Ion-Induced Leakage Currents
III. Percolation Model

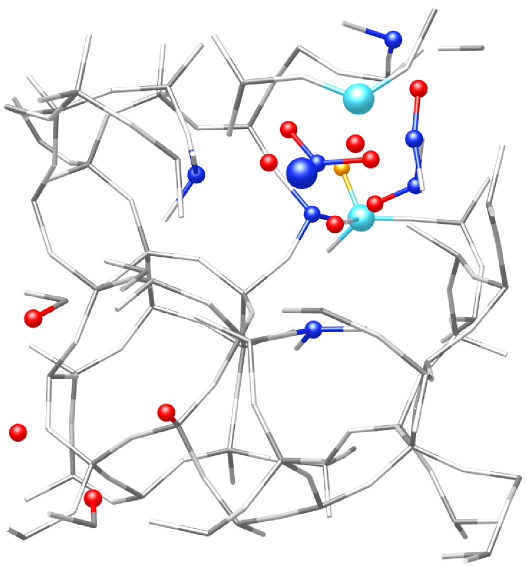
M. J. Beck[1,2], N. Sergueev[1], Y. S. Puzyrev[1],
K. Varga[1], R. D. Schrimpf[3], D. M. Fleetwood[3], S. T. Pantelides[1,3,4]

[1]Dept. of Physics & Astronomy, Vanderbilt University, Nashville, TN 37235
[2]Dept. of Chemical & Materials Engineering, University of Kentucky, Lexington, KY 40506
[3]Dept. of Electrical Engineering & Computer Science, Vanderbilt University, Nashville, TN 37235
[4]Oak Ridge National Laboratory, Oak Ridge, TN

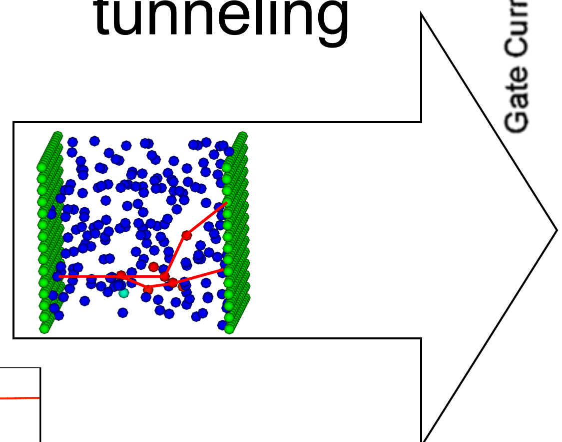
2009 MURI Review

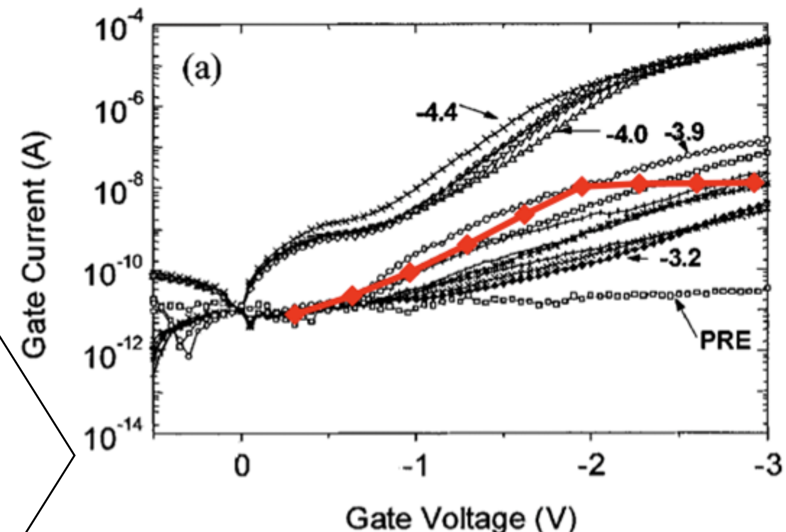
Multi-scale calculation

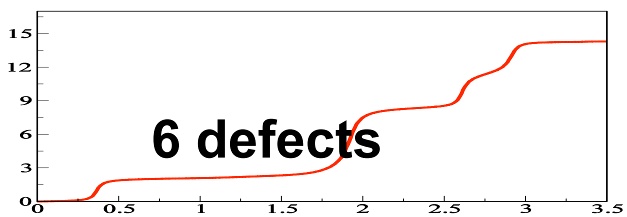
From QM transport to I-V device characteristics

