Spintronics: Transport phenomena in magnetic nanostructures

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Outline

- Electronic Structure
- Diffusive and ballistic Transport
- Transport Theory
- Giant MagnetoResistance
- Tunneling MagnetoResistance

Electronic structure: KKR scheme

- Kohn-Sham equation

$$\mathrm{H}\left|\Psi_k\right\rangle = (\mathrm{T} + \mathrm{V}_{eff})\left|\Psi_k\right\rangle = E_k\left|\Psi_k\right\rangle$$

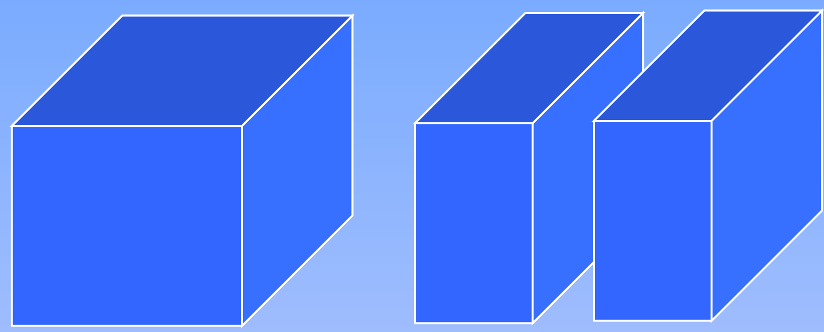
- Green's Function

$$\left(E - \mathring{\mathcal{H}}\right)\mathring{\mathcal{G}} = 1 \qquad\qquad (E - \mathcal{H})\,\mathcal{G} = 1$$

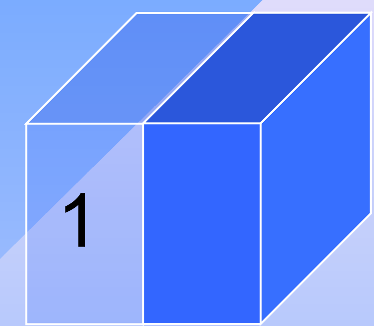
- Dyson Equation

$$\begin{aligned} \mathcal{G} &= \mathring{\mathcal{G}} + \mathring{\mathcal{G}}\,\Delta\mathcal{V}_{eff}\,\mathcal{G} \\ \Delta\mathcal{V}_{eff} &= \mathcal{V}_{eff} - \mathring{\mathcal{V}}_{eff} \end{aligned}$$

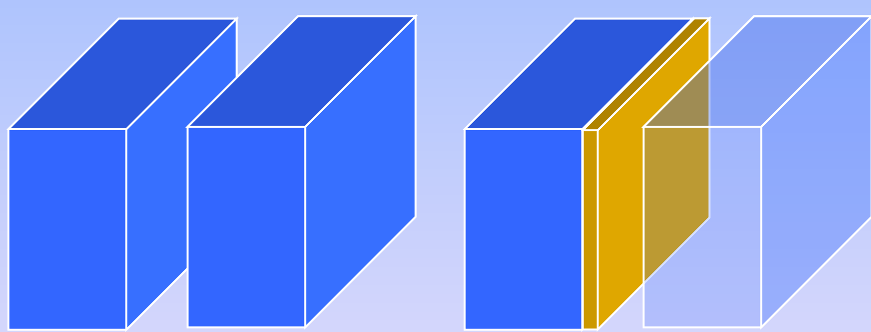
Treatment of different geometries



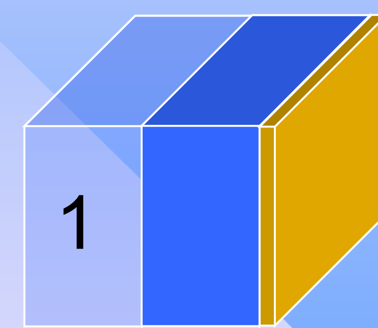
Surface



$$\mathcal{G}_{surf} = \mathcal{G}_{bulk} + \mathcal{G}_{bulk} \Delta V \mathcal{G}_{surf}$$

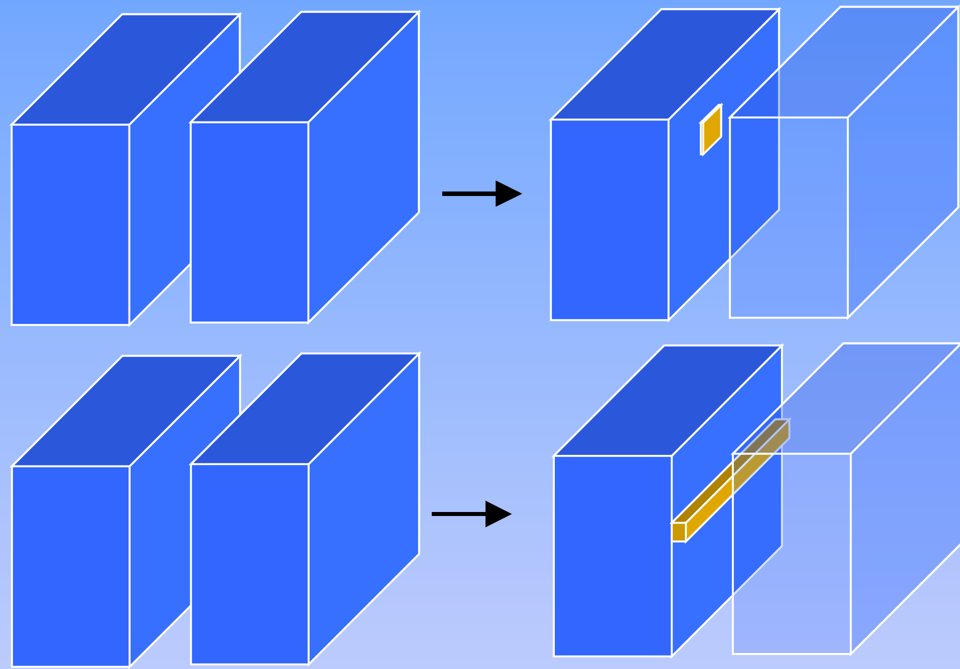


Adlayer



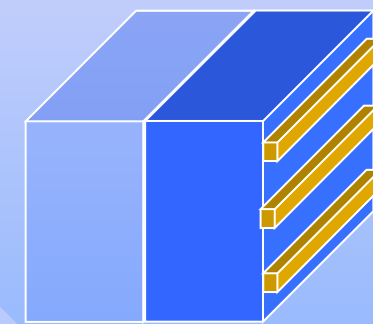
$$\mathcal{G}_{ad} = \mathcal{G}_{surf} + \mathcal{G}_{surf} \Delta V \mathcal{G}_{ad}$$

