Ferroelectric Diode Modeling

Zirun Han

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1 Introduction

This document outlines the calculations used to model and simulate a ferroelectric diode (FeD) with an MIM (Metal-Insulator-Metal) architecture. The model additionally accounts for the effects of a non-switching dead layer resulting from epitaxial growth of the ferroelectric on a metal electrode as well as the effects of inserting an insulating dielectric layer in the stack.

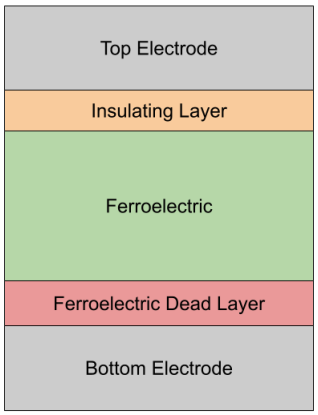

Figure 1: The FeD device architecture being modeled.

2 Variable Names and Abbreviations

$1, 2$	left and right electrodes
fe	ferroelectric layer
dl	dead layer
ox	oxide/insulator layer
d_i	thickness of layer i
λ_i	screening length of electrode i
$\bar{P}_i$	average polarization density of layer i
σ_s	screening charge density
ρ_0	free electron density

3 Potential Profile Calculations

The potential profile in this model is a superposition of two components, V_p, the electrostatic potential, and V_b, the barrier potential. The total potential is then calculated as $V_{total} = V_p + V_b$

3.1 Electrostatic Potential

The polarization of the ferroelectric layer induces surface charges that generate a depolarization field. Taking surface charge density on the ferroelectric layer i to be equal to the average polarization density $\bar{P}_i$, the depolarization fields are given by

$$\begin{aligned} \vec{E}_{p,fe} &= \frac{\sigma_s - \bar{P}_{fe}}{\kappa_{fe}\epsilon_0} \\ \vec{E}_{p,dl} &= \frac{\sigma_s - \bar{P}_{dl}}{\kappa_{dl}\epsilon_0} \\ \vec{E}_{p,ox} &= \frac{\sigma_s}{\kappa_{ox}\epsilon_0} \end{aligned} \tag{1}$$

by applications of Gauss's Law. Here, we note that the electric fields can point in different directions, resulting in an asymmetric potential profile depending on the direction of polarization. This is therefore a major contributor to the large change in electroresistance of the device in the on/off states. The screening charge density σ_s can be approximated from a Thomas-Fermi-type model[24].

Based on first-principles calculations, we make the approximation that the screening charge density $\sigma(x)$ of a metal in the presence of an external electric field takes the form[1]

$$\sigma(x) = \sigma_{max} \exp\left(-\frac{x}{\lambda}\right) \tag{2}$$

We can apply charge conservation and state that the total screening charge density in both electrodes should be equal: $\sigma_s = \sigma_{max_1}\lambda_1 = \sigma_{max_2}\lambda_2$ Integration yields that the electric potential $\phi(x)$ in the two electrodes should then be

$$\begin{aligned} \phi(x) &= \frac{\sigma_s\lambda_1 e^{-\frac{|x|}{\lambda_1}}}{\kappa_1\epsilon_0} - V_{ext} \quad x < 0 \\ \phi(x) &= -\frac{\sigma_s\lambda_2 e^{-\frac{|x-L|}{\lambda_2}}}{\kappa_2\epsilon_0} \qquad x > L \end{aligned} \tag{3}$$

To find σ_s, we combine equations 2 and 4:

$$\phi(0) - \phi(L) = \frac{\sigma_s\lambda_1}{\kappa_1\epsilon_0} + \frac{\sigma_s\lambda_2}{\kappa_2\epsilon_0} = \frac{\bar{P}_{fe} - \sigma_s}{\kappa_{fe}\epsilon_0}d_{fe} + \frac{\bar{P}_{dl} - \sigma_s}{\kappa_{dl}\epsilon_0}d_{dl} - \frac{\sigma_s}{\kappa_{ox}\epsilon_0}d_{ox} - \epsilon_0 V_{ext}$$

yielding

$$\sigma_s = \frac{\frac{\bar{P}_{dl}d_{dl}}{\kappa_{dl}} + \frac{\bar{P}_{fe}d_{fe}}{\kappa_{fe}} + \epsilon_0 V_{ext}}{\frac{\lambda_1}{\kappa_1} + \frac{\lambda_2}{\kappa_2} + \frac{d_{dl}}{\kappa_{dl}} + \frac{d_{fe}}{\kappa_{fe}} + \frac{d_{ox}}{\kappa_{ox}}} \tag{4}$$

