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Tsu-Esaki modeling of tunneling currents in ferroelectric tunnel junctions

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We model tunneling currents through step barrier structures representative of ferroelectric tunnel junctions wherein one of the electrodes contributes to the barrier potential profile or an extra layer is grown between the ferroelectric barrier and one of the electrodes. We study current density–voltage (J – V) and tunneling electroresistance (TER) curves using the Tsu-Esaki formula with numerically calculated transmission. This method is computationally robust, and the same results cannot be obtained with the standard methods usually applied for interpreting experimental I – V curves. Our results predict that the effect of resonant tunneling produces asymmetry in the J – V curves and negative differential resistance characteristics. We show that the asymmetry of the J – V curves can be tuned by adjusting the barrier heights and widths and that changing the extra barrier width affects the asymmetry the most. The barrier widths and the main barrier height affect the magnitude of the tunneling current the most. The change in the tilt of the main barrier is suggested to produce a significant TER of the order of 10^2 . Our numerical method provides a systematic way to study trends in tunneling currents through step barrier structures across a wide range of barrier parameters and bias voltages, in contrast to the necessity of employing several different approximations when using analytical formulae. Therefore, our method provides the means for interpreting existing and future experiments and can be used as a tool for designing new devices with desired functionalities. Published by AIP Publishing. <https://doi.org/10.1063/1.5001823>

I. INTRODUCTION

Quantum mechanical tunneling of electrons through thin insulating barriers forms the basis of many nanoelectronic devices, including resonant tunneling diodes (RTDs), resonant tunneling transistors, superconducting quantum interference devices, and magnetic tunnel junctions.^{1–4} The functionality of these multilayer structures stems from the quantization of energy levels in thin films, the quantum phase difference and critical current, or the spin polarization of electrons, properties that are determined mainly by the electrodes. III-V semiconductors and insulating nonpolar oxides such as Al_2O_3 are typical examples of tunnel barriers in such devices.^{5,6} The main role of the tunnel barriers is to quantize electron energy levels between two closely spaced barriers or to provide direct tunneling (DT) between electronic states in the electrodes.^{7,8} In these devices, the physical properties of the barriers do not change significantly during operation.

Tunneling devices with actively tunable barrier properties are also available. Prime examples are ferroelectric tunnel junctions (FTJs).^{9–15} In these devices, two electrodes sandwich a thin insulating ferroelectric tunnel barrier. Switching of the out-of-plane ferroelectric polarization by a large enough bias voltage changes the junction resistance, an effect known as tunneling electroresistance (TER). In junctions with different electrode materials, incomplete screening of polarization charges at the barrier/electrode interfaces can

cause large TER effects.^{16,17} In this case, electrostatic screening results in an asymmetrical deformation of the barrier potential with different average barrier heights for up and down polarization. Barrier heights for the two polarization states are often derived from fits to corresponding experimental I – V curves. For this, analytical formulas for direct tunneling (DT), thermionic emission (TE), and Fowler Nordheim tunneling (FNT) are in use.^{11,12,18} Each formula approximates quantum mechanical tunneling for limited bias voltage, barrier width, and temperature ranges. Complications may arise if several mechanisms contribute simultaneously to the tunneling current. Moreover, the analytical formulas assume a single trapezoidal barrier potential and, thus, do not accurately describe quantum mechanical tunneling in FTJs when the shape of the barrier is more complex.

Besides a change in the mean barrier height, polarization reversal in FTJs can also alter the effective barrier width. Several groups have demonstrated this effect for FTJs with a complex-oxide^{19–21} or a semiconductor^{22–27} electrode. In both cases, polarization reversal in the ferroelectric barrier changes the electronic properties of the electrode near the barrier/electrode interface via the accumulation or depletion of charge carriers. This leads to the formation of an additional insulating layer via a metal-to-insulator phase transition in selected oxides or the creation of a Schottky barrier in semiconductors. The interface layers of the electrode thus actively contribute to the barrier potential profile and polarization switching in the ferroelectric tunnel barrier turns the extra barrier either on or off. A controlled variation of the

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barrier width (in addition to a modulation of average barrier height) can be used to enhance the TER of FTJs.

Ion migration across a barrier/electrode interface of a tunnel junction can also change the width and shape of the barrier potential profile.^{28,29} Very large electric fields in tunnel barriers ($\mathcal{E} = V/d > 10^6$ V/cm) can activate ion migration even at low temperatures.³⁰ Reversible migration of, for example, oxygen vacancies into and away from the interface layers of a complex-oxide electrode modifies the electronic structure. If this migration process generates a metal-to-insulator phase transition, an additional barrier forms. Giant resistive switching effects with an OFF/ON resistance ratio of more than 10^5 in tunnel junctions with $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$ (LSMO) electrodes and a paraelectric SrTiO_3 (STO) tunnel barrier provide evidence for this scenario.²⁹ I - V curves of tunnel junctions with ionic interfaces are asymmetric in the high-resistance OFF state, reflecting a pronounced asymmetry in the barrier potential after the extra barrier has formed.

In the present work, we model quantum mechanical tunneling currents for junctions wherein one of the electrodes actively contributes to the barrier potential profile or an extra layer is grown between the ferroelectric barrier and one of the electrodes. The current density curves we obtain give insight into the characteristics of the currents through these structures. We use the Tsu-Esaki formula to calculate the J - V curves and solve the transmission coefficient numerically.³¹ For single trapezoidal barrier potentials, our approach reproduces the results from analytical formulas for direct tunneling (DT), thermionic emission (TE), and Fowler Nordheim tunneling (FNT). The standard way to analyze experimental data has been to apply several analytical approximations with narrow bias ranges and very limited possibilities to correctly represent the barrier structures. The Tsu-Esaki method allows for electrical transport calculations over much wider bias voltage and barrier width ranges and, thus, its application as a fitting tool for experimental data is less restricted. More importantly, calculations of tunneling currents through more complex and asymmetric barrier potentials are possible.