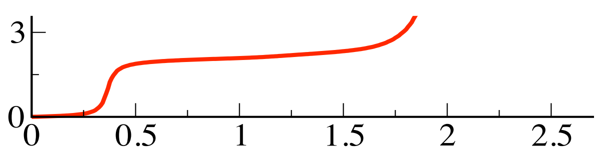


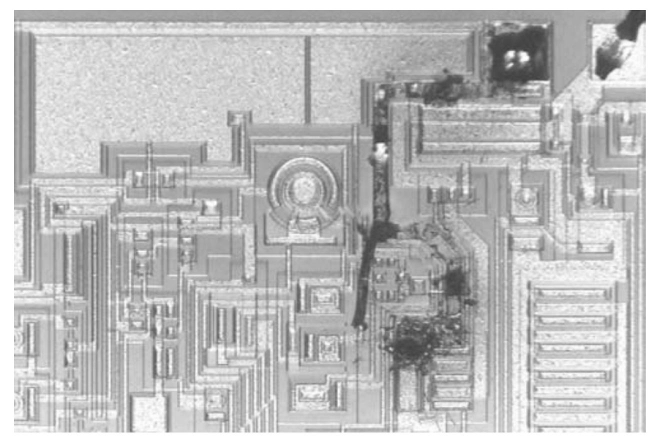
Mott's
defect-defect
tunneling







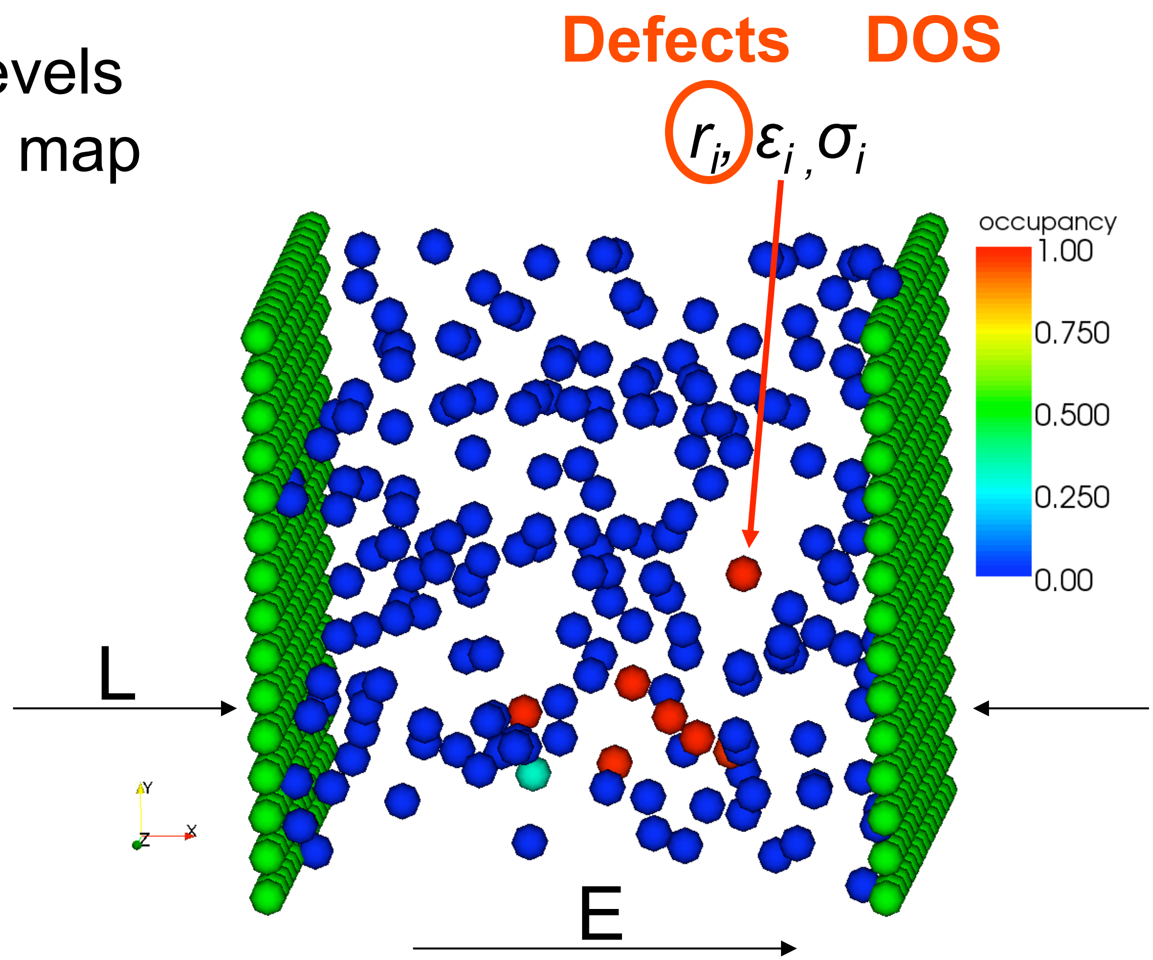


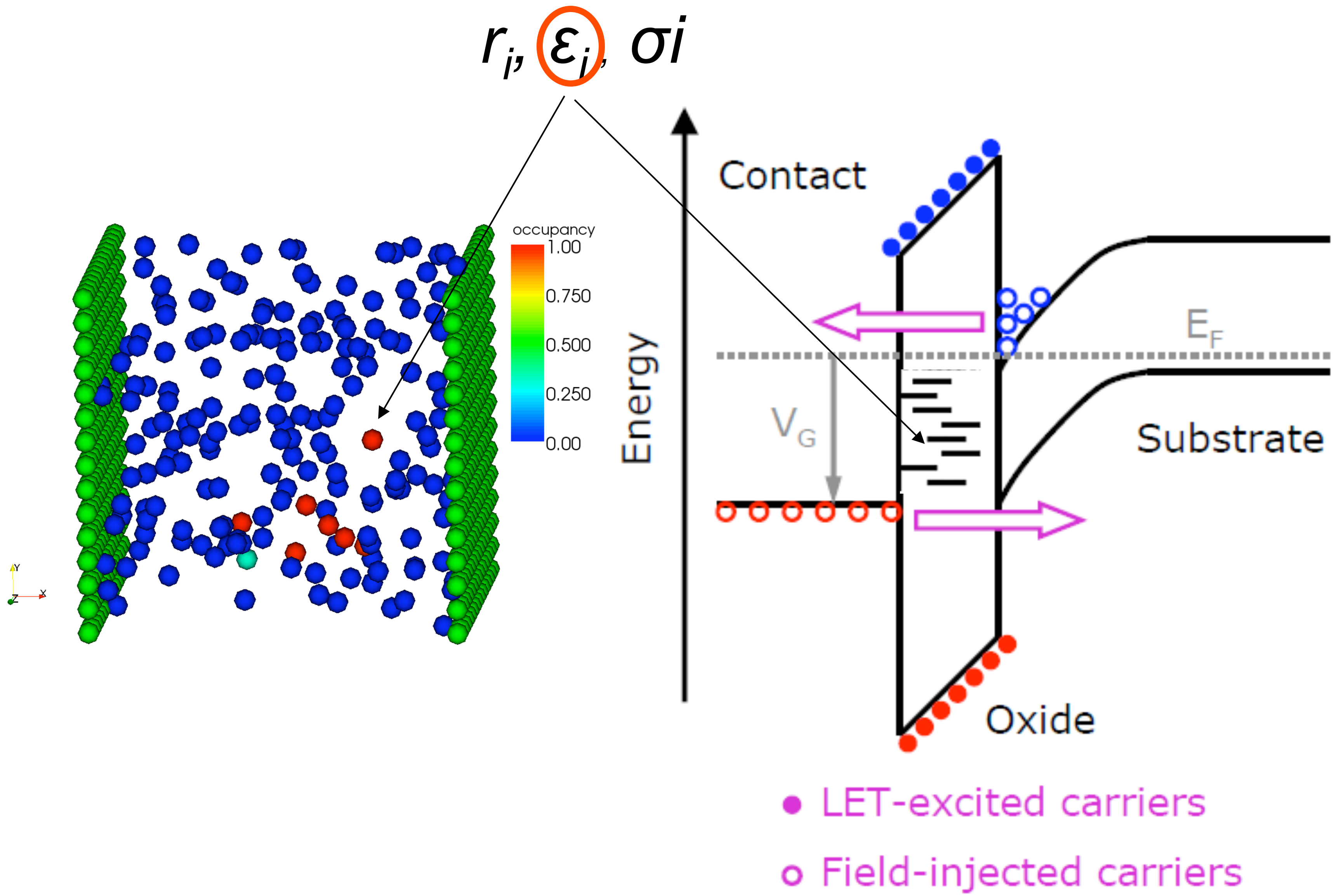


SEGR in SiO_2

- L =1.4 nm
- Defect energy levels
- Defect atomistic map

time = 78fs
22 defects





2009 MURI Annual review, Vanderbilt University, June 10 2009

