Quantum Transport Simulation on 2D Ferroelectric Tunnel Junctions

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Ferroelectric material has been recognized as an excellent candidate for the low-power non-volatile memories (NVM) due to its spontaneous polarization in the absence of an external bias. One of the NVM based on ferroelectric is ferroelectric tunnel junctions(FTJs) composed of insulating ferroelectric material sandwiched by metal plates. FTJs operate as resistive switching devices by modulating the tunneling potential barrier height. In this work, we consider a simple asymmetric structure of metal-ferroelectric-metal (MFM) FTJs with two different ferroelectric materials, Hf0.5Zr0.5O2(HZO) and CuInP2S6(CIPS), respectively. To investigate the performance of FTJs theoretically, we first explore complex band structures of HZO and CIPS with density functional theory (DFT) using Atomistic ToolKit(ATK) simulation[1]. Then, for the efficient device simulation using quantum transport, two bands k•p model[2] is established by fitting with DFT results as shown in Fig.1, 2. To calculate the transmission in FTJs, we develop the numerical quantum transport simulator based on Usuki's method[3] using a recursive scattering matrix. The potential profiles of MFM FTJs are self-consistently computed, as in Fig.3, 4, considering the Thomas-Fermi screening, P-V model for the ferroelectric polarization, and Poisson's equation. Calculating the transmission for a given potential profile, we can calculate the characteristics of FTJs operation. The barrier height modulation by polarization switching in ferroelectric leads to the different ON/OFF conductance and TER ratio. We investigate the dependency of TER ratio on the ferroelectric thickness and polarization and benchmark FTJs based on HZO and CIPS, as shown in Fig.5 and 6.

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References

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[2] Z. Dong et al., J. Appl. Phys. **123,** 094501 (2018).

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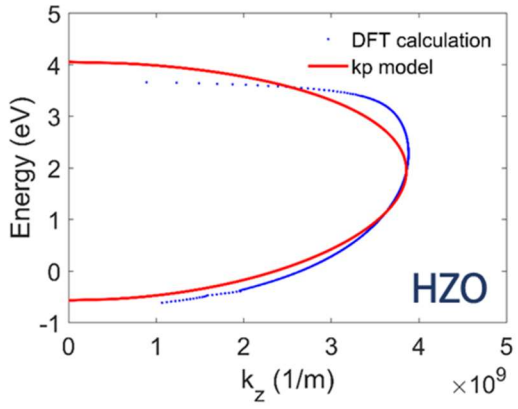

Fig.1: Fitting complex band structure of HZO

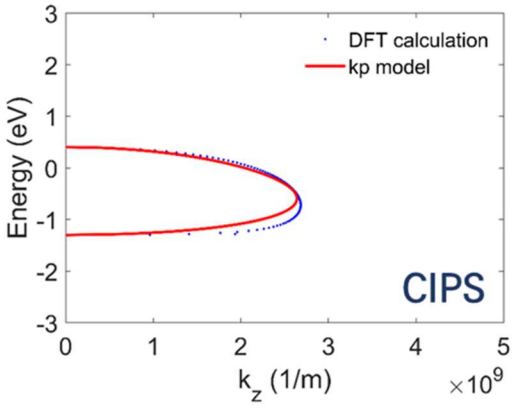

Fig.2: Fitting complex band structure of CIPS

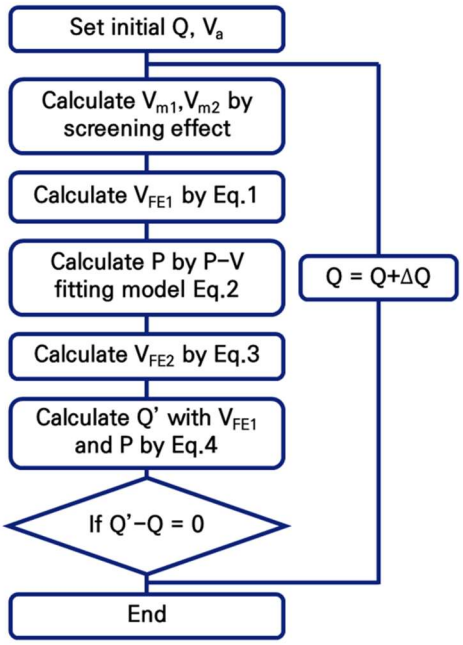

Fig.3: Self-consistent potential calculation workflow for MFM

- Thomas–Fermi screening

$$V_{m1} = -\frac{Q \cdot r_{m1}}{\varepsilon} e^{\frac{x}{r_{m1}}} \quad V_{m2} = \frac{Q \cdot r_{m2}}{\varepsilon} e^{-\frac{x}{r_{m2}}}$$

- Bias on FE by screening effect

$$V_{FE1} = V_{m1} - V_{m2} + V_a \quad \text{(Eq.1)}$$

- P–V fitting model

$$P(V) = P_s \tanh[w(V \pm V_c)]$$

$$W = \frac{1}{2V_c} ln \frac{P_s + P_r}{P_s - P_r} \quad \text{(Eq.2)}$$

- Poisson's equation

$$V_{FE2} = -\frac{(P-Q)t_{FE}}{\varepsilon_0 \cdot \varepsilon_{FE}} \quad \text{(Eq.3)}$$

- Surface charge on metal–FE surface

$$Q = P + \frac{V_{FE1} \varepsilon_0 \cdot \varepsilon_{FE}}{t_{FE}} \quad \text{(Eq.4)}$$

Fig.4: Underlying physical equations for FTJs

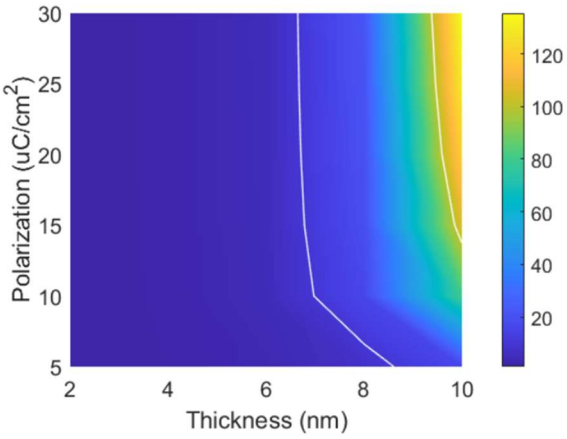

Fig.5: TER contour plot of HZO FTJ in log scale

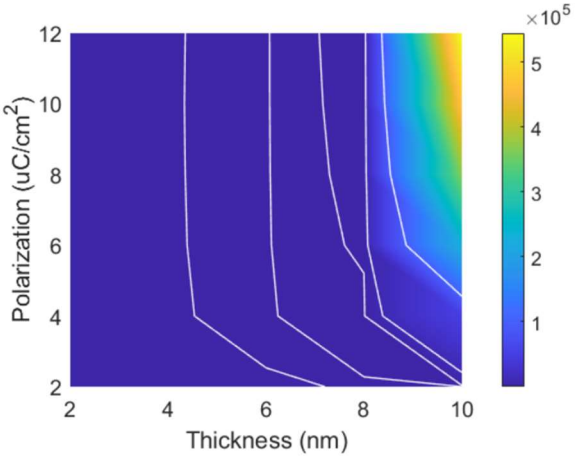

Fig.6: TER contour plot of CIPS FTJ in log scale