We focus on tunnel junctions that, in addition to the main tunnel barrier itself, comprise a thin insulating layer in or next to one of the electrodes. These structures are modeled using a step barrier profile consisting of two adjacent barriers. The width of the extra tunnel barrier is varied over an experimentally accessible range from 0 nm to 1 nm which mimics the length scale of both electrostatic and ion migration effects in oxide tunnel junctions. The Thomas-Fermi screening length, which for conducting oxides corresponds to a few unit cells at most, gives the extent of polarization-induced charge screening in FTJs. The rapid decay of electric fields in conducting electrodes also restricts the migration of ions to the immediate vicinity of barrier/electrode interfaces. Besides the width of the extra insulating layer, we also vary systematically other barrier parameters to gauge their influence on tunneling transport. We plot our results in the form of J - V and TER- V curves and identify characteristic changes in the magnitude and symmetry of the curves providing guidance for the interpretation of experiments.

II. MODELING OF TUNNELING CURRENTS IN FTJs

In this section, we first shortly review the literature concerning tunneling current calculations for FTJs and step potential barrier structures performed using different approaches. Then, in Subsection II A, we present the step potential barrier structure and the Tsu-Esaki method which we use in our current density calculations. Finally, in Subsection II B, we show how resonant tunneling, traditionally studied in the context of resonant tunneling diode (RTD) structures, affects the current through a step barrier structure.

A recent review by Velev *et al.* summarizes theoretical modeling of FTJ structures and materials.³² In many theoretical articles on FTJs, the conductance of the junction is calculated only for the zero-bias case. Since we are calculating the current as a function of bias voltage, the most relevant earlier reports concern calculations of J - V curves.^{16–18,33,34} In theoretical papers, usually the current density J , instead of the current I , is calculated as a function of bias voltage. The characteristics of the obtained J - V curves can be compared with experimental I - V curves assuming that the area through which the current flows stays constant.

Kohlstedt *et al.*¹⁷ studied the influence of the converse piezoelectric effect and imperfect screening effects on the J - V curves and calculated the currents using the Simmons' approximation.³⁵ Using the Landauer formula⁷ valid for small applied bias voltages, Zhuravlev and co-workers studied FTJs where the two metal electrodes have significantly different screening lengths.¹⁶ Both reports predict that asymmetric tunnel junctions with dissimilar electrodes produce large OFF/ON resistance ratios. Pantel and Alexe analyzed the tunneling currents in FTJs using a single tilted barrier model and analytical formulas for different transport regimes.¹⁸ They concluded that the dominating transport mechanism depends on the barrier thickness, bias voltage, and polarization direction. A report on symmetric FTJs predicts that a relatively large TER effect can be achieved also via a strong piezoelectric response to an applied bias.³³ Here the TER was calculated using the non-equilibrium Green's function (NEGF) formalism combined with the density functional theory (DFT). Useinov and co-workers used the NEGF method combined with the tight-binding model to calculate TER and tunneling magnetoresistance (TMR) effects as a function of bias voltage in FTJs with two magnetic electrodes.³⁴ They predict that TER exists at finite bias even in symmetric tunnel junctions and show that the bias dependence of TMR can be controlled via polarization switching in the ferroelectric tunnel barrier. In all the reports presented above, a tilted single barrier model was used for the tunnel barrier potential when calculating the tunneling current.

Structures with two adjacent barriers, i.e., step barriers, have also been modeled in the context of FTJs. Indlekofer and Kohlstedt simulated the current-voltage characteristics of FTJs using an NEGF approach with a self-consistent Hartree potential accounting for Coulomb charging effects.³⁶ The modeled tunnel junction was nominally a single barrier structure, but the results predicted that a partially depleted region arises close to the tunnel barrier, effectively adding an extra barrier to the structure. The current-voltage curves

showed bistable resistive switching behavior depending on the polarization state of the ferroelectric barrier. In FTJs with non-magnetic and ferromagnetic metal electrodes, the inclusion of an additional thin dielectric layer was predicted to enhance the TER ratio of both types of junctions.^{37,38} In the two reports, the TER ratio was calculated at zero-bias as a function of the dielectric layer thickness using the Landauer formula.³⁷ In a study of BaTiO₃/SrTiO₃ (BTO/STO) junctions, the currents were modeled either using an average barrier model or by using the Landauer formalism and approximating the transmission as $T_{\text{total}} \approx T_{\text{BTO}} * T_{\text{STO}}$.³⁹ In a recent paper, the NEGF method and the Landauer formula were used to model I - V curves of step barrier FTJs.⁴⁰ The results suggest that both the height and thickness of a CoO_x buffer layer forming at the Co/BaTiO₃ interface may change under bias.

Previous theoretical papers presenting J - V curves of quantum mechanical tunneling through step barriers have focused mainly on semiconductor diodes. Typically, the two barriers have a comparable width, e.g., around 5 nm, and the polarity of the applied bias voltage is fixed.⁴¹⁻⁴⁶ Both limitations should be lifted when calculating tunneling currents in FTJs as they comprise a nominal ferroelectric layer and, potentially, a narrower extra barrier either formed in the electrode or grown on purpose. Large asymmetries for positive and negative bias voltage are anticipated if the properties, i.e., the height, width, and tilt, of the adjacent barriers are different.

An early study using the Tsu-Esaki formula showed a negative differential resistance (NDR) in a step barrier structure for one bias polarity due to resonance tunneling through a quasibound state in the triangular well formed in the step barrier.⁴¹ In this study, the estimation of the bias voltage interval where resonant tunneling occurs is made based on geometric considerations. There is a peak in this interval in the calculated J - V curve and transmission probabilities are shown for selected bias values. However, no further analysis regarding the position of the peak with respect to possible resonance levels is made. Wang *et al.* investigated, both experimentally and theoretically, Al_xGa_{1-x}As/GaAs step barrier heterostructures, showing NDR for one bias polarity.⁴² They modeled the current using an envelope method for the band structure and a wave function matching technique for the Hamiltonian elements at the interface. A resonance peak was observed both in the calculated and in the experimental curves.

An interesting theoretical comparison between single barriers, asymmetric double barriers (i.e., asymmetric RTDs), and step barriers is presented in Ref. 43. The calculations were performed using the transfer-matrix technique. It is shown that the transmission and tunneling currents through step barriers resemble in many aspects those through asymmetric double-barrier structures. Compared to asymmetric double-barrier structures, step barrier structures have several useful features: wider NDR regions, easier fabrication, high-speed response, relatively lower transmission coefficients, and lower current peak-to-valley ratios.