Low-resistivity paths through oxide

$J = v_0 \Sigma_{ij} (\sigma_i^{boundary} - \sigma_j)$

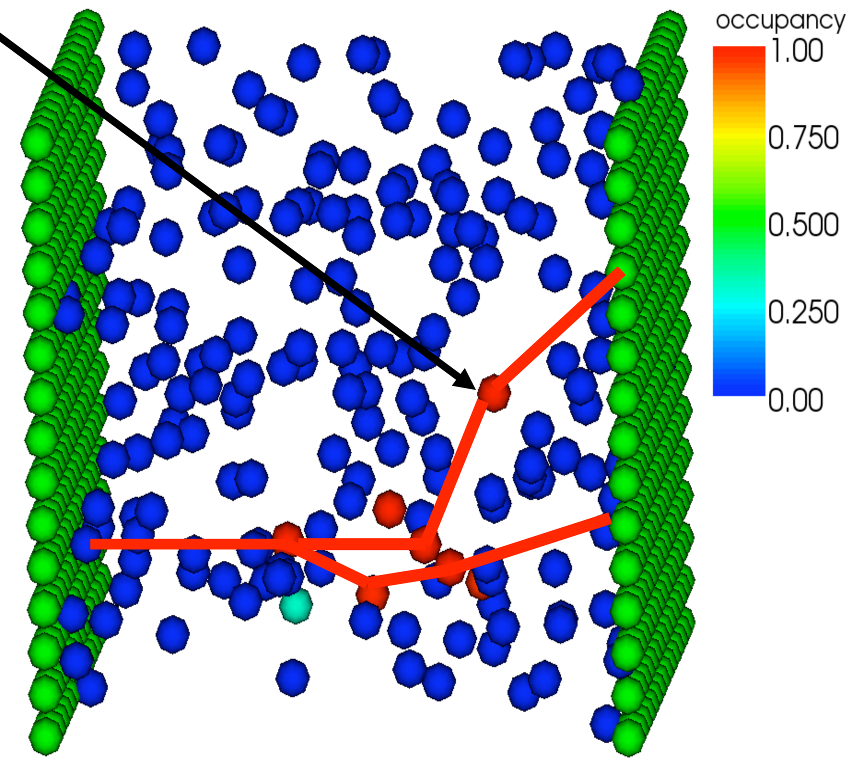
$v_0 = 1.15 \times 10^{13}\ s^{-1}$

Mott's defect-to-defect tunneling

$$\Delta\varepsilon_{i\to j} = \left(\varepsilon_j - \varepsilon_i\right) + qE\left[\hat{e}_x \cdot \left(\vec{r}_j - \vec{r}_i\right)\right]$$