Using the Thomas-Fermi model, we write the induced charge density per unit area as

$$\sigma(x) = \rho_0\left[1 - \frac{e^2\phi_{ext}(x)}{\epsilon_0 E_F}\right]^{\frac{3}{2}} - \rho_0 \approx -e^2\rho_0\frac{3\phi_{ext}(x)}{2E_F} \tag{5}$$

From here, we can substitute $\phi(0)$ for $\phi_{ext}(0)$ from equation 4 noting that no screening has occurred at that point and obtain that

$$\lambda_i^2 = \kappa_i\frac{2\epsilon_0 E_{F_i}}{3e^2\rho_{0_i}} = \kappa_i l_{TF}^2 \tag{6}$$

where l_{TF} is defined as the screening length in Thomas-Fermi theory.

3.2 Barrier Potential

This model calculates the effective barrier potential based on the metal work functions Φ_i and electron affinities χ_i and is given as follows for electrons at the Fermi level:

$$\begin{aligned} V_{b,fe} = V_{b,dl} \quad &= \Phi_1 - \chi_{fe} \\ V_{b,ox} \qquad\quad &= \Phi_2 - \chi_{ox} \end{aligned} \tag{7}$$

4 Calculating Tunneling Current

4.1 Tunneling Probability[3]

The tunneling probability $T(E)$ is set up to be calculated numerically from the Time-Independent Schrödinger Equation $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$. The potential profile ϕ can be divided into three segments, with ϕ_1 and ϕ_3 being constant, and ϕ_2 encompassing the non-constant tunneling barrier. The solution to the wavefunction of a right-traveling electron plane wave in regions 1 and 3 are

$$\begin{aligned} \psi_1(x) &= Ae^{ik_1x} + Be^{-ik_1x} \quad & k_1 &= \sqrt{\frac{2m_{\text{eff}}E_x}{\hbar^2}} \\ \psi_3(x) &= Ce^{ik_3x} & k_3 &= \sqrt{\frac{2m_{\text{eff}}(E_x - \Delta E)}{\hbar^2}} \end{aligned} \tag{8}$$

Setting the amplitude of transmitted wave C arbitrarily to 1, the tunneling probability is given by the expression

$$T(E_x) = \frac{k_3}{k_1}\left|\frac{C}{A}\right|^2 = \frac{k_3}{k_1}\left|\frac{1}{A}\right|^2 \tag{9}$$

To determine A, we apply the boundary conditions at the two interfaces and numerically integrate the ODE through region 2. The boundary conditions are

$$\begin{aligned} \psi(0) &= A + B \\ \psi'(0) &= ik_1(A - B) \\ \psi(L) &= Ce^{ik_3L} \\ \psi'(L) &= ik_3Ce^{ik_3L} \end{aligned} \tag{10}$$

Combining equations 7 and 8 yields an expanded expression for the tunneling probability

$$T(E_x) = \frac{k_3}{k_1}\left|\frac{2}{\psi(0) - i\psi'(0)/k_1}\right|^2 \tag{11}$$

4.2 Tunneling Current[5]

The forward tunneling current is given by $J_f = e \cdot n \cdot v_x$ where e is the elementary charge, n is the number density of tunneling electrons, and v_x is the drift velocity in the x direction. rewriting the equation in velocity space:

$$J_f = e\int_{\mathbf{v}} nv_x d\mathbf{v} \tag{12}$$

where the differential $d\mathbf{v} = dv_xdv_ydv_z$.

The number density of tunneling electrons n is equal to the density of states times the probability of successful tunneling. Making the assumption that the number of electrons that can occupy a unit volume of phase space $dxdydzdp_xdp_ydp_z$ is $\frac{2}{h^3}$ (factor of 2 due to spin degeneracy), the number of states in velocity space per unit volume is then $\frac{2m^3}{h^3}$. We multiply this by a Fermi factor based on the Fermi-Dirac distribution $f(E) = \left[1 + exp\left(\frac{E-E_F}{k_bT}\right)\right]^{-1}$ and obtain that the number density of electrons in electrode 1 is $\frac{2m^3}{h^3}f_1(E)$.