Chapline and Wang studied tunneling through step barriers using an analytical formula they derived for multilayer barriers.⁴⁶ The report is focused on finding a fitting formula

for quantifying individual barrier properties in a multilayer structure and shows that the analytical formula gives better fits than the Simmons' formula.³⁵ The derivation of the analytical formula is based on the WKB approximation, which is limited to small bias voltages and cannot account for wavefunction reflection and interference effects.⁴⁷

A. Tsu-Esaki method

In this work, we focus on direct tunneling processes where the tunneling probability, often called the transmission coefficient, is obtained by numerically solving the Schrödinger equation for a given potential profile. Inelastic and defect related tunneling processes, such as trap-assisted tunneling, are not taken into account.⁴⁸⁻⁵¹ A schematic illustration of quantum mechanical tunneling through a step barrier structure is shown in Fig. 1. We calculate currents for both positive and negative bias voltages. At negative bias voltages, electrons tunnel from the electrode with a narrow extra potential barrier. Figure 1 represents the positive bias voltage case.

For calculating the tunneling current density, we use the low-temperature Tsu-Esaki formula^{7,52} for a one-dimensional barrier potential varying along z

$$J_{T=0K}(V) = \frac{em^*}{2\pi^2\hbar^3} \left[eV \int_{eV}^{E_F} d\epsilon_z T_{tr}(\epsilon_z, V) + \int_{E_F}^{E_F+eV} d\epsilon_z T_{tr}(\epsilon_z, V)(E_F + eV - \epsilon_z) \right]. \quad (1)$$

Here, ϵ_z is the kinetic energy of the electron in the z -direction, m^* is the electron effective mass, V is the bias voltage, and $T_{tr}(\epsilon_z, V)$ is the transmission coefficient. Parabolic bands are assumed and the zero-reference of the potential energy is, referring to Fig. 1, at the conduction band minimum on the right-hand side of the barrier. Electron distributions on each side of the barrier are calculated using equilibrium Fermi-Dirac statistics and the Fermi levels are fixed at $\epsilon_{F,l} = E_F + eV$ and $\epsilon_{F,r} = E_F$ on the left and right-hand side of the barrier, respectively (E_F is the free-electron Fermi energy, i.e., the occupied conduction band width, see Fig. 1). The transmission coefficient is obtained by numerically solving the Schrödinger equation using the Numerov method.^{53,54} This method is computationally efficient and accurate and does not require any simplifying assumptions about the shape of the barrier potential profile. The method is also numerically robust enabling the modeling of the steep current rises originating from resonance phenomena. The

FIG. 1. Potential profile of a step barrier considered in this study. The schematic illustrates electron tunneling for a positive bias voltage.

details of our computational method are given in a previous article on tunneling through single tilted barriers.³¹

B. Resonant tunneling

Resonant tunneling diodes (RTDs), first proposed by Tsu and Esaki in 1973 and experimentally demonstrated in 1974, show NDR for a certain bias voltage range.^{52,55} The RTD structure consists of two barriers with a quantum well (QW) in between, and it forms the basis of many electronic devices,⁵⁶ such as terahertz oscillators and ultra-fast switching devices. In an RTD, the states in the QW are quantized and the lowest energy level, ϵ_1 , lies above the emitter Fermi level ϵ_F . Therefore at small bias values, there are no states available in the QW to tunnel to and the current, due to thermal emission, is very small. When bias is increased and ϵ_1 drops below ϵ_F , the current rapidly increases due to resonant tunneling through the quantized state. When bias is further increased, the energy level ϵ_1 drops below the energies of the electrons at the emitter causing the current to decrease. This results in an NDR region in the I - V curve.

Resonant tunneling can happen also in step barrier structures, where QW like states are induced in the notch between the barriers for one bias polarity. In the structures we consider here (see Fig. 1), this happens at positive bias voltages. Schulz and Gonçalves da Silva studied resonant transmission curves and, using geometrical considerations, showed that the peak in the transmission and the NDR region in the J - V curve appear at the same bias voltage interval.⁴¹ In a further study, Guo *et al.* concluded that resonant electron transmission validates the existence of quasibound states in step barrier structures and that, by properly adjusting the barrier parameters, the peak-to-valley ratio of the J - V curves can be enhanced.⁴⁴ A study on metal-insulator-insulator-metal (MIIM) diodes showed also that the quantum well needs to be wide enough, i.e., the lower barrier needs to be wide enough, to have a resonant energy level.⁵⁷

Figure 2(a) shows a typical zero-bias step barrier potential corresponding to our modeling presented in Sec. III and the ensuing J - V curve. We observe a sharp rise in the tunneling current in Fig. 2(b) at bias voltage $V_b = 1.2$ V and also at bias values $V_b = 1.8$ V and $V_b = 2.6$ V. Especially, the first steep rise makes the J - V curve prominently asymmetric. We estimate the energy levels of the confined states by those of an infinite triangular QW to see if the steep rises coincide with the bias voltages where the top of the band at the emitter crosses the QW levels and the resonant tunneling will take place. The analytical formula for the energy levels in an infinite triangular QW reads as $\epsilon_n = (\hbar^2/2m)^{1/3} \frac{2}{3} (\pi q \mathcal{E}) (n - \frac{1}{4})^{2/3}$, $n = 1, 2, \dots$, where q is the electron charge and $\mathcal{E}$ the electric field creating the triangular confining potential. $\mathcal{E}$ equals the slope of the main barrier in Fig. 3 where the step potentials and emitter Fermi levels together with the energy levels of the infinite triangular QW are plotted for three selected bias values.

At the bias value of 1.2 V, corresponding to the first steep rise in current in Fig. 2(b), the emitter Fermi level crosses with ϵ_1 [Fig. 3(a)]. For the bias value of 1.8 V,

FIG. 2. (a) Step barrier potential energy profile. The barrier parameters are $\phi_1 = 0.5$ eV, $d_1 = 2.5$ nm, $\phi_2 = 2.0$ eV, and $d_2 = 1.0$ nm. (b) The corresponding J - V curve. The other parameters used are $T = 0$ K, $E_F = 0.5$ eV, and $m^* = m_e$.

corresponding to the second steep rise in current in Fig. 2(b), ϵ_2 is slightly above the Fermi level as seen in Fig. 3(b). This is due to the QW well like states between the two barriers being less confined than those of an infinite triangular QW, especially in the case of the higher states with $n = 2, 3, \dots$. Therefore, the resonant levels in the step barrier structure have actually lower energies than those of the ideal triangular QW and the actual crossings and steep current rises take place at slightly lower bias voltages. The last steep rise in Fig. 2(b) occurs at a bias of 2.6 V due to the top of the higher barrier dropping below the Fermi level.