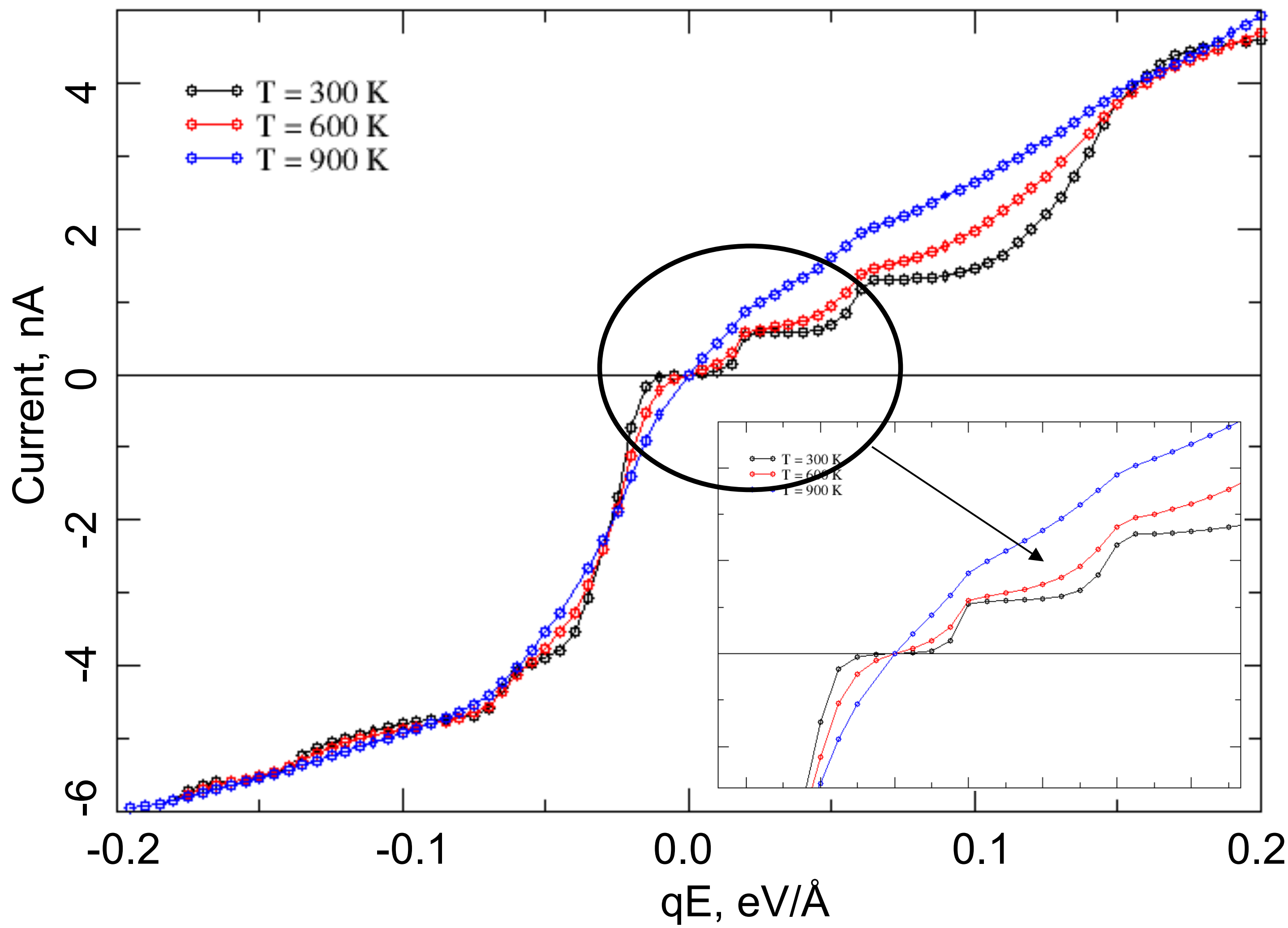
$$P_{i\to j} = \begin{cases} \exp\left(\dfrac{-\left|\vec{r}_j - \vec{r}_i\right|}{r_0}\right), & \Delta\varepsilon_{i\to j} \le 0 \\ \exp\left(\dfrac{-\left|\vec{r}_j - \vec{r}_i\right|}{r_0} + \dfrac{-\Delta\varepsilon_{i\to j}}{kT}\right), & \Delta\varepsilon_{i\to j} > 0 \end{cases}$$

$$\sigma_j^{s+1} = \sigma_j^s + \sum_i \left[\sigma_i^s\left(1-\sigma_j^s\right)P_{i\to j} - \sigma_j^s\left(1-\sigma_i^s\right)P_{j\to i}\right]$$