We now consider the probability of successful tunneling. In the previous section, the tunneling probability T is given as a function of electron energy in the forward direction E_x. We now additionally attach the probability of electrode 2 accepting the tunneling electron and write

$$\begin{aligned} P_{success} &= T(E_x)(1 - f_2(E + \Delta E)) \\ \Delta E &= E_{F,1} - E_{F,2} - eV \end{aligned} \tag{13}$$

where $1 - f_2(E + \Delta E)$ is the probability the energy state E of the tunneling electron is vacant in electrode 2. If it is not vacant, the tunneling cannot take place due to a phenomenon known as Pauli Blocking.

Note that the energy is shifted by ΔE in electrode 2 due to the applied voltage.

We finally note that $f_2(E + \Delta E) = f_1(E + eV)$ and write the number density of tunneling electrons as

$$n = \frac{2m^3}{h^3} T(E_x) f_1(E)(1 - f_1(E + eV)) \tag{14}$$

and

$$J_f = \frac{2m^3 e}{h^3} \int_{\mathbf{v}} T(E_x) f_1(E)(1 - f_1(E + eV)) v_x d\mathbf{v} \tag{15}$$

Applying the substitution $dE_x/m = v_x dv_x$ and converting the other two velocity components to polar form $dv_y dv_z = v_r dv_r d\theta = dE_r/m d\theta$,

$$J_f = \frac{2me}{h^3} \int_E T(E_x) f_1(E)(1 - f_1(E + eV)) dE_x dE_r d\theta \tag{16}$$

Integrating out θ and gathering terms results in

$$J_f = \frac{4\pi me}{h^3} \int_{E_{min}}^{\infty} T(E_x) dE_x \int_0^{\infty} f_1(E)(1 - f_1(E + eV)) dE_r \tag{17}$$

Taking into account that reverse tunneling could also occur, we calculate the reverse current density J_r using the same steps:

$$J_r = \frac{4\pi me}{h^3} \int_{E_{min}}^{\infty} T(E_x) dE_x \int_0^{\infty} f_1(E + eV)(1 - f_1(E)) dE_r \tag{18}$$

Setting overall current density $J = J_f + J_r$, we combine terms and integrate:

$$\begin{aligned} J &= \frac{4\pi me}{h^3} \int_{E_{min}}^{\infty} T(E_x) dE_x \int_0^{\infty} f_1(E) - f_1(E + eV) dE_r \\ &= \frac{4\pi me}{h^3} \int_{E_{min}}^{\infty} T(E_x) N(E_x) dE_x \end{aligned} \tag{19}$$

where

$$N(E_x) = kT ln \left[\frac{1 + exp\left(-\frac{E_x - E_{F,1}}{kT}\right)}{1 + exp\left(-\frac{E_x + eV - E_{F,1}}{kT}\right)} \right] \tag{20}$$

and $E_{min} = \max(0, \Delta E)$ as 0 is the minimum energy in electrode 1, and ΔE in electrode 2. Any wavefunction with lower energy will exponentially decay in these regions.

We note that the symmetric Pauli Blocking cancels each other. We can see that in this model, at low temperatures where almost all energy states are below the barrier height, Fowler-Nordheim tunneling is the dominant conduction mechanism. at high temperatures when the number density of states $N(E_x)$ larger than the barrier height is non-trivial, thermionic emission is taken into account.

5 Appendix: Numerical Integration of the Schrödinger Equation

An 8th order Runge-Kutta Method is used to numerically integrate the Schrödinger Equation across the potential barrier. To do this, it is necessary to set up the second-order equation as a system of coupled first-order ODEs as follows.

$$\frac{d}{dx}\begin{bmatrix}\psi\\ \dot{\psi}\end{bmatrix} = \begin{bmatrix}0 & 1\\ -\frac{2m}{\hbar^2}(E_x - V) & 0\end{bmatrix}\begin{bmatrix}\psi\\ \dot{\psi}\end{bmatrix} \tag{21}$$

A challenge in doing this is that the constants in the equation, e.g. m_e and $\hbar$ are small, leading to insufficient resolution using floating point numbers in Python. We then convert all calculations to atomic (Hartree) units, with $m_e = \hbar = e = a_0 = 1$. It is then possible to integrate the equation using a numerical solver, e.g. (solve_ivp in Scipy) with good precision.

References

[1] Charles T Black and Jeffrey J Welser. "Electric-field penetration into metals: consequences for high-dielectric-constant capacitors". In: *IEEE Transactions on Electron Devices* 46.4 (1999), pp. 776–780.

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