Surface Defects and Nanowires

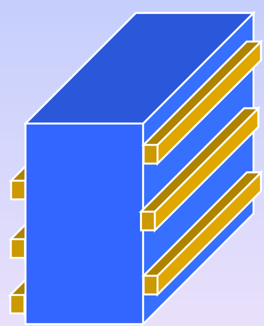


Surface defect

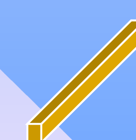
Nanowire



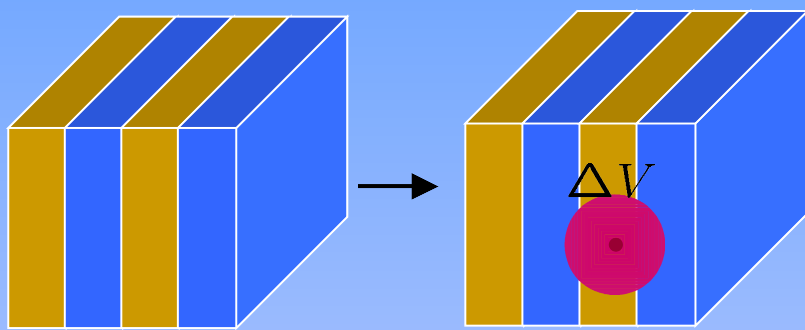
Nanowire (on a slab)
V. Bellini et al., PRB (2001)



Nanowire - free standing
J. Opitz et al., PRB (2002)

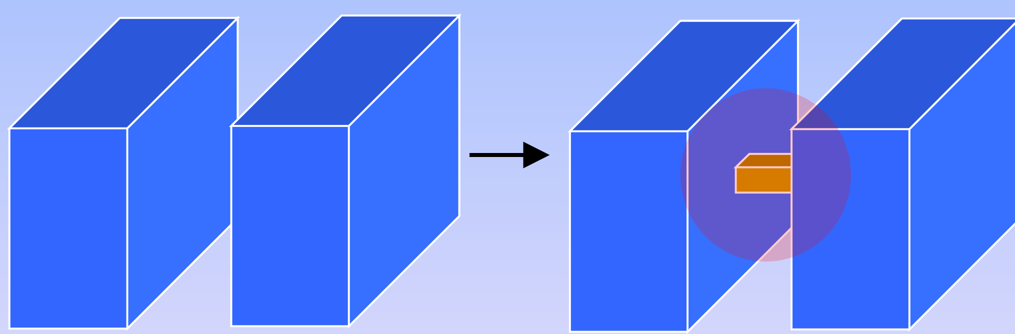


Bulk Defects and Nanocontacts



Defect in a multilayer

$$\mathcal{G}_{def} = \mathcal{G}_{bulk} + \mathcal{G}_{bulk} \Delta V \mathcal{G}_{def}$$

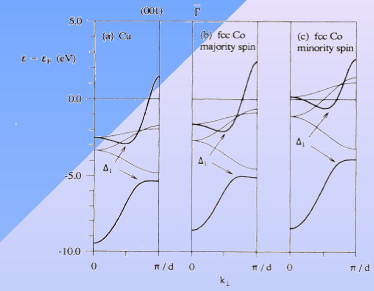


Nanocontact

$$\mathcal{G}_{def} = \mathcal{G}_{bulk} + \mathcal{G}_{bulk} \Delta V \mathcal{G}_{def}$$

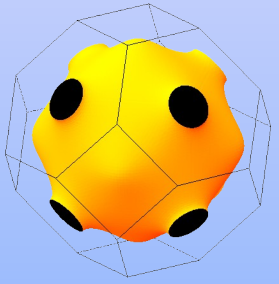
- Self consistent potential of region of interest

Output of electronic structure calculation



Dispersion relation: E_k^σ

Fermi surface: $E_k^\sigma = E_F$



Group velocity: $\mathbf{v}_k^\sigma = \frac{1}{\hbar}\frac{\partial E_k^\sigma}{\partial k}$

Wave function: $\psi_k^\sigma(\mathbf{r})^o, \ \psi_k^\sigma(\mathbf{r})$

Green function: $G^{\sigma\, o}(\mathbf{r}, \mathbf{r}', E), \ G^\sigma(\mathbf{r}, \mathbf{r}', E)$

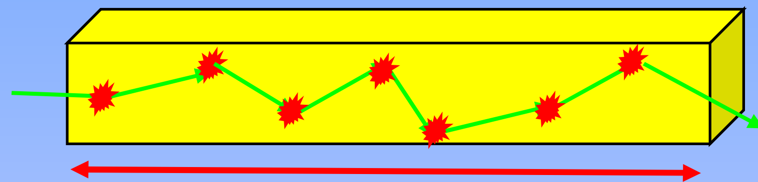
Transport Properties

Resistance

Diffusive

Conductance

$$R = \rho \frac{L}{A}$$



A

$$G = \sigma \frac{A}{L}$$

$$j(r) = \sigma E(r)$$

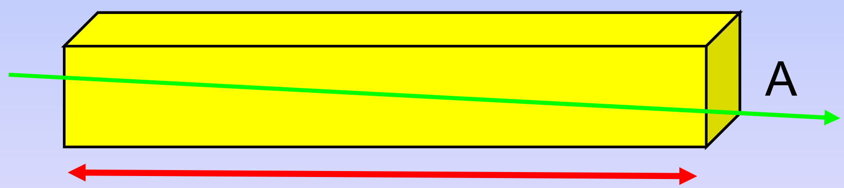
$$\lambda \ll L$$

Resistivity ρ

Conductivity σ

Ballistic

$$R \not\propto L$$

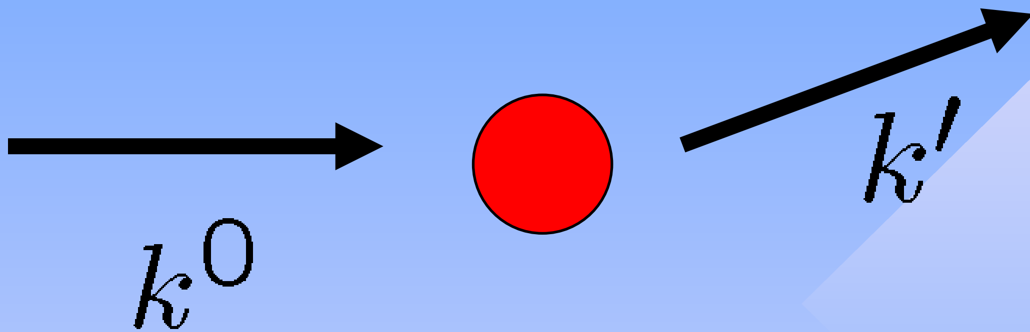


A

$$G \not\propto \frac{1}{L}$$

$$\lambda > L$$

Origin of Resistivity



Scattering centers:

- impurities, vacancies
- dislocations
- interfaces, surfaces
- disorder

T = 0

- phonons
- magnons

T > 0

Transport theory: Boltzmann equation

- One-particle distribution function

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\frac{\partial f_k}{\partial \mathbf{r}} + \frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t}\frac{\partial f_k}{\partial \mathbf{k}} - \frac{\partial f_k}{\partial t} = 0$$

Drift Field Scattering

- Scattering term

$$\left.\frac{\partial f_k}{\partial t}\right|_{scatt} = \sum_{k'} (f_{k'}(1 - f_k)P_{k'k} - (1 - f_{k'})f_k P_{kk'}$$

- Linear response

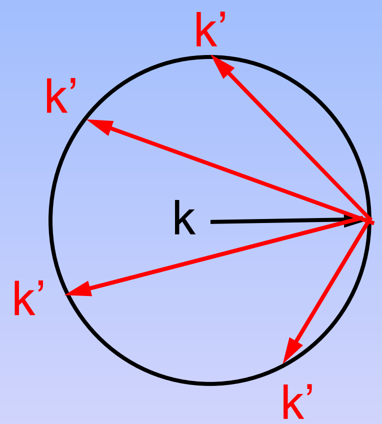
$$g_k = f_k - \mathring{f}_k = -e\frac{\partial \mathring{f}_k}{\partial E}\mathbf{\Lambda}_k\mathbf{E} \qquad |g_k| \ll \mathring{f}_k$$

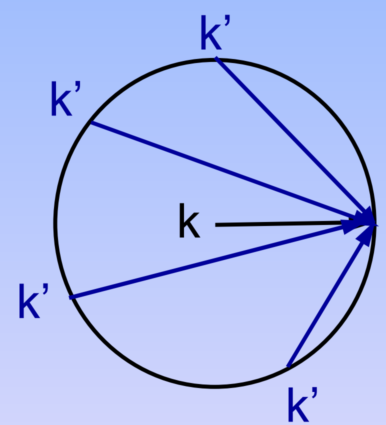
$$\left.\frac{\partial f_k}{\partial t}\right|_{scatt} = \sum_{k'} P_{kk'}\left(g_{k'} - g_k\right)$$

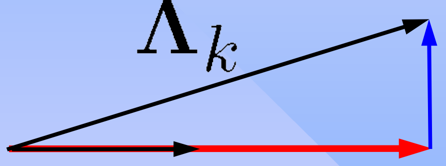
Linearized Boltzmann equation

to determine vector of mean free path

$$\boldsymbol{\Lambda}_k = \underbrace{\tau_k^B \Big[\mathbf{v}_k}_{} + \underbrace{\sum_{k'} P_{kk'} \boldsymbol{\Lambda}_{k'}}_{} \Big] \qquad \text{with} \qquad \tau_k^B = \Big[\sum_{k'} P_{kk'} \Big]^{-1}$$







$$\boldsymbol{\Lambda}_k \qquad \tau_k^B \sum_{k'} P_{kk'} \boldsymbol{\Lambda}_{k'}$$

$$\mathbf{v}_k \qquad \mathring{\boldsymbol{\Lambda}}_k = \tau_k^B \mathbf{v}_k$$

! Iterative solution

! Relaxation time approximation

$$\tau = \left\langle \tau_k^B \right\rangle_{E_k = E_F}$$

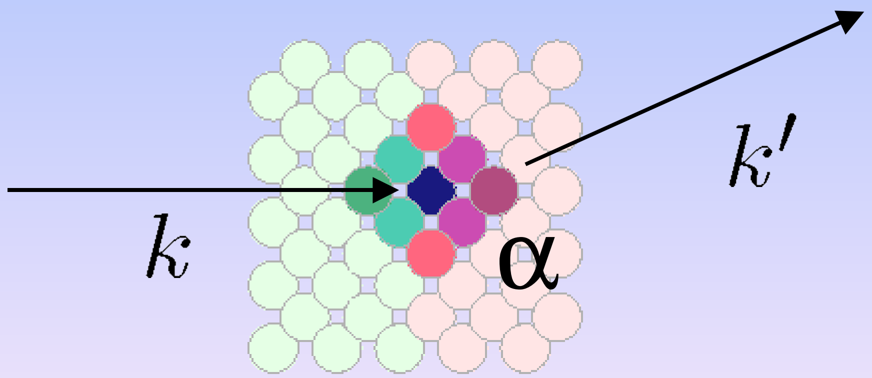
Transport theory: Transition probability

- Microscopic transition matrix

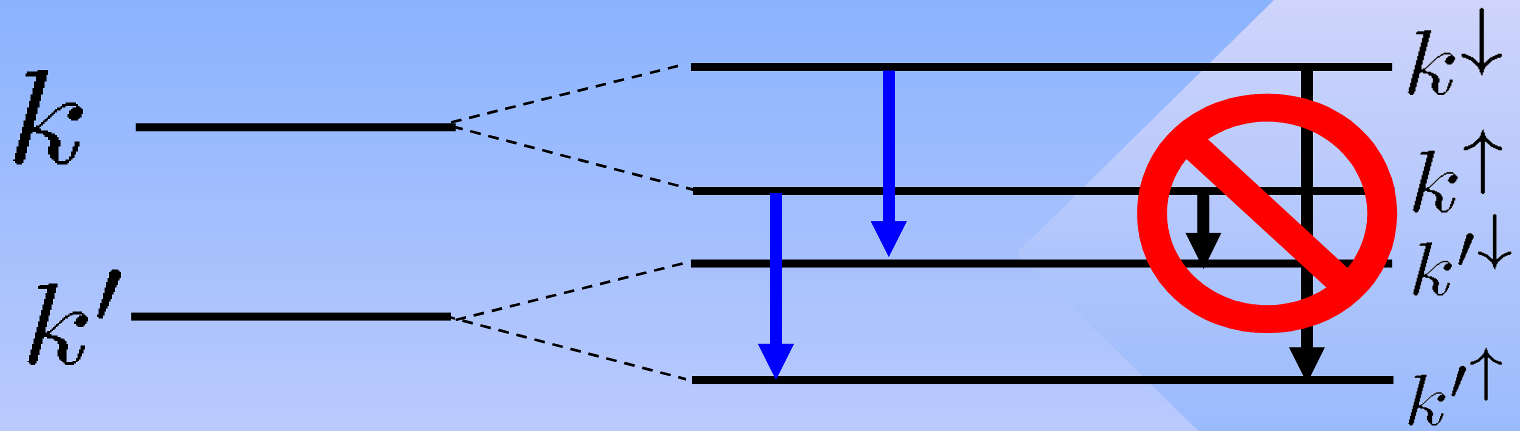
$$T^{\alpha}_{kk'} = \langle \mathring{\psi}_k | \Delta V^{\alpha} | \psi_{k'} \rangle = \langle \mathring{\psi}_k | \mathcal{T}^{\alpha} | \mathring{\psi}_{k'} \rangle$$

