Tunneling through Ferroelectric Insulators

Daniel Wortmann and Stefan Blügel
Institut für Festkörperforschung & Institute for Advanced Simulation,
Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

Motivation: Tunneling-electro-resistance

Some of the proposed novel functionalities of future oxide-based electronics will have their physical origin in the use of transition-metal oxide barrier materials, in particular of ferroelectric oxides. With different directions of the ferroelectric polarization the tunneling conductance is modified thereby allowing to utilize the polarization state for data storage. In direct analogy with the tunneling-magneto-resistance such devices are expected to show a tunneling-electro-resistance (TER) effect.

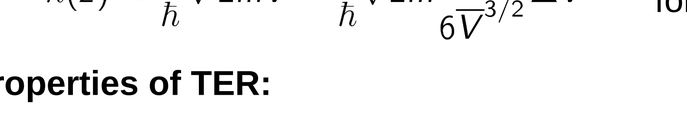
$$TER = \frac{\Gamma_{\leftarrow} - \Gamma_{\rightarrow}}{\Gamma_{\leftarrow} + \Gamma_{\rightarrow}}$$

Three possible mechanisms:

I. Change in barrier thickness (piezoelectric effect)

II. Change of interface transmission

III. Change of the barrier shape



Simple model for influence of barrier shape

Two basic approximations:

I. Tunneling in WKB approximation:

$$\Gamma = C\, e^{-2\int_0^d \kappa(z)dz} = C\; e^{-2\overline{\kappa} d}$$

II. Simple effective mass model of tunneling

$$\kappa(z) = \frac{1}{\hbar}\sqrt{\frac{2m}{d}(V_1(d-z) + V_2 z)}$$

Leads to: $TER \approx \tanh d\,(\overline{\kappa_{\rightarrow}} - \overline{\kappa_{\leftarrow}})$

with

$$\kappa(z) \approx \frac{1}{\hbar}\sqrt{2m\overline{V}} - \frac{1}{\hbar}\sqrt{2m}\frac{1}{6\overline{V}^{3/2}}\Delta V^2$$ for a simple barrier

Basic properties of TER:

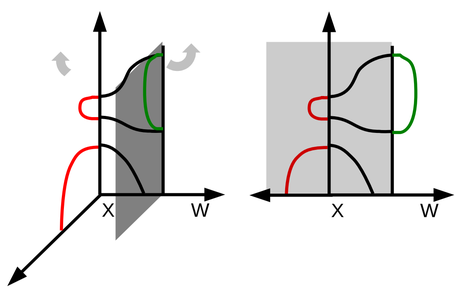
- Can arise from change in the average potential height $\overline{V}$ (Probably undesirable effect)
- Can arise from change of slope of the barrier ΔV
- TER due to the different decay constants scales with the barrier thickness

Complex bandstructure calculations: Green function embedding for FLAPW

- DFT treatment (GGA)
- All-electron full-potential linearized augmented plane wave (FLAPW)
- Based on FLEUR code ↦ **http://www.flapw.de**
- **Green function embedding & Transfer matrix calculation**
- Generalized k-vectors from diagonalizing transfer matrix

$$k = \Re(k) + i\Im(k) = q + i\kappa$$

- Visualization in **Complex Bandstructure**

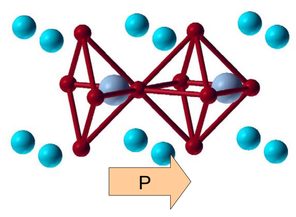


$BaTiO_3$ and $PbTiO_3$

$BaTiO_3$:

- Ferroelectric phase of $BaTiO_3$

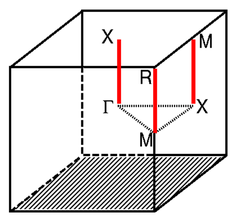
$49\mu C/cm^2$

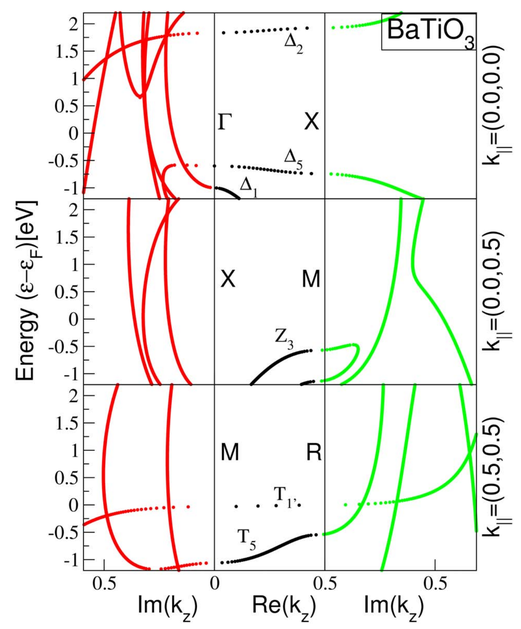


Displacements:
Ti - 0.05Å
O 0.24Å
O 0.15Å

Complex bandstructure:

- Valence band top and conduction band bottom show little dispersion
- Slowly decaying states in gap not directly derived from bandedges
- Bands have very similar decay constants for all energies in gap



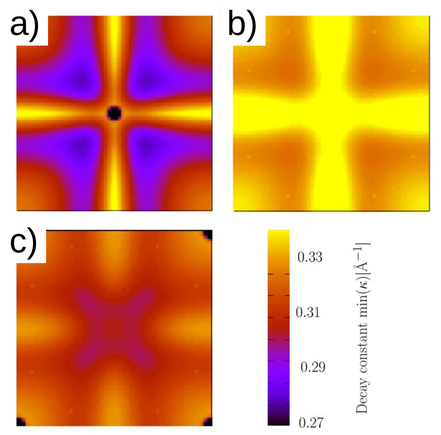


Smallest decay constant over Brillouin-zone

- Simplest example: vacuum

$$\kappa(k_{\parallel}) \propto \sqrt{(2m\epsilon + k_{\parallel}^2)}$$

- Three plots at different energies
  a) close to conduction band
  b) middle of gap
  c) close to valence band
- All show similar pattern
- Little variation of decay constant with energy or k-vector

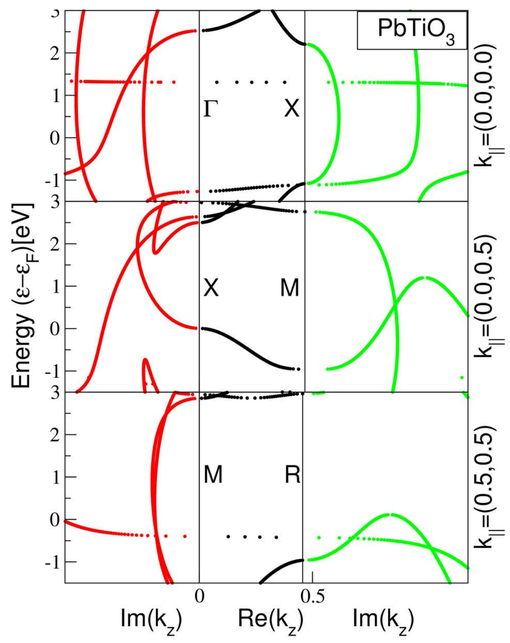


$PbTiO_3$:

- Structure from experimental data

Complex bandstructure:

- Similar to $BaTiO_3$
- Close to valence band: slowly decaying states
- At larger energy: little variation of the decay constant



Summary & Conclusions

- At least for $BaTiO_3$ and $PbTiO_3$ the decay of the wavefunction in the barrier is little depended on energy, i.e. the barrier shape has little influence on the tunneling.
- The simple effective mass model of tunneling cannot be expected to provide reasonable estimates of the TER effect.
- We did not include interface effects which can be expected to dominate the effect.

References:

- Kohlstedt, Tsymbal, Science 14, 181 (2006)
- Wortmann, Ishida, Blügel, PRB 65, 165103 (2002)
- Freimuth, Mokrousov, Wortmann, Heinze, Blügel. PRB **78**, 035120 (2008)