As shown in Fig. 2(b), the asymmetry due to the first steep rise in the positive voltage region of the J - V curve is a prominent effect of the resonant tunneling. The features at higher voltages, including also the NDR effects, are not so strong, at least on the logarithmic scale. The experimental high-resistance-state I - V curve for positive bias voltages in Ref. 58 exhibits oscillations that look similar to the oscillations in Fig. 2(b). The experimental junction consists of a

FIG. 3. Potential curves for three positive bias values: (a) 1.2 V, (b) 1.8 V, and (c) 2.6 V. The Fermi level at the emitter, $\epsilon_{F,l}$, and the analytically calculated energy levels of an infinite triangular quantum well, ϵ_1 , ϵ_2 , and ϵ_3 are shown. The parameters of the step barrier are given in the caption of Fig. 2.

ferroelectric layer combined with MoS₂, a two-dimensional (2D) semiconductor. It is argued that in the high resistance state, the polarization in the ferroelectric (FE) layer induces an additional barrier in the semiconductor. Thus, this can be considered as a step barrier structure and the oscillations observed in Ref. 58 could be due to a resonant tunneling effect. Similarly, resonant tunneling could be at the origin of the oscillations observed in the I - V curve at high voltages in Ref. 59. However, these experimental curves do not show clear NDR and the oscillations are clearly weaker than in our calculations. In addition, these oscillations do not seem to be a typical phenomenon observed in FTJ I - V curves. It should be kept in mind that in our calculations, the step barrier structure is a simplified model of the actual device. The oscillations and eventual NDR may be smoothed out in experiments due to, e.g., barrier interface roughness or slight non-uniformity of barrier thicknesses.

The resonances observed in our calculations are further confirmed by peaks in the transmission. For each bias voltage, the transmission T_{tr} is calculated for energies within the range $[eV, E_F + eV]$, i.e., corresponding to the integration interval in the Tsu-Esaki formula of Eq. (1). As an example, the calculated transmission $T_{tr}(\epsilon, V)$ curves for the step potential barrier in Fig. 2(a) are shown in Fig. 4 for selected bias voltages. For negative bias values, the transmission shows no peaks and the same goes for small positive bias voltages. As examples of this, the transmission curves for $V_b = -2.0$ V and $V_b = 0.5$ V are shown in Figs. 4(a) and 4(b). At $V_b = 1.2$ V, Fig. 4(c), the transmission shows a pronounced peak and this corresponds to the onset of resonant tunneling seen as a steep rise in the J - V curve in Fig. 2(b). The energy

of the lowest level, ϵ_1 , for the infinite triangular QW, is shown as a reference in the transmission curve. As discussed above, the QW like state in the step barrier potential is less confined and therefore lower in energy than ϵ_1 . Consequently, also the peak in transmission occurs at a slightly lower energy than ϵ_1 . In Fig. 4(d), the transmission even shows two peaks for $V_b = 2.0$ V corresponding to the first and second levels of the triangular QW like state.

As can be seen in Fig. 4, the transmission peaks are very narrow and intense. Due to this, the discretization around the peaks needs to be extremely dense for both dx and $d\epsilon$. We calculated the currents by using an adaptive grid spacing scheme. We also studied the convergence of the results, and with decreasing grid spacing in both x and ϵ , the results converged towards smooth and unique solutions for the J - V curves.

III. RESULTS

In the following, we systematically study quantum mechanical tunneling through step barriers. The barrier potentials we consider are representative for FTJs where the step barrier shape is due to either effects of electrostatic or ionic charge modulation near the barrier electrode/interface or the intentional growth of a bi-layer barrier. As a result, different experimentally realized junctions can be modeled using the step barrier approach. Because the extra barrier can form unintentionally, the possibility of a step barrier shaped potential should always be taken into account when interpreting experimental I - V curves, even for nominally single barrier structures.

For developing new devices, the study of the trends in J - V curves as a function of device parameters is crucial. Our

FIG. 4. Transmission curves for the step potential barrier in Fig. 2(a) for bias voltages (a) $V_b = -2.0$ V, (b) $V_b = 0.5$ V, (c) $V_b = 1.2$ V, and (d) $V_b = 2.0$ V. The vertical lines indicate the energy levels ϵ_1 and ϵ_2 of the infinite triangular QW. The parameters of the step barrier are given in the caption of Fig. 2.

results are not only applicable in understanding the results of certain specific experiments, but, in addition, they bring insight into designing new kinds of devices with desired functionalities. It should be noted, however, that our calculations represent idealized barrier structures. In experiments, the situation is typically more complex.

We note that we already used a step barrier potential to fit experimental data in a recent study on $\text{Pb}(\text{Zr,Ti})\text{O}_3$ (PZT) tunnel junctions with LSMO electrodes.²⁹ The best fit for the experimentally observed highly asymmetrical I - V curve of the high-resistance OFF state was obtained using a step barrier potential with a high and narrow (≈ 0.8 nm) extra barrier. Both the OFF and ON state I - V curves could be fitted using this step barrier model when taking into account the effect of series resistance (see Subsection III C) and changing only the extra barrier height. The formation of this extra barrier was attributed to oxygen migration across the interface between the LSMO electrode and the PZT tunnel barrier. A similar phenomenon is discussed in Ref. 60.

In another experimental study of a nominally single layer junction, a comparison was made between *ex situ* and *in situ* fabrication of the top Pt electrode in a Nb-doped STO/BTO/Pt structure.⁶¹ The junctions with *ex situ* fabricated top electrodes showed much larger OFF/ON ratios, suggesting that a passive interface layer forms at the top electrode resulting in a step barrier potential profile.