- Transition probability

$$P_{kk'} = 2\pi \sum_{\alpha} c_{\alpha} N \left| T^{\alpha}_{kk'} \right|^2$$

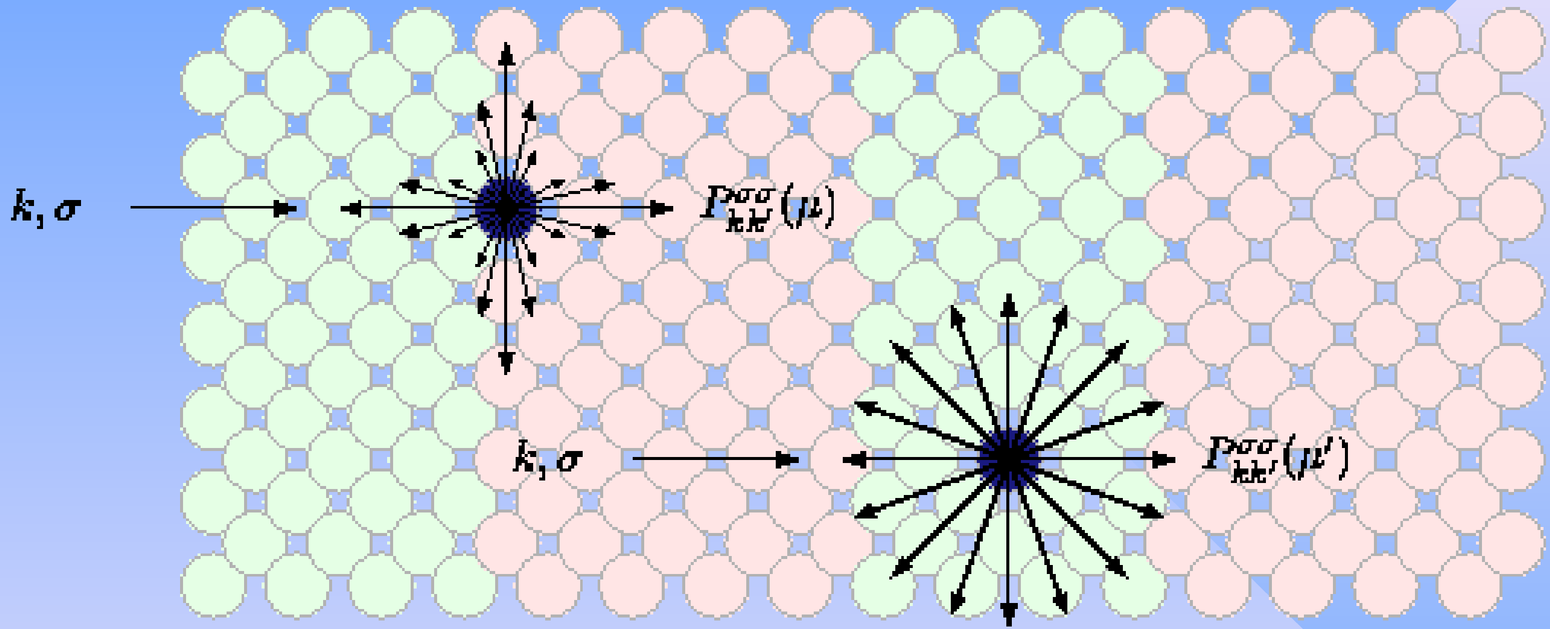


Neglecting spin-flip processes



3d transition metals: in most cases spin-flip cross section one to two orders smaller

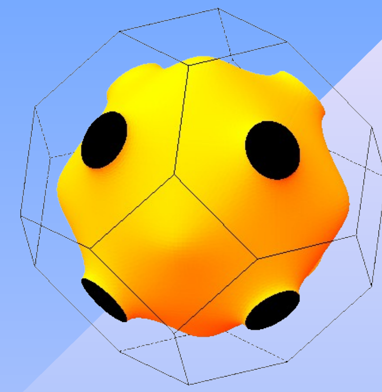
Scattering in nanostructures



- Scattering properties depend on:
  - Type of impurity
  - Position of impurity

Two current model

Co Majority Fermi Surface



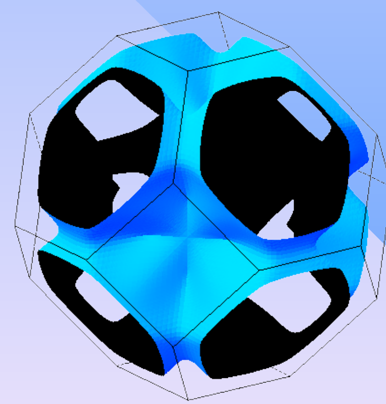
Conductivity Tensor

$$\mathbf{j} = \hat{\sigma}\mathbf{E}$$

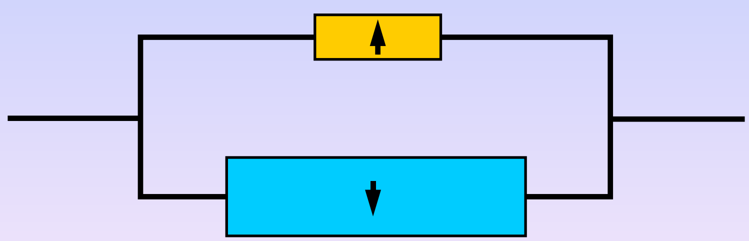
$$\sigma^{ij} = \frac{e^2}{(2\pi)^3} \oint_{E_k=E_F} \frac{\mathrm{d}S}{v_k}\, v_k^i \Lambda_k^j$$

$$= \frac{e^2}{(2\pi)^3} \int_{E_k=E_F} \frac{\mathrm{d}S}{v_k} v_k^i v_k^j \tau_k^B$$