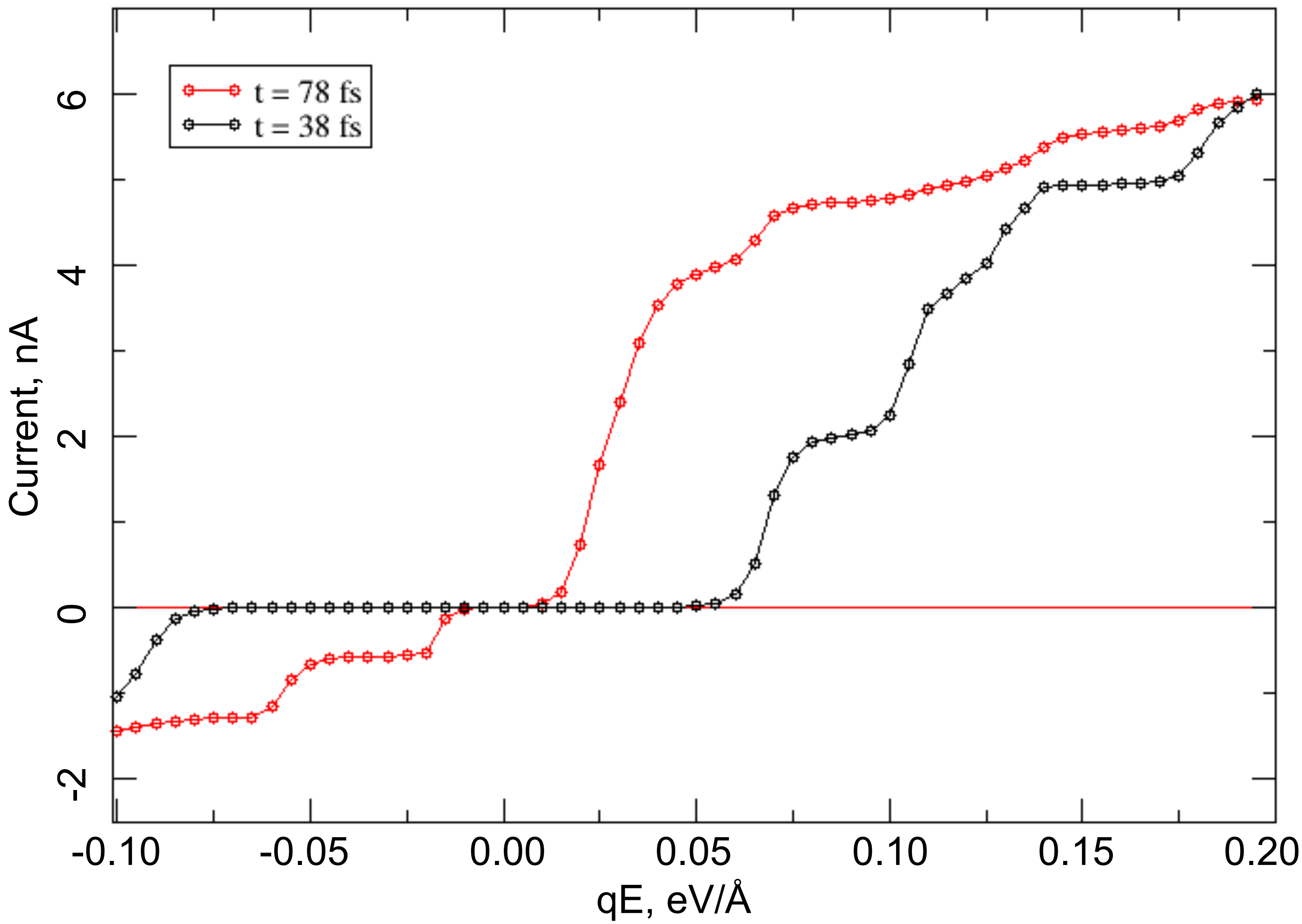
2009 MURI Annual review, Vanderbilt University, June 10 2009