Efforts have also been made to increase TER by adding an extra barrier adjacent to the FE layer.^{19,39,58,62} Experimental Au/Co/BTO/LSMO/NdGaO₃ (NdGaO₃ is the substrate) junction was described with a step barrier potential consisting of the BTO ferroelectric layer and a passive layer

of CoO_x at the Co/BTO interface. The resistive switching was attributed to the field-induced charge redistribution at the ferroelectric-electrode interface changing the CoO_x barrier height.⁶² LSMO/BTO/LCMO/LSMO junctions, where a thin La_{0.5}Ca_{0.5}MnO₃ (LCMO) interlayer was inserted at one of the electrodes, exhibited large TER effects in experiments.¹⁹ This was shown to be due to a metal-to-insulator phase transition in LCMO caused by the modulation of carrier density through ferroelectric polarization switching, effectively adding an insulating barrier of LCMO next to the BTO layer in the high resistance state. BTO/STO composite barriers, i.e., step barrier structures, have been compared to single BTO barriers, and the composite barriers show enhanced TER and enable effective control of the barrier potentials.³⁹ Recent experiments⁵⁸ of a hybrid structure with a ferroelectric thin film and a 2D semiconductor layer showed an OFF/ON resistance ratio of 10^4 . The reversible accumulation-depletion of majority carriers in the 2D semiconductor occurs in response to the switching of the FE barrier, thus altering the barrier at the interface between these two layers.

The step barriers we consider consist of a low main tunnel barrier, depicting the ferroelectric layer, and an additional narrow but higher barrier at one of the electrode interfaces. The thicker and lower barrier is referred to as the “main barrier” (parameters d_1 and ϕ_1), whereas the thinner and higher barrier is labeled as the “extra barrier” (parameters d_2 and ϕ_2). Fits to experimental I - V curves indicate that the heights of ferroelectric tunnel barriers are rather small. In Refs. 12–15, 19, and 29, mean barrier heights ranging from 0.1 to 0.8 eV have been obtained from fits to I - V curves for

FIG. 5. (a) Step barrier potential energy profiles with different main barrier widths and (b) the corresponding J - V curves. The main barrier height is $\phi_1 = 0.2$ eV and the three different widths are $d_1 = 2.0$ nm, 4.0 nm, and 6.0 nm. The extra barrier parameters are $\phi_2 = 1.2$ eV and $d_2 = 1.0$ nm. The other parameters used are $T = 0$ K, $E_F = 0.5$ eV, and $m^* = m_e$.

BTO and PZT junctions. Referring to these results, we use for the main barrier height ϕ_1 values in the range of $0.2 \dots 0.8$ eV. The main barrier width d_1 is varied over typical experimental values of $2 \dots 6$ nm. We change the width of the extra barrier d_2 from 0 to 1 nm. The use of this parameter range is motivated by effective screening of electric fields in conducting oxide electrodes, which restricts charge accumulation and ion migration effects to the immediate vicinity of the electrode/barrier interface. Also in the case of an intentionally grown extra barrier, the extra dielectric layer is often much thinner than the ferroelectric layer.^{39,58} The height of the extra barrier ϕ_2 is varied from 0 to 3.0 eV.

In this work, the width, height, and tilt of the barriers are varied to gauge their influence on J - V transport curves. The results are grouped into two main sections, depending on whether the parameters of the main barrier or those of the extra barrier are varied. For certain barrier configurations, we calculate also the TER as a function of bias voltage. In addition to varying the barrier parameters, we show the effect of an additional series resistance, typically present in experiments, on J - V curves. It is important to note that as our calculations represent idealized barrier structures, comparing directly theoretical and experimental J - V curves is not feasible. Instead, our method allows analyzing trends and prominent features such as the asymmetry in measured J - V curves with varying barrier parameters.

A. Main barrier

In a layered structure where a second barrier forms due to effects of electrostatic charge modulation or ion migration, typically only the parameters of the main barrier can be

controlled. Therefore, we first study how the main barrier height, width, and tilt affect the shape of the J - V curves.

1. Main barrier width

We have calculated two different cases where the main barrier width changes. The extra barrier parameters are $\phi_2 = 1.2$ eV and $d_2 = 1.0$ nm in both cases. The main barrier height is $\phi_1 = 0.2$ eV in the first case, shown in Fig. 5(a), and $\phi_2 = 0.5$ eV in the second, shown in Fig. 6(a). The main barrier width is varied in the range $d_1 = 2.0 \dots 6.0$ nm, corresponding to typical values in experimental devices. The corresponding J - V curves are shown in Figs. 5(b) and 6(b). In all the following calculations, we set $E_F = 0.5$ eV.

The interesting feature seen in Fig. 5(b) is that as the main barrier width is increased, the steep rise in the current occurs at a lower bias voltage. This happens because the potential is less steep when the main barrier is wider (since it is assumed that the potential drops linearly) making the confinement weaker and hence the QW states lower in energy and more closely spaced. With increasing main barrier height, the currents diminish and increase more slowly as a function of the bias voltage as seen by comparing Figs. 5(b) and 6(b). With increasing barrier width, the current profile narrows, i.e., the current rise is steeper at lower bias voltages, in both cases $\phi_1 = 0.2$ eV and $\phi_1 = 0.5$ eV. Moreover, the currents at low bias voltages are more symmetrical when the main barrier is wider.

2. Main barrier height

The main barrier height can be tuned by changing the materials of the junction, either the barrier material or the

FIG. 6. (a) Step barrier potential energy profiles with different main barrier widths and (b) the corresponding J - V curves. The main barrier height is $\phi_1 = 0.5$ eV and the three different widths are $d_1 = 2.0$ nm, 4.0 nm, and 6.0 nm. The extra barrier parameters are $\phi_2 = 1.2$ eV and $d_2 = 1.0$ nm. The other parameters used are $T = 0$ K, $E_F = 0.5$ eV, and $m^* = m_e$.