Co Minority Fermi Surface

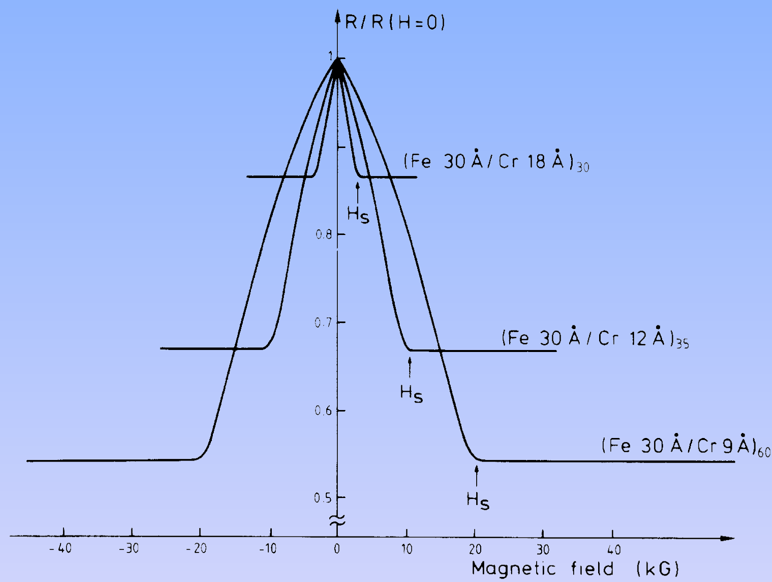


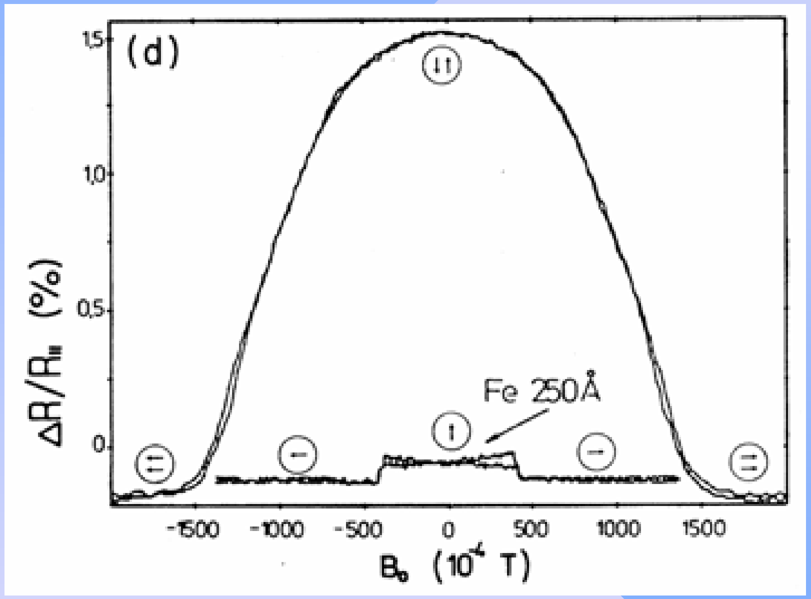
$$\sigma = \sigma^{\uparrow} + \sigma^{\downarrow} \qquad \beta = \frac{\sigma^{\uparrow}}{\sigma^{\downarrow}}$$

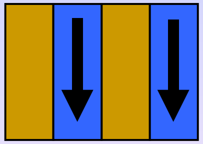


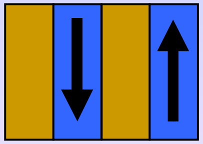
Giant MagnetoResistance

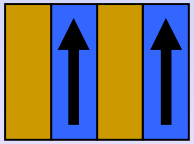
$$GMR = \frac{\rho^{AP} - \rho^{P}}{\rho^{P}} = \frac{\sigma^{P}}{\sigma^{AP}} - 1$$











M.N. Baibich et al., PRL **61**, 2472 (1988)

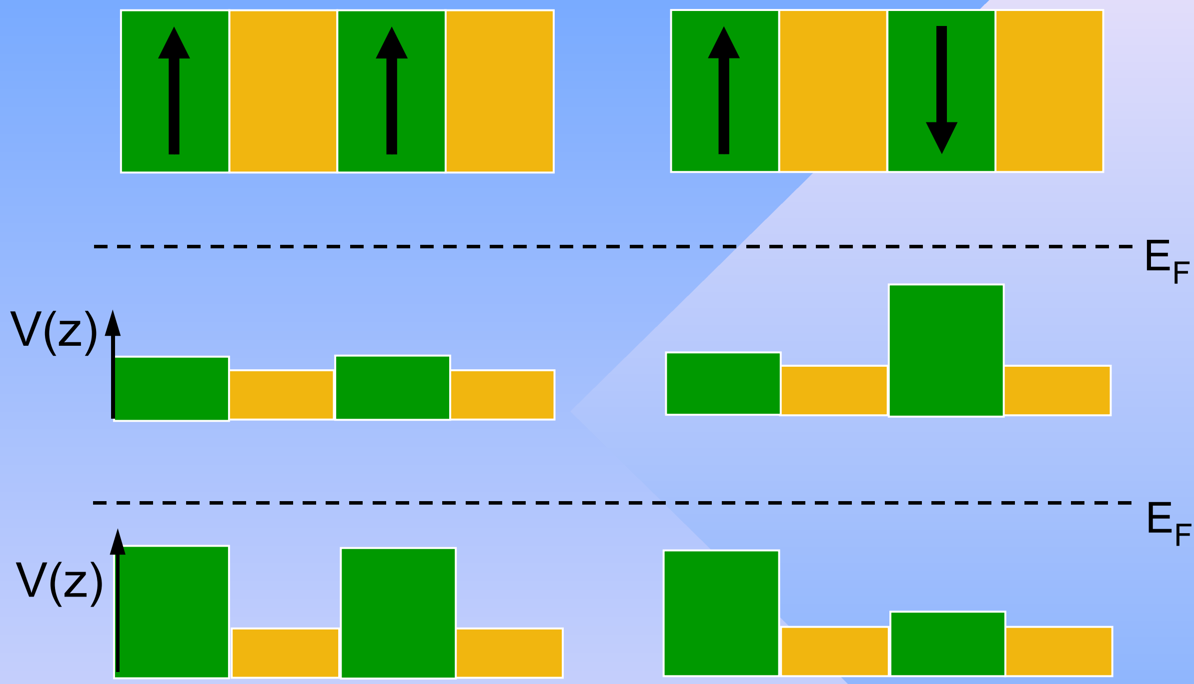
G. Binasch et al., PRB **39**, 4828 (1989)