Leakage Current Temperature Dependence

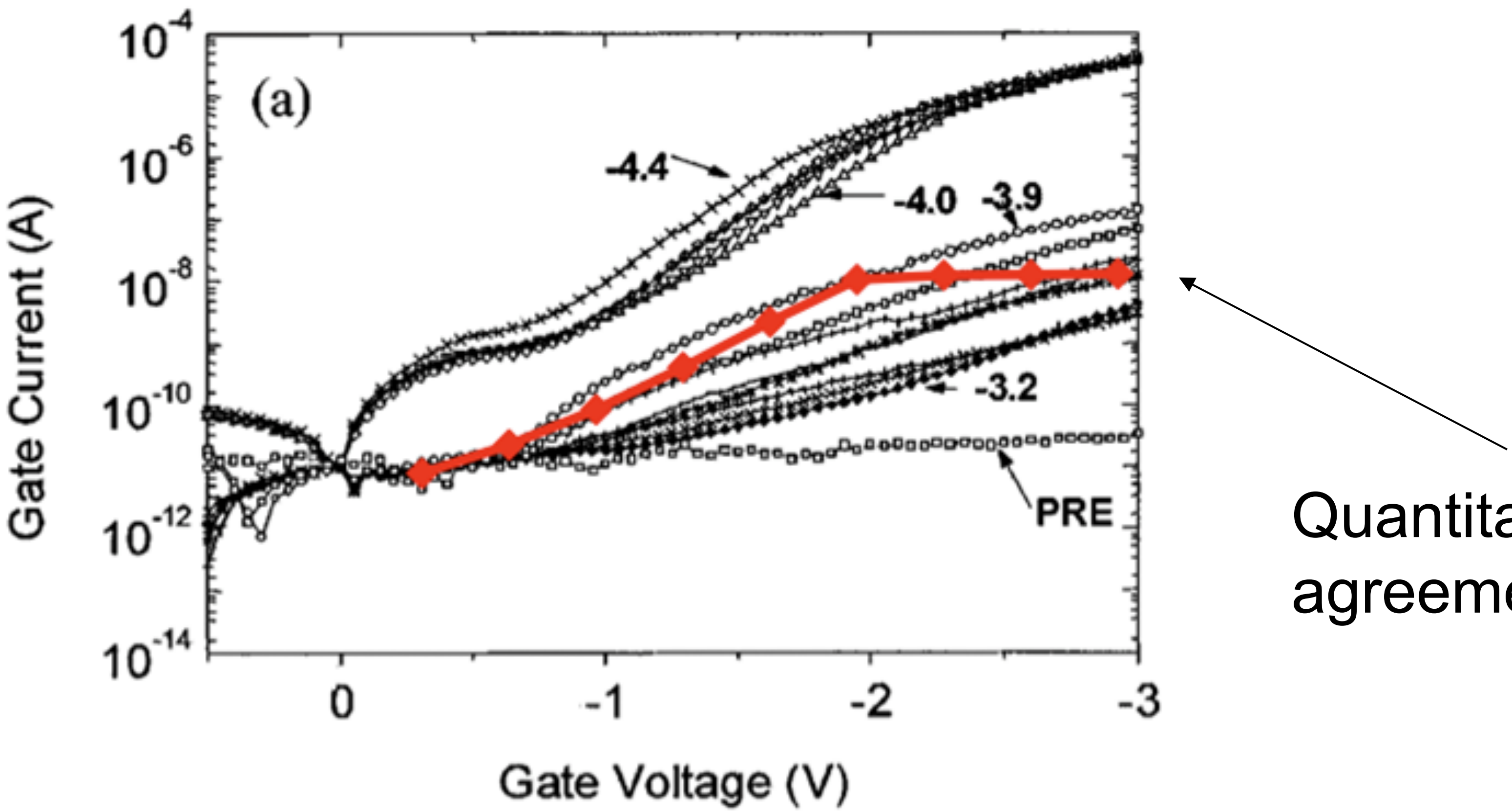


2009 MURI Annual review, Vanderbilt University, June 10 2009

Leakage Current Time Dependence



