Supporting Information

for *ACS Appl. Electron. Mater.*

DOI:

Tunnel electroresistance in $Hf_{0.5}Zr_{0.5}O_2$-based ferroelectric tunnel junctions under hysteresis: approach of the point-like contact model and linearized Thomas-Fermi screening

Artur Useinov*, Deepali Jagga, Edward Y. Chang

International College of Semiconductor Technology, National Yang Ming Chiao Tung University, Hsinchu 30010, Taiwan.

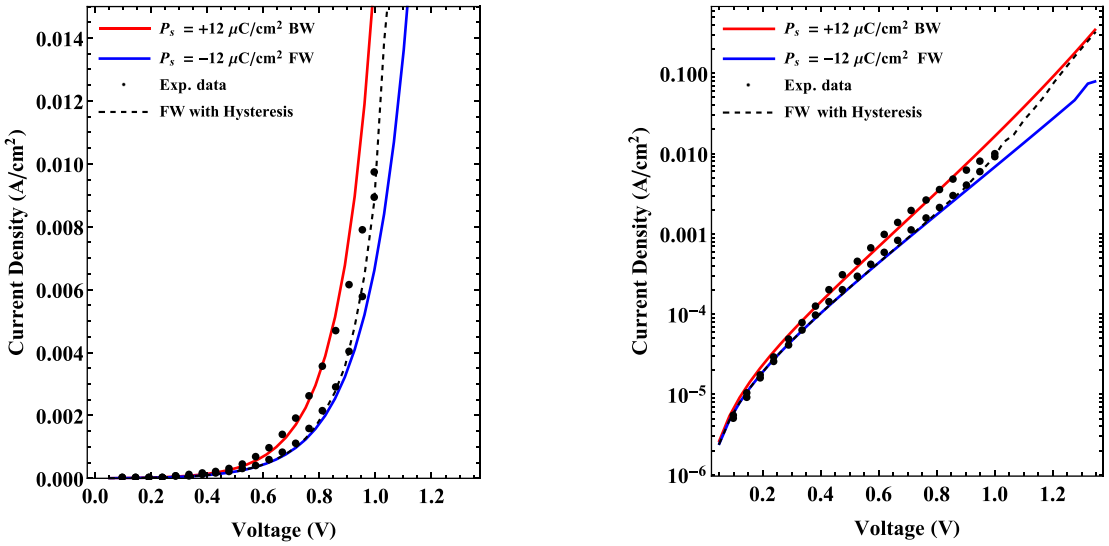
*Email: arthur.useinov@gmail.com

KEYWORDS: *Tunnel electroresistance, ferroelectric tunnel junction, hysteresis, I-V simulation, point-like contact model, monodomain (multidomain) ferroelectric barrier, linearized Thomas-Fermi screening, metal/ferroelectric interface, FeRAM*

Quantum transmission coefficient (transmittance) of the ferroelectric tunnel junction (FTJ) is found on the bases of transfer matrix technique. An example for the rectangular barrier with a brief description is shown in the file ExampleOfTransferMatrixApplication.pdf, which is accessible also as a program and developed in Wolfram Mathematica 11.3: ExampleOfTransferMatrixApplication.nb.

An example of the program for the Sample 1 (S1) is saved in CodeAndDataForSample1 folder. This folder includes input and output files, pdf and CodeSample1.nb code. Program consists from different modulus: *e.g.* wave functions can be found according “(Appendix II - WAVEFUNCTIONS) How Wave Functions were derived”, it is used for a finding the transfer matrix and related probability amplitude; Modulus “(Run first) Transmittance I (Airy-fun. based solution from section "WAVEFUNCTIONS")” constructs a transmittance from probability amplitude Q11. Module “3. Special (Run Set of initial parameters: 4nm symmetric) + POTENTIAL plotting” is responsible for an initial input, *etc.* Before the program launch, please copy “4nm.txt” as input file into the local disk folder Documents. See also output files in Documents after program execution.

CodeSample1.nb generates the following result:



SI Figure 1: FTJ forward (FW) and backward (BW) J-V curves at linear (left) and log scales (right) for S1.