Influence of multilayer potential: intrinsic GMR

Magnetic configuration

Majority electrons

Minority electrons

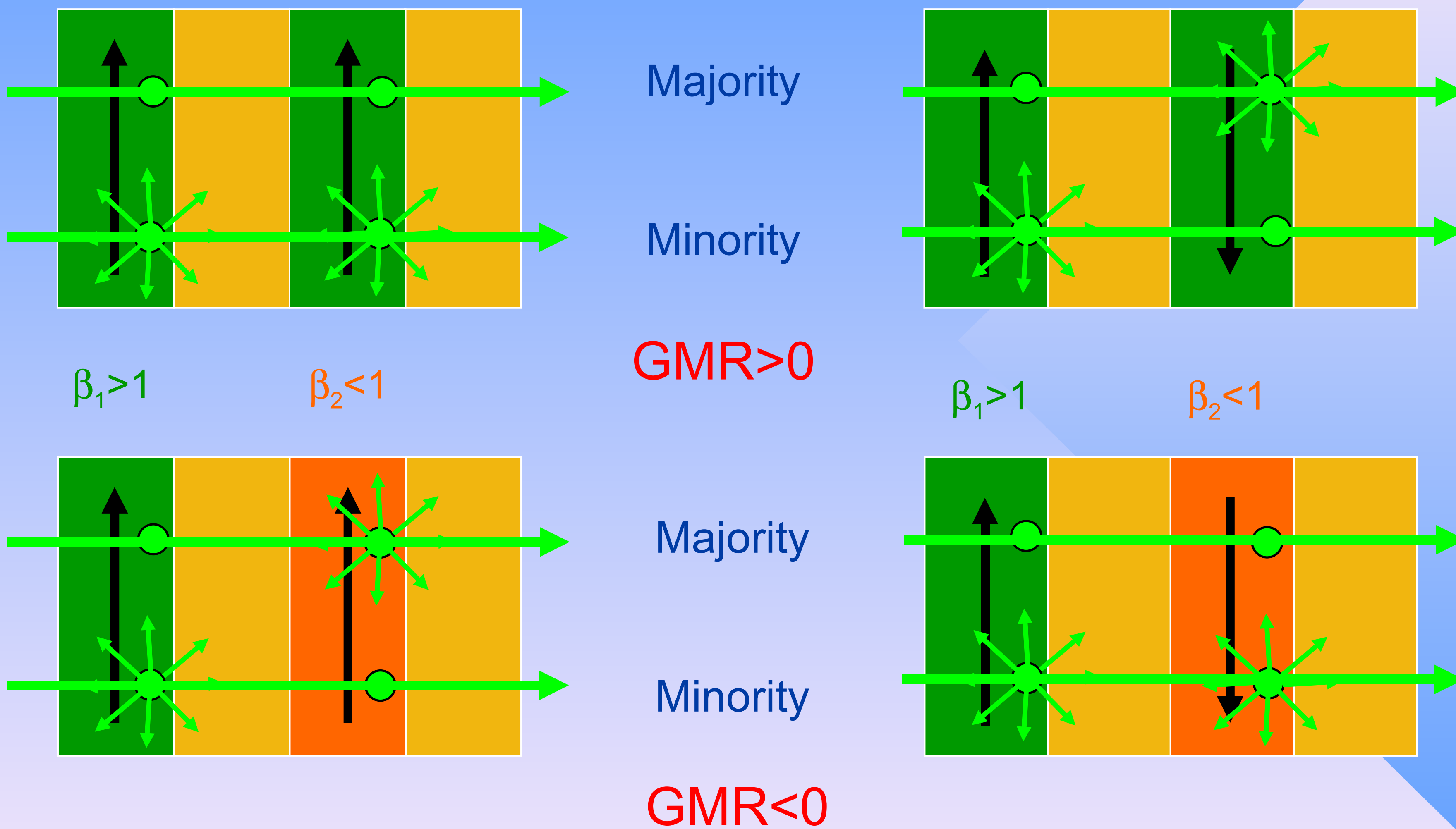


Fermi velocity: $V_F^{Min} < V_F^{AP} < V_F^{Maj}$

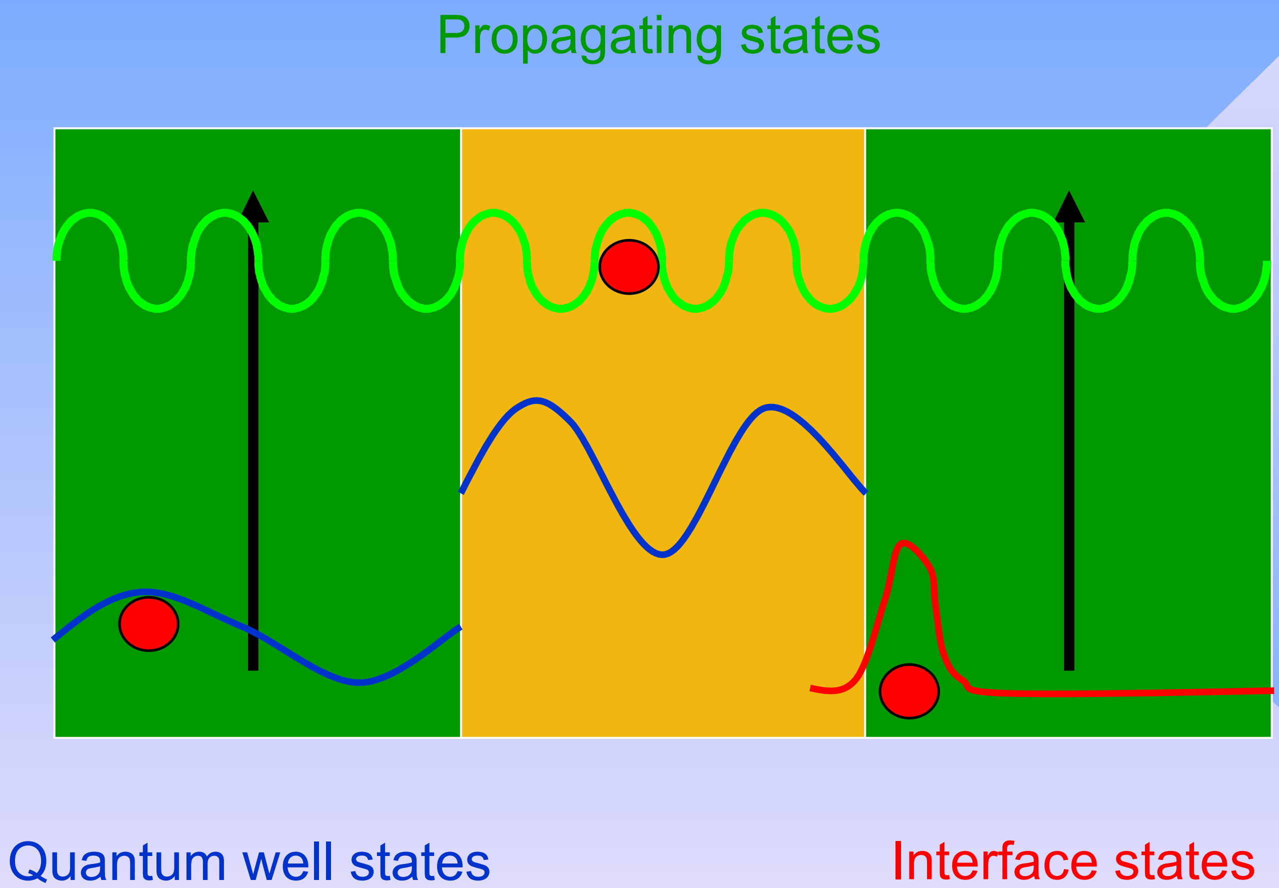
Resistance: $\rho^P < \rho^{AP}$

GMR: GMR > 0

Influence of Impurities: extrinsic GMR

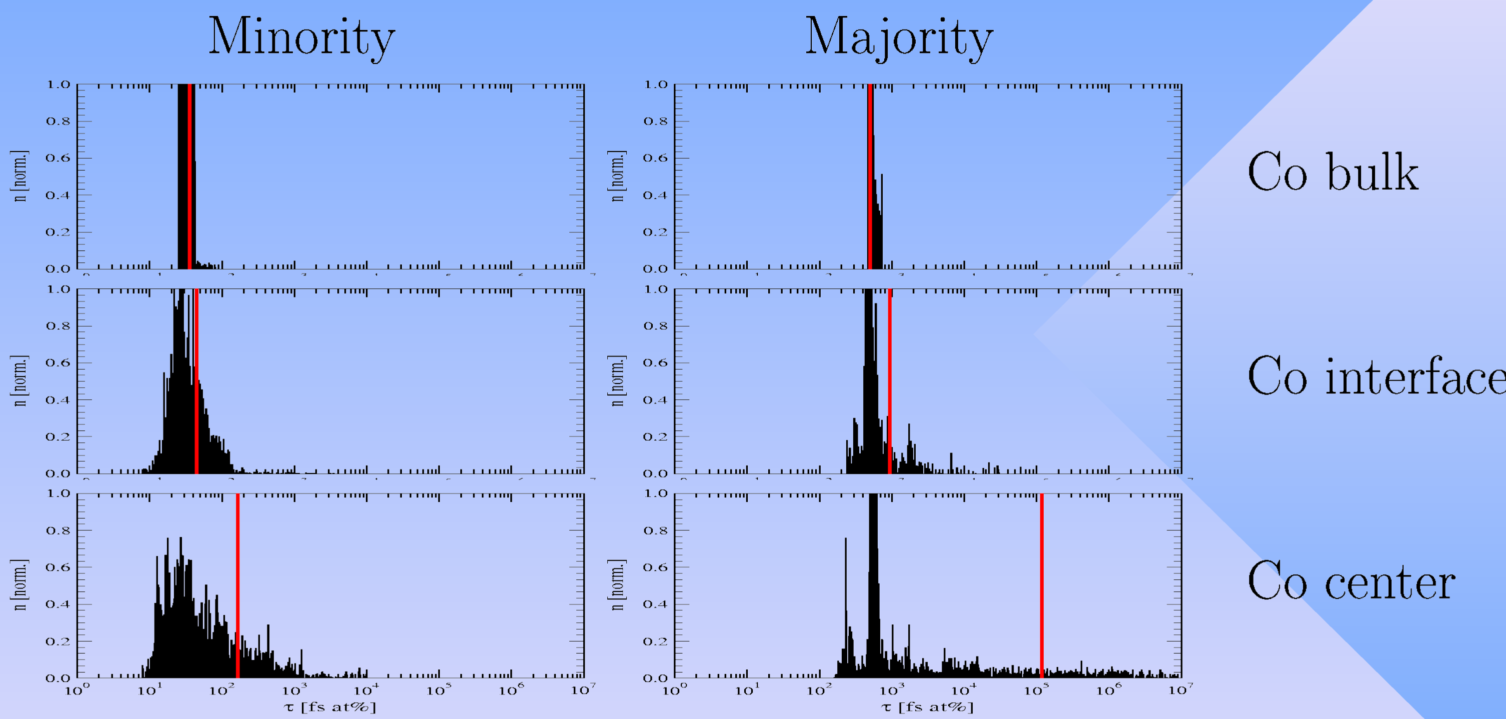


