masses ($m^* = 0.1 \dots 5.0 m_e$). Barrier heights $\phi_1 = 0.95$ eV and $\phi_2 = 1.05$ eV, and a barrier width of $d = 3$ nm are used. Moreover, $T = 0$ K and $E_F = 0.1$ eV are assumed.

reasonable that the effective mass would be strongly dependent on the bias voltage, the implications of the magnitude of the effective mass should be considered to check whether the high bias results are compatible with the fitting within the low-bias DT regime.

IV. CONCLUSIONS

We have modeled tunneling currents through layered heterostructures using the Tsu-Esaki approach with numerically calculated transmission. The tilted barrier, including image force lowering and rounding, was chosen as our model potential since it is a simple structure, but yet, it has useful applications, *e.g.*, for the modeling of FTJs. J - V curves obtained using analytical formulae agree well with our calculations for thicker barriers for both low and high temperatures. For thin barriers, the WKB approximation used in the analytical formulae breaks down, whereas the numerically solved transmission is accurate for extremely thin barriers as well.

With our approach, we are able to produce the oscillations that do not show up when using the analytical formulae. In addition, we can calculate the currents continuously for a wide bias voltage range and for different Fermi energies and temperatures in the electrodes. When using analytical formulae for fitting, first the dominant tunneling process has to be identified and, if more than one process needs to be considered, the compatibility of the results from the different fittings should be checked. With the Tsu-Esaki model, the fitting can be performed at once for the whole bias range, thereby avoiding these considerations.

In order to show what kind of I - V curve features are reproducible by using a single tilted barrier model, we calculated currents for different tilts and widths of the barrier. According to our results, in asymmetrical I - V curves, differences of about two orders of magnitude can be explained by a change in the tilt of the barrier. Asymmetries of several orders of magnitude in current, which have been observed in experiments, require the use of a more complicated barrier model such as a step barrier. We also found that the currents may increase with increasing barrier thickness if barrier rounding due to, *e.g.*, image force lowering, is taken into

account and a constant electric field within the barrier is assumed.

As a slightly unexpected phenomenon for the simple tilted barrier model, we discovered in our simulations a “leaf-like” shape, which is also observed in certain experimental I - V curves. According to the modeling, it can be explained by a small change in the effective thickness of the tunnel barrier rather than changes in the barrier height or tilt. In this model, two different effective widths correspond to two different resistance states and the characteristics of the calculated currents are similar to the experimental data in both low and high bias voltage regions.

Our results give guidelines for the use of analytical formulae for fitting and provide a useful tool for distinguishing features related to single barrier structures in experimental I - V curves. In the future, we will look at currents through step barrier structures, enabling the study of resonance effects and more complicated I - V curve features.

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