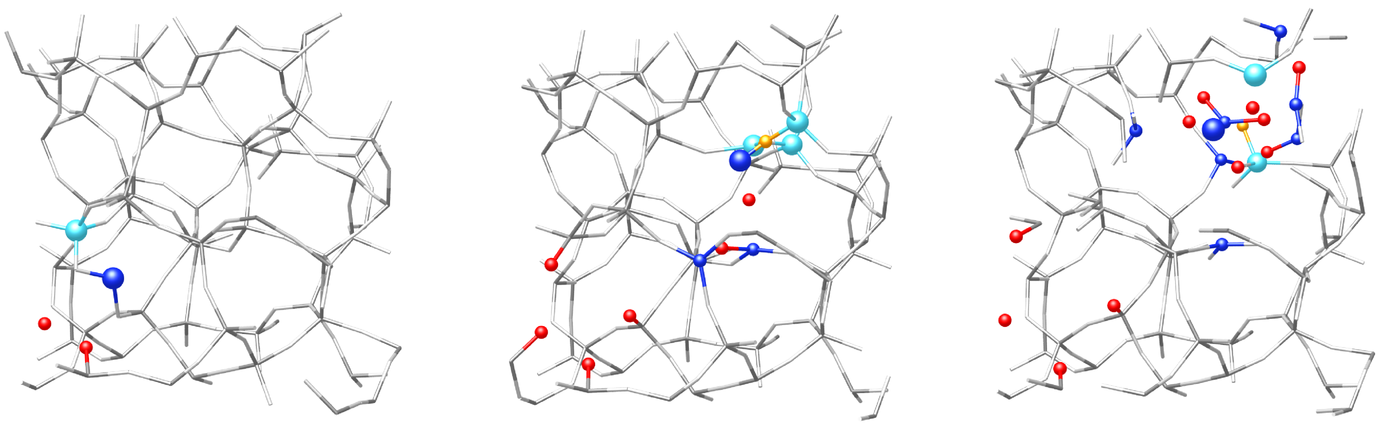
Direct comparison with experiment

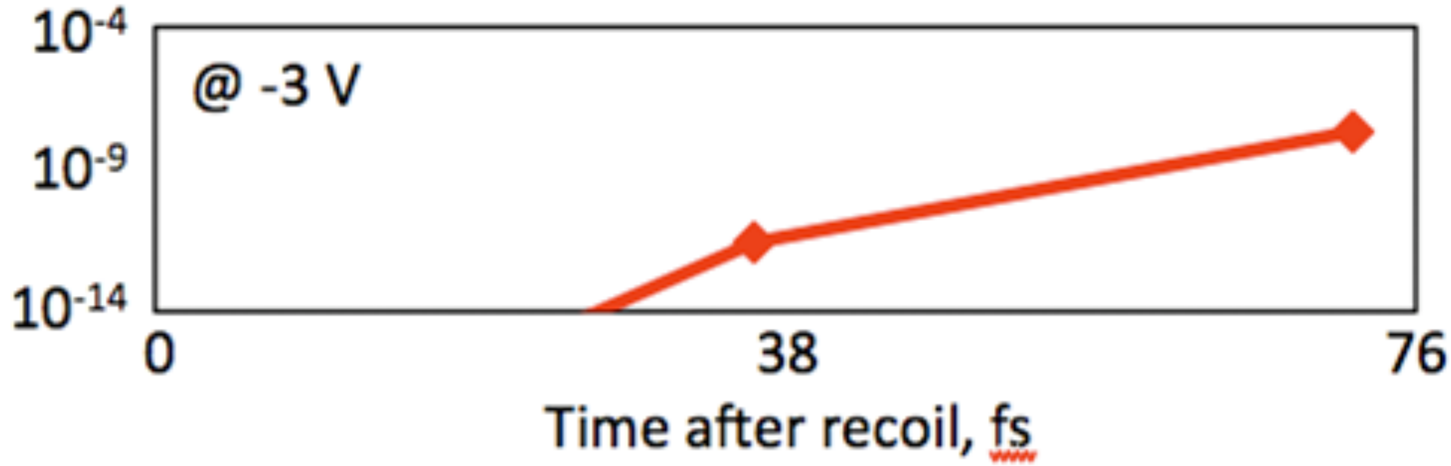


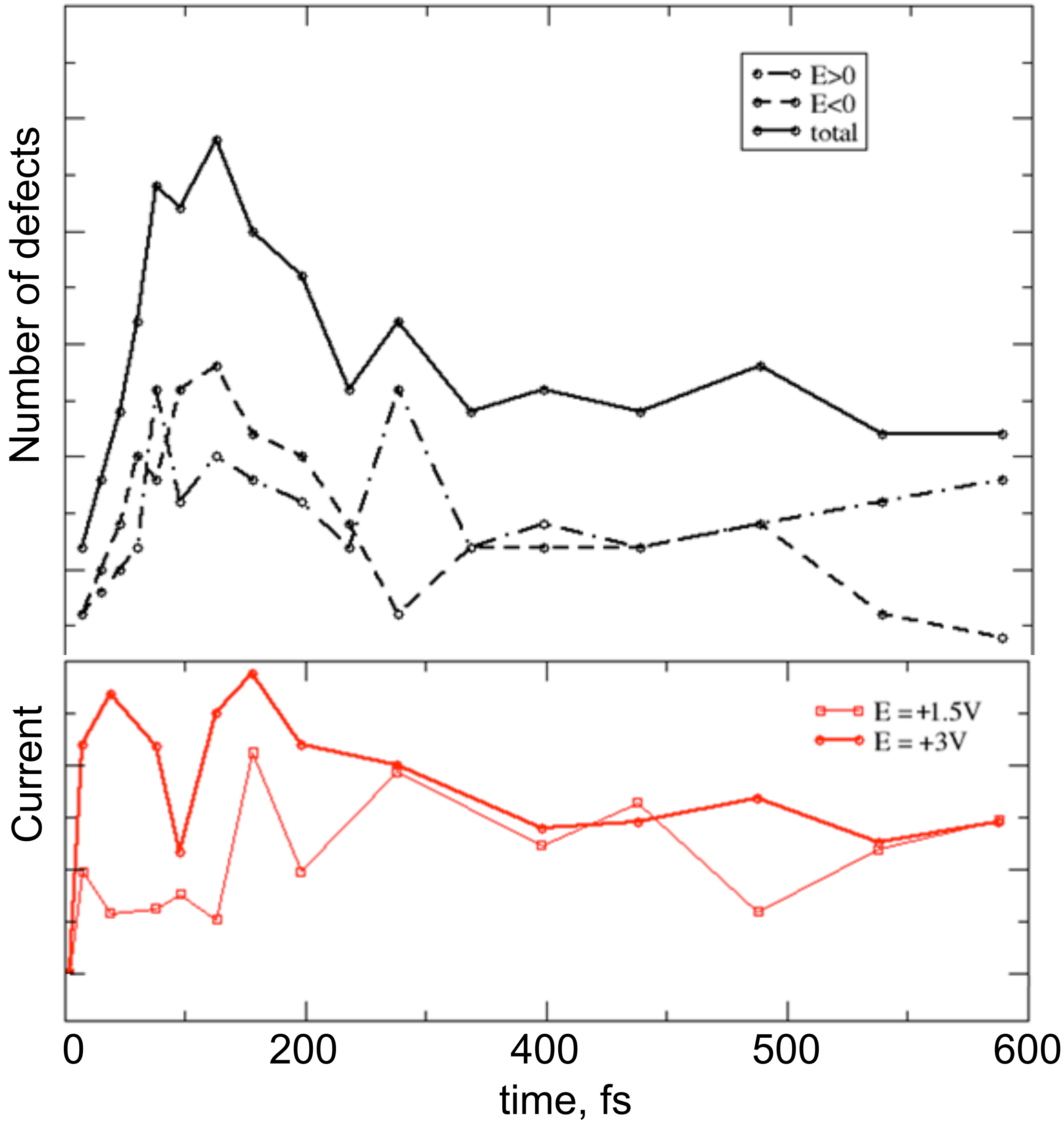
Quantitative agreement!

