Multiscale Modeling of Memristor Devices for Novel Memory and Logic Architectures

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Outline

• Multiscale modeling platform
  – Physics

• Simulation results
  – HfO$_x$ RRAM for memories
  – RRAM devices for neuromorphic

• Conclusions
A multiscale modeling platform

• Connects atomic material properties to electrical device characteristics
• Focus on novel materials, charge and ion transport, and structural changes, consistently modeled in a friendly environment
• kMC description to account for variability and reliability
Ginestra™ Physics

- Novel devices (e.g. memories, neuromorphic computing) need to account for structural material changes, ion/vacancy migration, individual species contribution, ferroelectric effect, phase change, ...
Ginestra TAT charge transport models

- Mechanisms: DT and FN tunnel, D Poole-Frenkel, TE, hopping, Trap-Assisted Tunneling (TAT)
- Defects (oxygen vacancies) assist trap-assisted-tunneling (TAT)
- Electron-phonon coupling and lattice relaxation included

L. Vandelli et al., TED 58, 2011 - L. Larcher, TED 50, 2003
Power dissipation & temperature increase

- 3D power dissipation map calculated from the power released at every defects by TAT electrons and within the conduction/valence band
- 3D temperature map calculated by solving the heat Fourier equation with imposing appropriated boundary conditions

L. Vandelli et al., IMW 2011 - L. Vandelli et al., IEDM 2011 – L. Larcher et al., IEDM 2012
Stress-induced structural material changes

• Generation of vacancies (O) and interstitial ions (O, H, ..) due to atomic bond breakage induced by:
  – Temperature and field driven (thermochemical model)
  – Precursors and defect assisted defect generations
  – Electron injection and impact ionization
  – Material morphology (grain vs GBs)

L. Vandelli et al., TED 2013
Stress-induced structural material changes

- Phase changes, including ferroelectric
- Morphology: e.g. GBs and grains
- Diffusion of O ions and vacancies
  - depends on field, temperature, morphology, stoichiometry, cohesion/isolation forces
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RRAM modeling purposes

- Goal: connect material properties to the electrical device operations: from charge transport, to forming, switching and reliability
Preforming current simulations - HfO$_x$

- **TAT current** assisted by O vacancies on grains and (mostly) GBs - CAFM
- T & V dependence across large area MIM cap with different stoichiometry

![Diagram of TiN/Ti/5nm HfO$_x$/TiN](image)

- **HfO$_x$**
  - $N_T=7\cdot10^{20}\text{ cm}^{-3}$

- **HfO$_2$**
  - $N_T=1.2\cdot10^{19}\text{ cm}^{-3}$

O. Pirrotta et al., JAP 2013 – A. Padovani et al., EDL 2013
HfO$_x$ RRAM forming simulations

- Multiple grains and GB spots included: abrupt current increase due to a single spot that gets converted into the CF
- Forming involves breakage of Hf-O bonds, and out-diffusion of released O ions: dominant mechanism assisted by electron injection and preexisting vacancies

L. Vandelli et al., IEEE-IMW, 2011 - L. Larcher et. al., Journ. on Comp. El., 2013
Generation of O vacancies & ions in HfO$_2$

- Electron injection & preexisting O vacancies reduce the activation energy for defect creation in their proximity.

\[ \text{O}_{\text{vac}}^0 + \text{O}_{\text{int}}^{2-} \quad \text{Barrier} = 1.96 \text{ eV} \]

HfO$_x$ RRAM forming kinetics simulations

RVF (Ramped Voltage forming)

L. Vandelli et al., IEEE-IMW, 2011
HfO$_x$ RRAM forming simulations

- Accurate simulation of forming voltage $V_F$ and TDDB distributions
- Temperature and voltage dependences correctly reproduced

B. Butcher et al., A. Padovani et al., IMW 2012 - A. Kalatarian et. al., IRPS 2012
HfO$_x$ RRAM reset simulations

L. Vandelli et al., IEEE-IMW, 2011
LRS - HRS current distribution - HfO$_x$

- $I_{\text{LRS}}$ due to electron drift through O vacancy sub-band
- Lognormal $I_{\text{HRS}}$ distribution due to a $\sim$1-2nm barrier thickness depending on $V_{\text{reset}}$

F. Puglisi et al., ICICDT 2013 - L. Larcher et al., 2014, TED - G. Bersuker et al., JAP 2011
Current fluctuations: RTN

- Multi-level RTN signal decomposed into two-level signals through FHMM
- Relative current fluctuations higher in HRS compared to LRS
- RTN in HRS due to the activation/deactivation of defects supporting TAT

D. Veksler et al., IEDM 2012
F. Puglisi et al., ESSDERC 2012, IRPS 2014, IRPS2015
HRS RTN physical mechanisms

- Trap activation/deactivation due to 2 different mechanisms
  - Coulomb blockade due to trapping in adjacent slower traps (O ions)
  - Metastable states of O vacancies

F. Pugliese et al., IRPS 2015, TED 2015
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**HfOx RRAM under pulse switching regime**

- Pulse regime proposed for a more gradual change of CF/ interface properties for analog conductance modulation
- Forming simulations to determine initial O/Vo distributions

![Diagram](image)

- **I_{CC}=20uA**
- **V_{SET} = 0.8V**
- **V_{READ} = 25mV**
- **V_{SET} = -0.8V**

**Pulse SET sequence**
- Set pulse ~100ns

**Pulse RESET sequence**
- Read pulse ~1µs
Pulsed SET simulations in HfO$_x$ RRAM

- Simulations explain current trend vs pulse set voltage and time

EDL data – collaboration with Prof. Hwang’s group, Postech
Pulsed SET simulations in HfO$_x$ RRAM

- The first voltage pulse creates Vo-O pairs due to the high field: the most of the CF is reconstructed after the first pulse, explaining the abrupt current increase.
- Subsequent pulses do not affect significantly the CF.

Unpublished data – collaboration with Prof. Hwang’s group, Postech
Pulsed RESET simulations in HfO$_x$ RRAM

- Reset is much more gradual than set due to O ion diffusion
- The CF rupture/oxidation is controlled by the O ion supply – it more gradual compared to bond breakage (no field/temperature feedback)

![Graph showing current versus pulse number](image-url)
**AlO$_x$-HfO$_x$ RRAM for analog switching**

- AlO$_x$-HfO$_x$ stacks show a linear current increase with subsequent pulses, more suitable for neuromorphic devices.
- Field redistribution across two layers (one has to be very thin) allows for better control of O ion supply, enabling a more gradual modulation of CF conductance.

H. Hwang et al., EDL, 2016
Analog switching in TiO$_x$/TaO$_y$ RRAM

- Simulation of Ti/35nmTiO$_x$/2nmTaO$_y$/TiN RRAM shows that the quasi-linear resistance changes during potentiation and depression are due to the higher control on the O ion supply, i.e. diffusion into switching and/or O reservoir layers.
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• Dynamic simulation platform connecting material properties to electrical device performances essential to engineer novel memories and neuromorphic computing devices

• Same approach allows targeting selectors (OTS, tunneling barriers), ferroelectric memories, PCM, ...
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RRAM technology issues

- Selector for cross-bar and 3D integration
- Analog switching for neuromorphic
- Variability & RTN
- Full understanding missing
  - $V_{\text{RESET}} > V_{\text{SET}}$
  - O ion reservoir
  - High endurance