FIG. 7. (a) Step barrier potential energy profiles with different main barrier heights and (b) the corresponding J - V curves. The different main barrier heights are $\phi_1 = 0.2$ eV, 0.4 eV, 0.6 eV, and 0.8 eV and the width is $d_1 = 3.0$ nm. The extra barrier parameters are $\phi_2 = 1.2$ eV and $d_2 = 1.0$ nm. The other parameters used are $T = 0$ K, $E_F = 0.5$ eV, and $m^* = m_e$.

material of the electrodes. We calculated currents as a function of the main barrier height for two different main barrier widths, $d_1 = 3.0$ nm and $d_1 = 5.0$ nm. In both cases, the extra barrier width and height were kept constant as $d_2 = 1.0$ nm and $\phi_2 = 1.2$ eV. The main barrier height ϕ_1 values are varied in the range of $0.2 \dots 0.8$ eV, corresponding to values obtained from fits to I - V curves for BTO and PZT junctions.^{12–15,19,29} The potential energy profiles and the corresponding J - V curves for $d_1 = 3.0$ nm are presented in Fig. 7 and for $d_1 = 5.0$ nm in Fig. 8.

For both main barrier widths, we can see that increasing the main barrier height decreases the asymmetry of the currents for both low and high bias voltages in Figs. 7(b) and 8(b). This is because with the increasing barrier height the barrier starts to resemble a single barrier structure. With the increasing barrier height, the steep rise in current moves to higher bias values and the rise becomes more moderate. This is in contrast to the previous case [Figs. 5(b) and 6(b)] where widening the barrier moved the onset of the steep rise in current to smaller bias voltages.

3. Main barrier tilt

In FTJs, the main barrier is tilted due to the polarization in the barrier material. The barrier polarization can be reversed by large enough bias voltages resulting in changes in the magnitude and/or the direction of the barrier tilt and hence the mean barrier height. This is the origin of the TER effect in FTJs.^{16,17} To see what kind of features the changing tilt produces in the J - V curves, we studied two different cases where we varied the tilt of the main barrier and the extra barrier height $\phi_2 = 1.5$ eV was kept constant. In both

structures, the main barrier width $d_1 = 2.0$ nm and the extra barrier width $d_2 = 1.0$ nm.

In the first case, the main barrier height next to the electrode is fixed to $\phi_{1,\text{left}} = 0.2$ eV and the barrier height at the interface of the extra barrier is varied in the range $\phi_{1,\text{right}} = 0.1 \dots 0.7$ eV. The potential energy profiles and the corresponding J - V curves are shown in Fig. 9. In the second case, the main barrier height next to the electrode is fixed to $\phi_{1,\text{left}} = 0.5$ eV and the barrier height at the interface of the extra barrier is varied in the range $\phi_{1,\text{right}} = 0.1 \dots 0.7$ eV. The potential energy profiles and the corresponding J - V curves are shown in Fig. 10. This situation reflects a ferroelectric tunnel barrier with an adjacent passive dielectric layer where the reversal of the polarization alters the tilt of the main barrier but not the properties of the extra barrier.

For the lower main barrier height, the steep rise in the current at positive bias voltage values starts to disappear with increasing $\phi_{1,\text{right}}$ as shown in Fig. 9(b). In addition, the J - V curves become almost exponential (i.e., linear on the logarithmic scale) at higher bias voltages shown in Fig. 9(b). This can be seen also in the results of Secs. III A 1 and III A 2. However, now it is more visible due to a thinner main barrier and higher current values. Linearity in the logarithmic scale is obviously the result of the dominance of tunneling through the extra barrier. Since the confinement starts to diminish when $\phi_{1,\text{right}} > \phi_{1,\text{left}}$, this leads to the disappearance of the resonant tunneling effect and the ensuing steep rise in current. When $\phi_{1,\text{left}} = 0.5$ eV, the steep rise in current stays prominent with increasing $\phi_{1,\text{right}}$ as shown in Fig. 10(b).

The TER ratio defined by the help of the resistances in the high (R_{OFF}) and low (R_{ON}) resistance states, i.e.,

FIG. 8. (a) Step barrier potential energy profiles with different main barrier heights and (b) the corresponding J - V curves. The different main barrier heights are $\phi_1 = 0.2$ eV, 0.4 eV, 0.6 eV, and 0.8 eV and the width is $d_1 = 5.0$ nm. The extra barrier parameters are $\phi_2 = 1.2$ eV and $d_2 = 1.0$ nm. The other parameters used are $T = 0$ K, $E_F = 0.5$ eV, and $m^* = m_e$.

FIG. 9. (a) Step barrier potential energy profiles with different main barrier tilts and (b) the corresponding J - V curves. The main barrier parameters are $\phi_{1,\text{left}} = 0.2$ eV and $d_1 = 2.0$ nm. The barrier height $\phi_{1,\text{right}}$ is varied resulting in different slopes $\mathcal{E}$ of the main barrier. The extra barrier parameters are $\phi_2 = 1.5$ eV and $d_2 = 1.0$ nm. The other parameters used are $T = 0$ K, $E_F = 0.5$ eV, and $m^* = m_e$.

FIG. 10. (a) Step barrier potential energy profiles with different main barrier tilts and (b) the corresponding J - V curves. The main barrier parameters are $\phi_{1,\text{left}} = 0.5$ eV and $d_1 = 2.0$ nm. The barrier height $\phi_{1,\text{right}}$ is varied resulting in different slopes $\mathcal{E}$ of the main barrier. The extra barrier parameters are $\phi_2 = 1.5$ eV and $d_2 = 1.0$ nm. The other parameters used are $T = 0$ K, $E_F = 0.5$ eV, and $m^* = m_e$.

$\text{TER} = (R_{\text{OFF}} - R_{\text{ON}})/R_{\text{ON}}$ is equivalent to $\text{TER} = (J_{\text{ON}} - J_{\text{OFF}})/J_{\text{OFF}}$. We calculated the TER in the two cases presented above considering $\phi_{1,\text{right}} = 0.1$ eV and $\phi_{1,\text{right}} = 0.7$ eV as the two resistance states. The potentials of the high and low resistance states and the calculated TER as a function of bias for both main barrier heights are shown in Figs. 11 and 12.

We can compare these TER values to the theoretical results by Zhuravlev *et al.* in Ref. 37. They calculated TER of FTJs with a composite barrier, i.e., a barrier consisting of a functional ferroelectric film and a thin film of a nonpolar dielectric material. In their model, the switching of the main barrier polarization changed both the tilt of the main barrier and the height of the adjacent dielectric barrier. The TER was calculated using the Landauer formula for conductance, and the bias dependence of TER was not studied. For a step barrier with dimensions $d_1 = 2.5$ nm and $d_2 = 1.0$ nm, a TER of the order of 10^2 – 10^3 was obtained. The barrier heights

were $\phi_1 \approx 0.6$ eV and $\phi_2 \approx 2.5$ eV and the switching of the polarization in the main barrier altered the extra barrier potential height by about 0.5 eV.