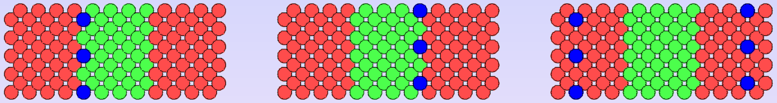
Quantum confinement



GMR: Influence of interface scattering

Co/Cu multilayer   Relaxation times



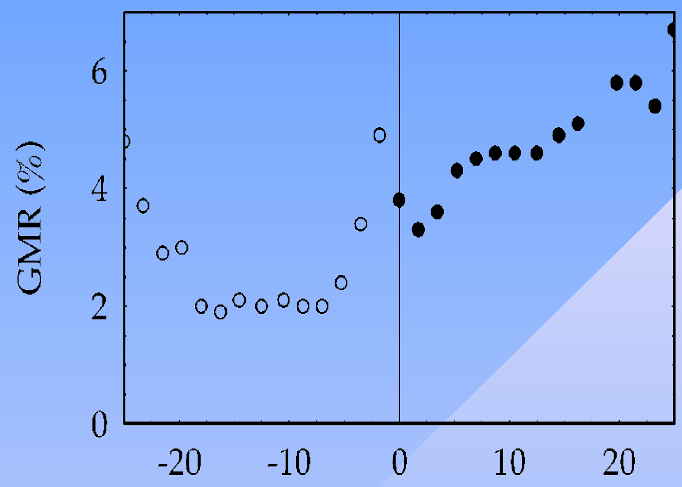


J. Binder et al., J. Appl. Phys. **89**, 7107 (2001)

GMR: dependence on impurity position

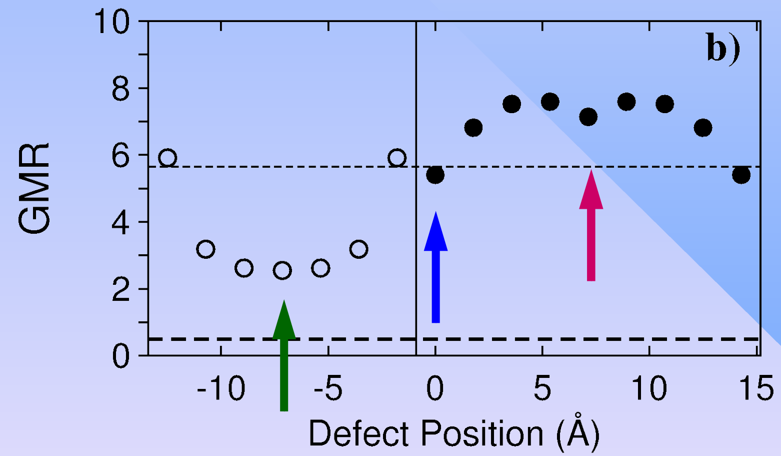
Experiment:

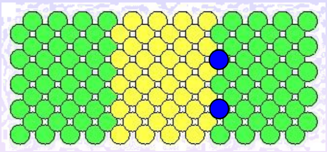
C. Marrows et al., PRB **63**, 220404 (2001)