It should be noticed that mistakes of the Airy-function integration are possible to obtain in the cases when one of the sections of the potential profile is flat (*e.g.* at some finite V the potential energy of the screening region can be flat). To avoid these mistakes the voltage step ΔV can be changed, or transmittance can be calculated only for this voltage point separately. At most cases of the problematic integration, the program makes data reconstruction/improvement automatically, like this:

```
Tab1c = Table[{Tab2pos[[i, 1]],
  If[NumberQ[Tab1b[[i, 2]]] == False,
   Tab1b[[i, 2]] =
    N[Tab2pos[[i,
      2]]*(2.0*Tab1b[[i - 1, 2]]/Tab2pos[[i - 1, 2]] -
       Tab1b[[i - 2, 2]]/Tab2pos[[i - 2, 2]])], Tab1b[[i, 2]]]}, {i,1, Length[Tab2pos]}]
```

To avoid similar problems for the 4th section with FE barrier an exponent wave function solution is also involved into consideration for current density simulation.

Hysteresis-based *J-V* behavior can be calculated by two equivalent ways:

A) Tab3:= Table[{eVa, CurrentDensityJ[E1p, k1, k7, eVshift + eVa, Ubp, Lp, Slp,

Slrp, PpVFuncNegtoPosR[-Pp, eVa], U3p]}, {eVa, Vmin, Vmax, ndeltaV}]; *where*

PpVFuncNegtoPosR[P_, eV_] :=

P*Tanh[Slope*(eV - Shift)] + (1 - Abs[Tanh[Slope*(eV - Shift)]])*P*

RandomReal[{-RandomnessIs, RandomnessIs}]; (*Eq.*(10) *of the main manuscript*)

B) Tab3 = Table[{Tab1[[i,1]], (Tab1[[i, 2]]*(1 - PpVFuncNegtoPosR[1, Tab1[[i, 1]]]) +

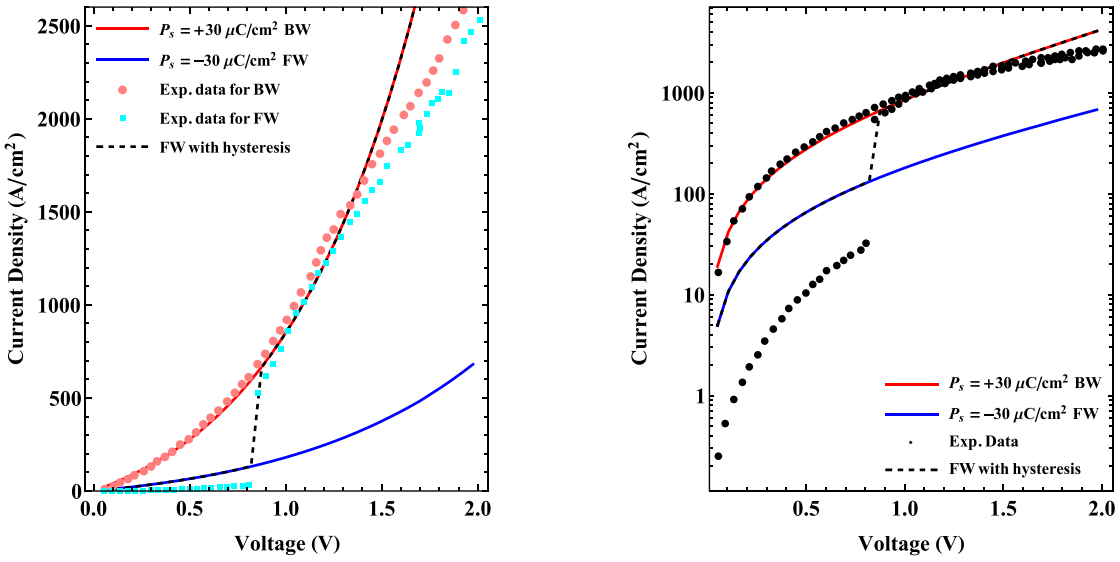
Tab2[[i, 2]]*(1 + PpVFuncNegtoPosR[1, Tab1[[i, 1]]]))/2.0 }, {i,1, Length[Tab1]}]

In terms of speed and minimization of integration mistakes the way **B** was used as a preferred one.

Using this program, it is also possible to reproduce results for S2 and S3 substituting parameters from Table 1, taking input parameters from "Initial experimental data from VLSI.zip".

The example of the program for Sample 4 (S4) CodeSample4.nb is saved inside CodeAndDataForSample4. Before the program launch, please copy "1nm_HZO_Alan1_fromLog.txt" and "1nm_HZO_Alan2_fromLog.txt" from InputData folder as input files into your local disk folder Documents. See also output files in Documents after the program execution by *Shift-Enter*.

Results for S4:



SI Figure 2: J-V curves in linear (left) and log scales (right) for the FTJ S4.