For small bias voltages, i.e., comparable to the results obtained using the Landauer formula, we get a TER of the order of 10^2 for both of our systems as can be seen from Figs. 11(b) and 12(b). Our potential parameters are similar to those of Ref. 37 with the exception that in our calculations, the extra barrier height stays constant. However, a change in the extra barrier height by as much as 1 eV (see Fig. 17) has at most an order of magnitude effect on the TER ratio at low bias. Hence, our results suggest that the change in the main barrier tilt is more important for the TER ratio than a possible change in the extra barrier height, as long as there is a second insulating layer in the junction. As a function of bias, the TER ratio increases up to 10^6 [see Fig. 12(b)] due to resonance tunneling in the high conductance state.

FIG. 11. The potential profiles of the low (ON) and high (OFF) resistance states (a) and corresponding TER as a function of bias voltage (b). Main barrier heights for the low resistance state are $\phi_{1,\text{left}} = 0.2$ eV and $\phi_{1,\text{right}} = 0.1$ eV, and for the high resistance state $\phi_{1,\text{left}} = 0.2$ eV and $\phi_{1,\text{right}} = 0.7$ eV. The other parameters used are as in Fig. 9(a).

FIG. 12. The potential profiles of the low (ON) and high (OFF) resistance states (a) and corresponding TER as a function of bias voltage (b). Main barrier heights for the low resistance state are $\phi_{1,\text{left}} = 0.5 \text{ eV}$ and $\phi_{1,\text{right}} = 0.1 \text{ eV}$, and for the high resistance state $\phi_{1,\text{left}} = 0.5 \text{ eV}$ and $\phi_{1,\text{right}} = 0.7 \text{ eV}$. The other parameters used are as in Fig. 10(a).

FIG. 13. (a) Barrier potential energy profiles with different extra barrier widths and (b) the corresponding J - V curves. The single barrier case (black dashed line) is shown as a reference. The barrier parameters are $\phi_1 = 0.2 \text{ eV}$, $d_1 = 2.0 \text{ nm}$, and $\phi_2 = 1.2 \text{ eV}$, and the curves are calculated for three different extra barrier widths $d_2 = 0.2 \text{ nm}$, 0.6 nm , and 1.0 nm . The other parameters used are $T = 0 \text{ K}$, $E_F = 0.5 \text{ eV}$, and $m^* = m_e$.

B. Extra barrier

When the extra barrier forms due to, e.g., electrostatic charge modulation or ion migration, its properties may be difficult to control. Still, it is useful to see how the width and height of the extra barrier affect the current behavior, in order to provide examples for interpreting experimental data. There are also studies where an extra layer is intentionally grown on top of the FE layer and in this case also its width and height can be varied.^{37,63,64}

1. Extra barrier width

We studied the effects of the extra barrier width by comparing the currents of the step barrier structure to the J - V curve of a single barrier structure, $d_1 = 2.0 \text{ nm}$ and $\phi_1 = 0.2 \text{ eV}$, without an extra barrier. In the first case, presented in Fig. 13, the height of the extra barrier was

$\phi_2 = 1.2 \text{ eV}$ and the width was varied within the range $d_2 = 0.2 \dots 1.0 \text{ nm}$. This range mimics the length scale of both electrostatic and ion migration effects in oxide tunnel junctions.

The J - V curves in Fig. 13(b) show that with the increasing barrier width, the steep rise in current at positive bias voltages moves to higher values. The current values drop with increasing barrier width, but for large positive bias voltage values, the drop is negligible. This happens because the extra barrier drops below the emitter Fermi level and therefore has a negligible effect on the current. As a result, the addition of an extra barrier increases the asymmetry of the currents both at low voltages and especially at high bias voltages.

In the second case, presented in Fig. 14, the extra barrier height was fixed to $\phi_2 = 2.0 \text{ eV}$. The J - V curves in Fig. 14(b) show that, again, with the increasing barrier width, the

FIG. 14. (a) Barrier potential energy profiles with different extra barrier widths and (b) the corresponding J - V curves. The single barrier case (black dashed line) is presented as a reference. The barrier parameters are $\phi_1 = 0.2 \text{ eV}$, $d_1 = 2.0 \text{ nm}$, and $\phi_2 = 2.0 \text{ eV}$. The curves are calculated for three different extra barrier widths $d_2 = 0.2 \text{ nm}$, 0.6 nm , and 1.0 nm . The other parameters used are $T = 0 \text{ K}$, $E_F = 0.5 \text{ eV}$, and $m^* = m_e$.

FIG. 15. TER as a function of bias voltage for different extra barrier widths for (a) $\phi_2 = 1.2$ eV and (b) $\phi_2 = 2.0$ eV. The potential barrier profiles are shown in the insets of both figures. The low resistance (ON) state corresponds to the single potential barrier case (black dashed line) and the colors refer to the different extra barrier widths representing the different high resistance (OFF) states. The barrier potential parameters used for calculating the results in Figs. 15(a) and 15(b) are as those for Figs. 13(a) and 14(a).

steep rise in current moves to higher bias voltage values. Moreover, the current values drop with the increasing barrier width and the second kink at positive bias voltages disappears. Since the extra barrier is now relatively high, the current values drop also for large positive bias voltages, though still not as much as at large negative bias voltage values. In summary, the extra barrier width has a much larger effect on the asymmetry of the currents than changes in the width and height of the main barrier.

FIG. 16. (a) Barrier potential energy profiles with different extra barrier heights and (b) the corresponding J - V curves. The single barrier case (black dashed line) is presented as a reference. The main barrier parameters are $\phi_1 = 0.2$ eV and $d_1 = 2.0$ nm. The extra barrier width is $d_2 = 0.5$ nm and the curves are calculated for three different extra barrier heights: $\phi_2 = 1.0$ eV, 2.0 eV, and 3.0 eV. The other parameters used are $T = 0$ K, $E_F = 0.5$ eV, and $m^* = m_e$.

