Supporting Information

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

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The goal of the Supporting Information is demonstrating additional results for J-V curves in S1-S3 with the same set of E_F , effective mases and U_B parameters (Fig. S1, Table S1); presentation of the technical detail for better results reproducibility.

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 as CodeAndDataForSample1.zip. Zip archive includes input and output files, pdf and CodeSample1S1.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 amplitudes; Modulus " (Run first) Transmittance I (Airy-fun. based solution from section "WAVEFUNCTIONS")" constructs a transmittance from probability amplitude Q11. Module "3. Initial parameters + 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.

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:

```
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.

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}];
```

that is Eq.(10) of the main manuscript. Other definitions of variables see in the Table S1, page S3 below.

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

Using the program CodeSample1S1.nb as a basic model, it is also possible to reproduce results for S2 and S3 substituting parameters from Table S1, 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.zip. 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 (execution command: Ctrl+All, Shift-Enter).

Table S1

Parameter in manuscript	**Definition in code**	**Sample 1**	**Sample 2**	**Sample 3**
d **- (λ_L + λ_R)**	Lp+delta1+delta2 (Å)	43.5 Å	33 Å	26.2 Å
$\lvert P_s \rvert$ ($\mu C/cm^2$)	Pp ($\mu C/cm^2$)	12.0	10.0	10.0
λ_L (nm)	Slp	0.16	0.06	0.21
λ_R (nm)	Slrp	0.16	0.12	0.06
λ_L/ λ_R	Slp/ Slrp	1.0	0.5	3.5
δ_1 (nm)	delta1	10^{-4}	10^{-4}	0.11
δ_2 (nm)	delta2	10^{-4}	10^{-4}	0.41
ϕ_1 (nm)	Fi1	2.5 10^{-5}	0.025	-0.025
ϕ_2 (nm)	Fi2	4.4 10^{-5}	0.025	-0.044
ΔV (V)	deltaV	0.035	0.075	0.035
V (V)	eVa	[Vmin, Vmax]	[Vmin, Vmax]	[Vmin, Vmax]
m_1/m_e	m1	0.8	0.8	0.8
m_2/m_e	m2	0.6	0.6	0.6
m_3/m_e	m3	0.4	0.4	0.4
m_4/m_e	m4	0.4	0.4	0.4
m_5/m_e	m5	0.4	0.4	0.4
m_6/m_e	m6	0.6	0.6	0.6
m_7/m_e	m7	0.8	0.8	0.8
E_F (eV)	E1p	2.5	2.5	2.5
U_B (eV)	Ubp	1.7	1.7	1.7
U_0 (eV)	U3p	0.0	0.0	-1.4
H_{SL}	Slope	4.8	9.8	2.8
V_c (V)	Shift	1.15	0.9	0.55
R_m	RandomnessIs (=RrM/2)	0.15	0.15	0.025

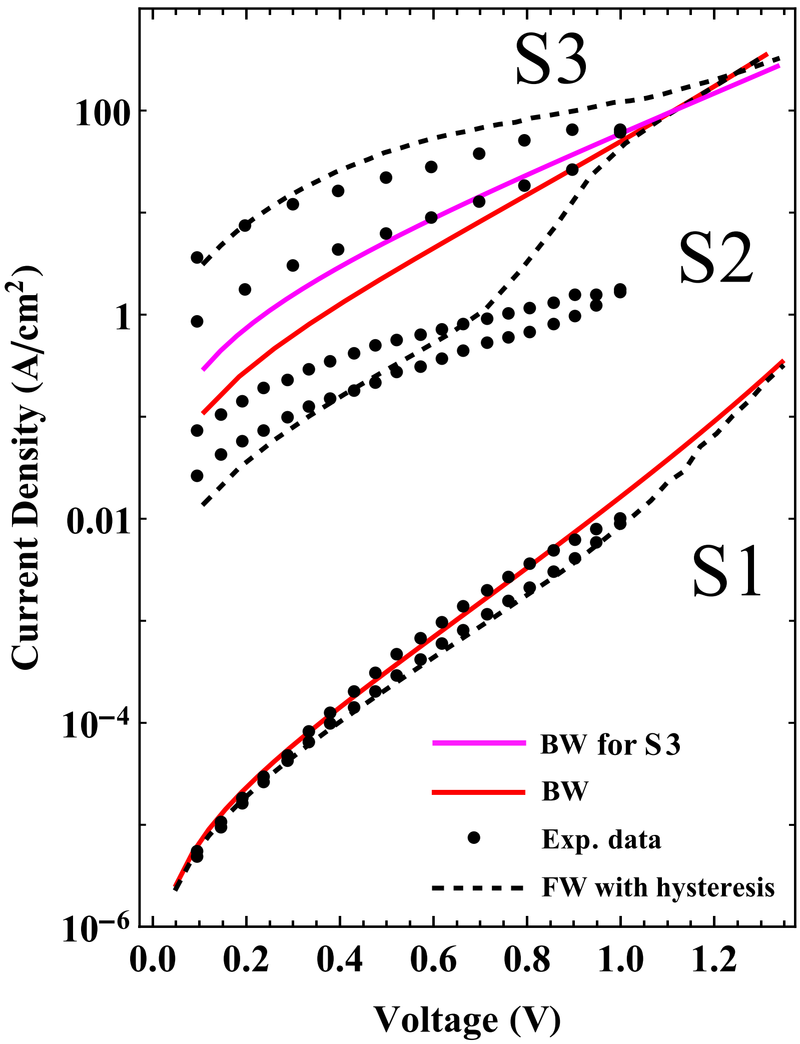

Figure S1: Representation of the J-V curves for samples S1, S2 and S3 with the same initial set of effective masses, following reference sample parameters according Table S1. This figure is build from JoinedCurvesS1S2S3.nb (JoinedResults.zip)