Massengill, et al., IEEE TNS 48 1904 (2001)

Model results in real-time defect evolution and transient currents







Defect time evolution

Energy

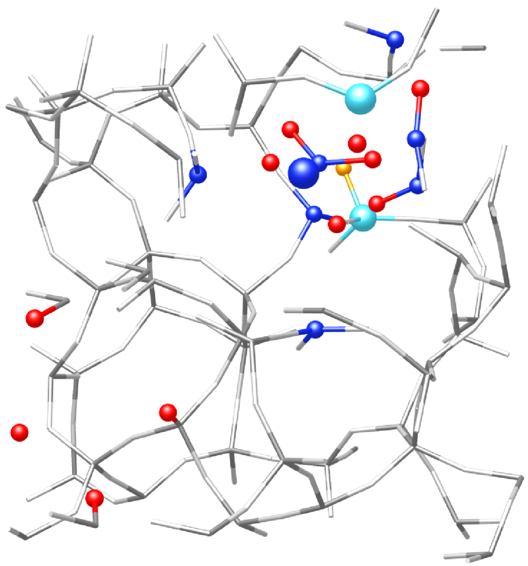
Space

Transient current
Keeps going

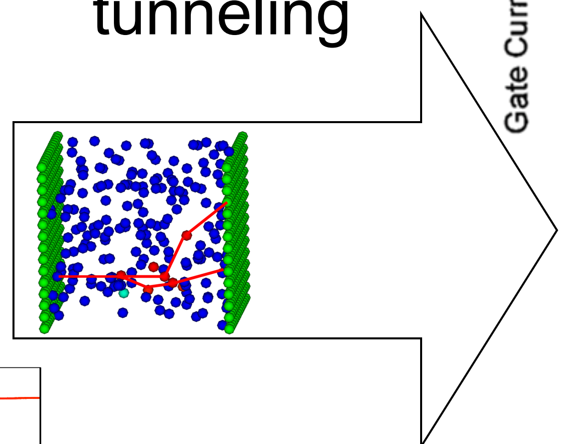
- 3D Mott defect-to-defect calculation of leakage currents
- Low-resistivity paths through oxide layers
- Displacement damage lead to appreciable current

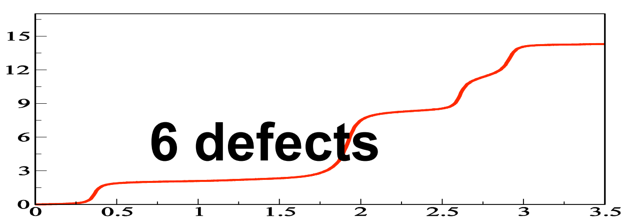
Multi-scale calculation

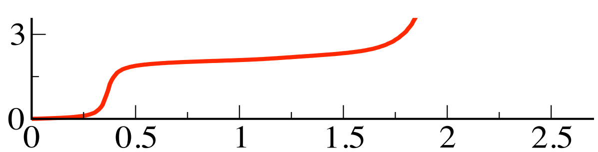
From QM transport to I-V device characteristics

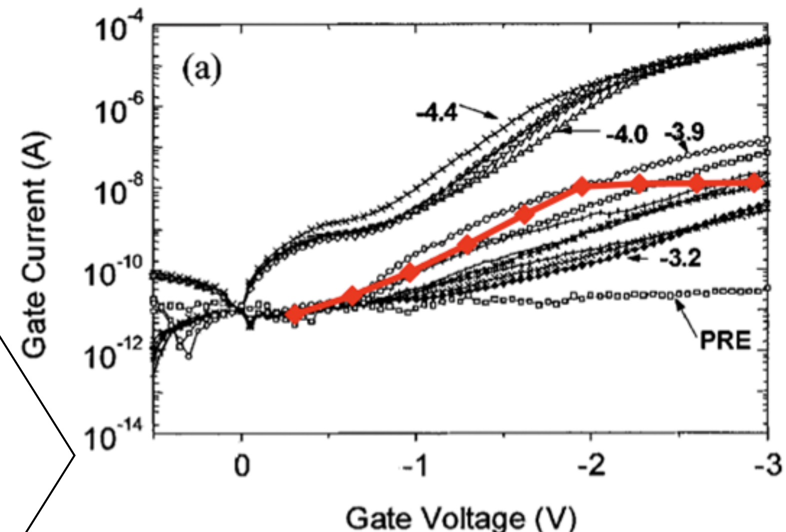


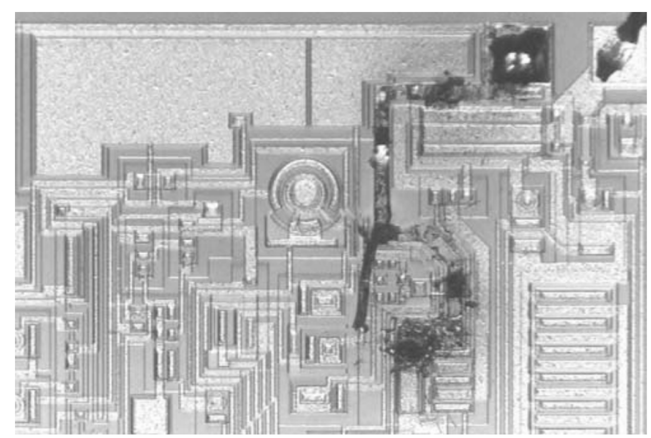
Mott's
defect-defect
tunneling











2009 MURI Annual review, Vanderbilt University, June 10 2009