For calculating the TER, we consider the single barrier case, i.e., no extra barrier, as the low resistance (ON) state. The different extra barrier cases represent different high resistance (OFF) states. The TERs as a function of bias for different barrier widths for the two cases $\phi_2 = 1.2$ eV and $\phi_2 = 2.0$ eV are shown in Fig. 15. The biggest TER value of the order of 10^6 – 10^7 is obtained for the highest ($\phi_2 = 2.0$ eV) and thickest ($d_2 = 1$ nm) extra barrier, and in all cases, the TER value is at its highest at small bias values. For large positive voltages, the TER decreases rapidly for all barrier configurations, whereas for large negative bias values, it reaches a more or less constant value. As could be expected, the largest changes in TER are obtained by increasing the thickness of the higher ($\phi_2 = 2.0$ eV) extra barrier [see Fig. 15(b)].

2. Extra barrier height

The effect of changing the extra barrier height was studied by comparing the J - V curves to the same single barrier structure as in Sec. III B 1 and varying the height of the extra barrier between $\phi_2 = 0 \dots 3.0$ eV. This large variation is motivated by our finding in Ref. 29 that a relatively large difference between ϕ_1 and ϕ_2 is required to reproduce experimentally observed asymmetries. The width of the extra barrier was kept constant, $d_2 = 0.5$ nm. The potential energy profiles and corresponding J - V curves are presented in Fig. 16.

As shown in Fig. 16(b), the steep rise in the current occurs approximately at the same bias voltage regardless of the extra barrier height and current values drop at all bias voltages. Overall, the change in the extra barrier height has a relatively small effect on the shape of the J - V curves. Comparing Figs. 13(b), 14(b), and 16(b), we can see that in case of the extra barrier, its width is what influences the J - V curves the most.

The TER as a function of bias for different barrier heights with $d_2 = 0.5$ nm is shown in Fig. 17. Comparing to Fig. 15, changing the extra barrier height has a much smaller effect on the TER than changing the extra barrier width. Qualitatively the TER as a function of bias voltage behaves similarly as when increasing the width of the barrier.

C. Series resistance

Series resistance in experiments can also affect the shape of the J - V curves and diminish the asymmetry related

FIG. 17. TER as a function of bias voltage for different extra barrier heights. The potential barrier profiles are shown in the inset. The low resistance (ON) state corresponds to the single potential barrier case (black dashed line) and the colors refer to the different extra barrier heights representing the different high resistance (OFF) states. The barrier potential parameters of the inset are as in Fig. 16(a).

to the tunnel junction structure. As an example, we have calculated the J - V curves of the two step-barrier structures shown in Fig. 18(c) with different extra barrier heights ϕ_2 . The corresponding J - V curves are plotted both without a series resistance, Fig. 18(a), and with a series resistance taken into account, Fig. 18(b).

In Fig. 18(a), the J - V curves are similarly asymmetrical with respect to the bias direction, as expected, since the

underlying potential energy profiles are qualitatively similar, i.e., step barriers. Assuming a junction area of $A = 5000 \mu\text{m}^2$ and a series resistance $R_s = 250 \Omega$, the J - V curve of the low resistance state, i.e., when $\phi_2 = 0.8 \text{ eV}$, shows, in contrast, almost no asymmetry [Fig. 18(b)]. Here the resistance at high bias voltages in the $\phi_2 = 0.8 \text{ eV}$ case becomes so low that the current is in practice limited by the series resistance and not by the tunnel junction. Simply looking at the J - V curves in Fig. 18(b) can therefore give a misleading idea of the changes in the underlying potential structure.

IV. CONCLUSIONS

We have made numerically accurate calculations for step potential energy barrier structures using the Tsu-Esaki formalism. The systems studied represent typical potential barrier profiles of experimental FTJ structures with a relatively low main barrier modeling the FE layer and an adjacent narrower but higher extra barrier. Naturally, our barrier profiles represent an idealized situation compared to experiments where the actual structures tend to be more complex. Still, our method allows analyzing prominent features and trends in the J - V characteristics.

Resonant tunneling through the notch states in the triangular QW that forms at the interface between the two barriers is predicted to produce NDR characteristics and ensuing asymmetry in the J - V curves. The most prominent characteristic, the steep increase in current density, is studied as a function of the barrier parameters. This asymmetry of the J - V curves can be tuned by adjusting the barrier heights and widths in the range of typical experimental values.

The barrier widths and the main barrier height affect the magnitude of the tunneling current the most. The extra

FIG. 18. J - V curves of two potential energy barrier structures with different high barriers ϕ_2 (a) without and (b) with taking a series resistance into account. (c) The two potential energy profiles at zero bias for the two values of $\phi_2 = 0.8 \text{ eV}$ and 3.5 eV . The barrier widths are $d_1 = 2 \text{ nm}$ and $d_2 = 1 \text{ nm}$, and for both structures $\phi_1 = 0.2 \text{ eV}$. The series resistance used $R_s = 250 \Omega$ and the assumed area of the junction $A = 5000 \mu\text{m}^2$. The other parameters used are $T = 0 \text{ K}$, $E_F = 0.5 \text{ eV}$, and $m^* = m_e$.

barrier height has a much smaller effect on the absolute current values and also on the TER effect. The change in the extra barrier width affects strongest the asymmetry of the J - V curve. Changes in the TER ratio of the order of 10^2 can be obtained by increasing the thickness of the extra barrier by only 0.4 nm. Regardless of the height of the extra barrier, the change in the tilt of the main barrier is suggested to produce a significant TER of the order of 10^2 . This is due to the earlier onset of the steep rise in current in the case when the tilt descends toward the extra barrier interface. Finally, the effect of series resistance is shown to significantly decrease the asymmetry of the J - V curves in the low resistance state.

The J - V curves presented here give an overview of typical features that can be related to tunneling through step barriers. These results cannot be obtained with the standard methods usually applied for interpreting experimental I - V curves. Our method enables us to analyze the effects of various barrier parameters on the J - V curves providing a basis for interpreting existing and future experiments. In our previous article on single tilted barrier structures, we showed that, e.g., large asymmetries between different bias polarities suggest that a step barrier structure should be considered.³¹ The characteristics of the curves presented here can be used to further interpret experimental features and to design new barrier configurations with desired functionalities.

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