Interface-controlled tunneling spin polarization

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Supported by National Science Foundation
Outline

- Introduction
- Tunneling conductance in a simple tight-binding model
- Spin-polarized tunneling from clean and oxidized Co surfaces through vacuum
- Spin polarization in Co/Al₂O₃/Co tunnel junctions
- Interface resonant states in Fe/MgO/Fe tunnel junctions
Tunneling magnetoresistance (TMR)

Magnetic tunnel junction

\[
TMR = \frac{R_{\uparrow\downarrow} - R_{\uparrow\uparrow}}{R_{\uparrow\uparrow}}
\]

Experimental values at room temperature:

- FM|Al₂O₃|FM MTJs: TMR~70%
- Fe|MgO|Fe MTJs: TMR~200%
Symmetry arguments

**Insulator**

Complex band structure:

\[ E = E(k_{||}, k_z), \text{ where } k_z = q + i\kappa, \quad \psi \propto e^{-\kappa z} \]

- State of smallest \( \kappa \) dominates in conductance
- States of different symmetry tunnel with a different decay length
- Often this state belongs to the identity representation

**Ferromagnet**

Fe [001]

Graph showing band structure with labels for \( \Gamma[000] \), \( \Delta \), and \( H[001] \).
Deficiencies

Symmetry arguments

- limited only by special k-points
- assume sufficiently thick barrier
- do not take into account electronic and atomic structure of ferromagnet/insulator interfaces
1D tight-binding model

\[ G(E) = \frac{4\pi^2 e^2}{h} V_b^2 \rho_i(E) e^{-2\kappa d} \rho_r(E) \]

Conductance (high barrier):

- Conductance depends strongly on interface bonding
3D tight-binding model

In-plane dispersion: $E_{||}(k_{||}) = -2 \left[ \cos(k_x) + \cos(k_y) \right]$

$k_{||}$-resolved interface DOS

- Interface potential and bonding control the conductance

$V_i = 1$

$V_i = 1.5$
Spin-dependent tunneling from clean and oxidized Co surfaces

Electrodes: Co (111) and Al (111)
Co surface: clean or oxidized (absorbed O monolayer)
Tunneling barrier: vacuum

- Relevance to spin-polarized STM
- Relevance to Tedrow-Meservey experiments
Calculation methods

Atomic structure:
• Plane-wave pseudopotential method

Electronic structure:
• Tight-binding linear muffin-tin orbital method
• Fully self-consistent potentials

Conductance:
• Layered Green’s function approach
• Transmission matrix formalism

\[ G = \frac{e^2}{h} \text{Tr}\left\{ \hat{G}_R \hat{\Gamma}_R \hat{G}_A \hat{\Gamma}_L \right\} \]
Fermi surface of bulk fcc Co along [111] direction

- Holes of different diameter near the $\Gamma$ point
\( K_{||} \)-resolved transmission from clean Co surface to Al

- Negative spin polarization (-60%)
- Majority spins dominate at large barrier thickness
- Crossover only at \(~10\text{nm}\)
$K_{\parallel}$-resolved transmission from oxidized Co surface to Al

- Minority conductance is filtered out by O layer
- Spin polarization is close to +100%
Density of states for oxidized Co surface

O-surface

Co-surface

Co-subsurface

Co-bulk

Energy (eV)

DOS (eV$^{-1}$ atom$^{-1}$)
$K_{\parallel}$-resolved DOS for oxidized Co surface

- Surface Co-O antibonding state creates an additional tunneling barrier in minority-spin channel
Bulk states strongly mix with Co-O antibonding states and extend to the O layer.
Spin-dependent tunneling in Co/Al₂O₃/Co tunnel junctions

Model 1: O-terminated Al₂O₃
Model 2: Adds O(II) atoms adsorbed at the interfaces

- Structure is relaxed
- Strong bonding between Co(II) and O(II) atoms
Transmission function

Majority

Minority

Spin polarization

Model 1

negative

Model 2

positive
Co-O bonding at the interface

- Exchange-split antibonding Co(II)-O(II) states
$K_{||}$-resolved majority DOS

- Co-O antibonding state controls spin polarization
Interface resonance in Fe/MgO/Fe junctions

- Minority interface resonant state is filtered out by Ag
Conclusions

- Tunneling spin polarization in magnetic tunnel junctions is controlled primarily by the interface bonding and structure.

- A monolayer of oxygen on Co (111) surface reverses the spin polarization from negative to positive due to the Co-O bonding. This phenomenon can be detected by spin-polarized STM.

- Oxygen absorbed at the Co surface in Co/Al₂O₃/Co tunnel junctions controls positive spin polarization. Oxidation of a ferromagnet at the interface might be important for obtaining large magnetoresistance.

- Interface resonant states control spin polarization in Fe/MgO/Fe junctions at small barrier thickness. This states can be filtered out by a thin Ag layer.