MODELING OF ELECTRON TRANSPORT THROUGH FERROELECTRIC TUNNEL JUNCTIONS

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Modeling of tunnel junctions in ferroelectric materials is an important tool for understanding their properties [1]. An adjacent barrier next to the ferroelectric layer often exists in experiments, introduced either on purpose or formed due to interfacial interactions. Along this line we have studied tunneling currents through single and step barrier structures using the Tsu-Esaki formalism with numerically solved transmission coefficients [2].

Using a step barrier model (Fig. 1(a)) we are able to reproduce the experimental I–V curves (Fig. 1(b)) of all-oxide LSMO/PZT/LSMO junctions exhibiting high-bias-induced resistive switching [3]. The height of the extra barrier, ϕ_2, is the only difference between the two resistance states. We discuss, based on our modeling, the atomic and electronic structures of the bilayer barrier in the low and high resistance states (LRS and HRS).
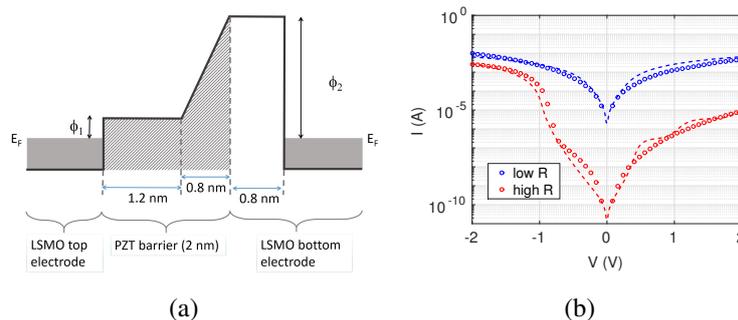

(a)   (b)

Figure 1: Model potential (a) and the corresponding I–V curves (b) (circles=experiment, line=calculated, LRS: ϕ_1=0.15 eV and ϕ_2=0.58 eV, HRS: ϕ_1=0.15 eV and ϕ_2=2.00 eV).

We have also studied how different parameters in a step barrier structure, *e.g.*, the widths of the barriers, affect the shape of the I–V curve. The aim of this study is to give insight for the design of tunnel junctions and to provide a useful computational tool for interpreting experimental results.

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[2] C. B. Duke, "Tunneling in Solids", *Sol. State Phys.* **10** (Suppl.), (New York, Academic Press, 1969).
[3] Q.H. Qin, L. Äkäslompolo, N. Tuomisto, L.D. Yao, S. Majumdar, J. Vijayakumar, A. Casiraghi, S. Inkinen, B.B. Chen, A. Zugarramurdi, M. Puska, and S. van Dijken, "Resistive switching in all-oxide ferroelectric tunnel junctions with ionic interfaces", *submitted for publication*.