ION TRANSPORT IN MEMRISTIC DOUBLE BARRIER DEVICES

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The memristive double barrier device is an ultra-thin four-layer system (Nb/Al/Al₂O₃/NbOₓ/Au). The memristive layer (NbOₓ) is sandwiched between a Schottky barrier and a tunneling barrier. It has been recently shown that such devices offer a number of potentially interesting features [1]. An intrinsic current compliance, improved retention, and no need for an initial electric forming procedure. The latter is particularly attractive for applications in highly dense random access memories and also neuromorphic mixed signal circuits.

**Analog Memristive Tunneling Device**

- Analog resistance change devices are of particular interest for its application in neuromorphic systems.
- One of such devices which allows continuous resistance change over a wide parameter range consists of an Al₂O₃ tunneling barrier, a NbOₓ solid state electrolyte and a Schottky barrier at the bottom Au electrode.
- An interesting feature of these devices is that the resistance change is due to a spatially homogenous resistive switching mechanism, rather than due to filamentary resistive switching.
- Inside the solid state electrolyte mobile oxygen and positively charged immobile defects are present.
- In the high resistance state the oxygen is randomly distributed, whereas in the low resistance state the oxygen is transported in front of the Schottky barrier.
- The goal of this work is a model which i) allows real-time simulation of the switching dynamics and ii) provides insight into the underlying physics, which are not accessible by experimental approaches.

**Kinetic Monte Carlo Approach**

- Since we are interested in the complete dynamics range of the device, rather than in the ultrafast dynamics of the switching phenomena itself, we have to cope with a serious time-scale problem.
- An atom performs a jump every 10⁻⁶ s, whereas the actual process takes only 10⁻⁵⁻⁻² s.
- An infrequent-event system is one in which the dynamics is characterized by occasional transitions from one state to another, with long periods of relative inactivity between these transitions.
- With respect to the rare jumps, the system thus performs nothing but a simple Markovian walk.

**Procedure of Potential and Current Calculation**

- The Coulomb potential within the device due to positively charged defects and negatively charged ions is based on of Poisson’s equation, \( \nabla \cdot (-\varepsilon \nabla \Phi) = -\rho(x) \).
- The boundary conditions at the top and bottom electrode are given by \( \Phi(x = 0) = \Phi(x = L) = 0 \).
- At all remaining boundaries, periodic boundary conditions are used. Within the solid state electrolyte and the tunneling barrier the permittivities are assumed to be constant, \( \varepsilon_{SS} = 42 \) and \( \varepsilon_{TB} = 9 \).
- Continuity equation is satisfied at all time. Therefore \( \nabla \cdot J = 0 \) can be used to iteratively match the current equations for the three distinct parts of the device:
  - Simmons equation for the tunneling barrier
  - Ohm’s law in the solid state electrolyte
  - Schottky current for the Schottky barrier
- From these current-voltage relations, we can obtain the voltage drops across the three distinct layer, and therefore the boundary conditions for the potential distribution within the solid state electrolyte and the tunneling barrier.

**Results**

So far a deeper physical understanding of the interplay between the current transport mechanism and inner atomic device structure is missing. In this contribution, we report on results of kinetic Monte-Carlo simulations of transport phenomena in these devices. We identify the ion drift of charged point defects within the NbOₓ layer as a key factor for the resistive switching behavior. We discuss the related current-voltage characteristics which is in excellent agreement with experimental data.

**Conclusion**

The main result of this work is that the influence of charges on the effective Schottky barrier height, given by \( \Phi_b = \Phi_{b0} + \Phi_d \), as well as adsorption mechanisms have to be taken into account. Here \( \Phi_{b0} \) and \( \Phi_d \) denote the equilibrium Schottky barrier height and the surface potential at the Au surface, respectively.

In our work, we allow for:
- surface states located at Au surface,
- adsorption of oxygen at Au surface, and
- resonant charge transfer with Bloch states of Au
in order to be able to find simulation results in excellent agreement with experimental data.


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