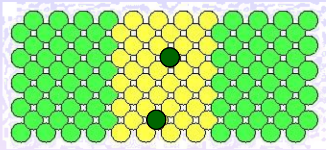


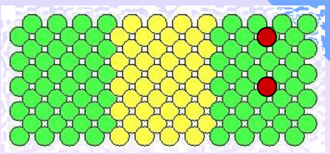
Theory:

P. Zahn et al., PRB **68**, 100403(R) (2003)

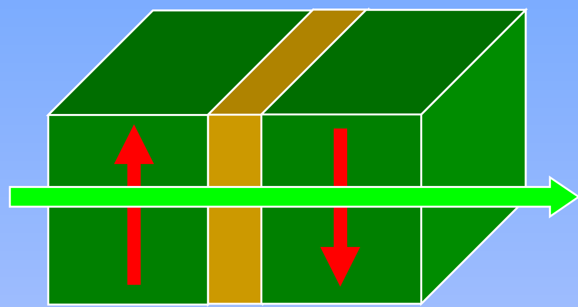




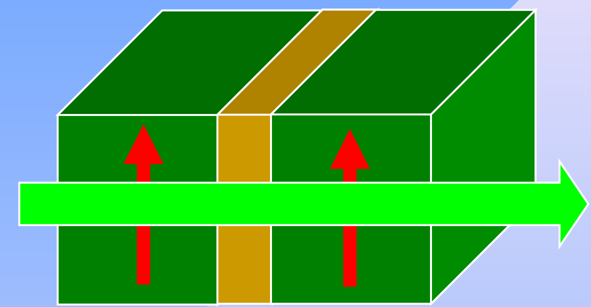




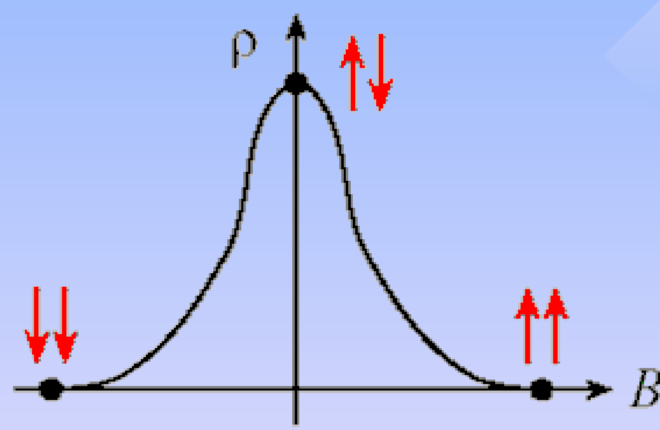
Tunneling MagnetoResistance



g^{AP}



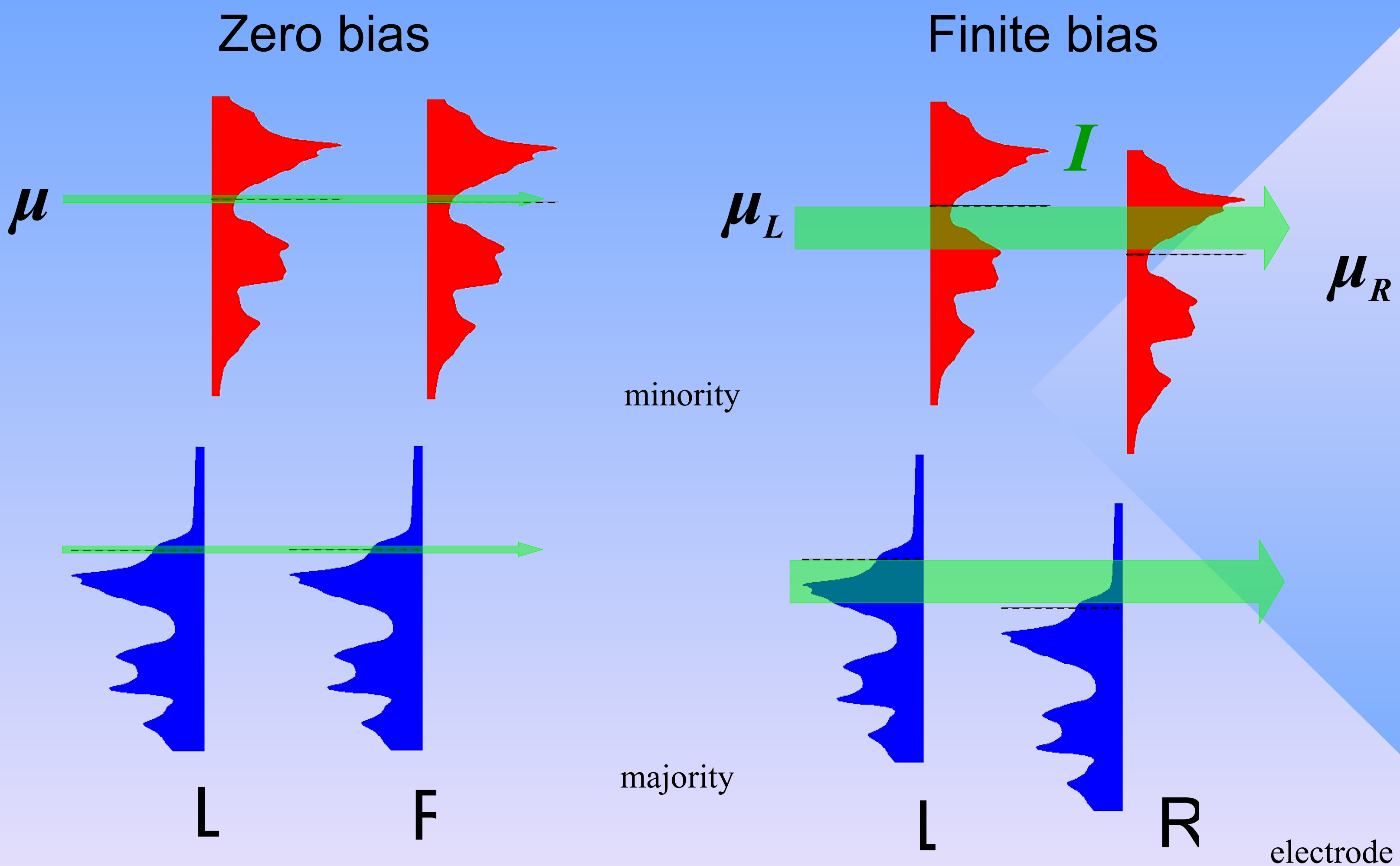
g^{P}



$$\boxed{TMR = (g^{P} - g^{AP}) / g^{AP}}$$

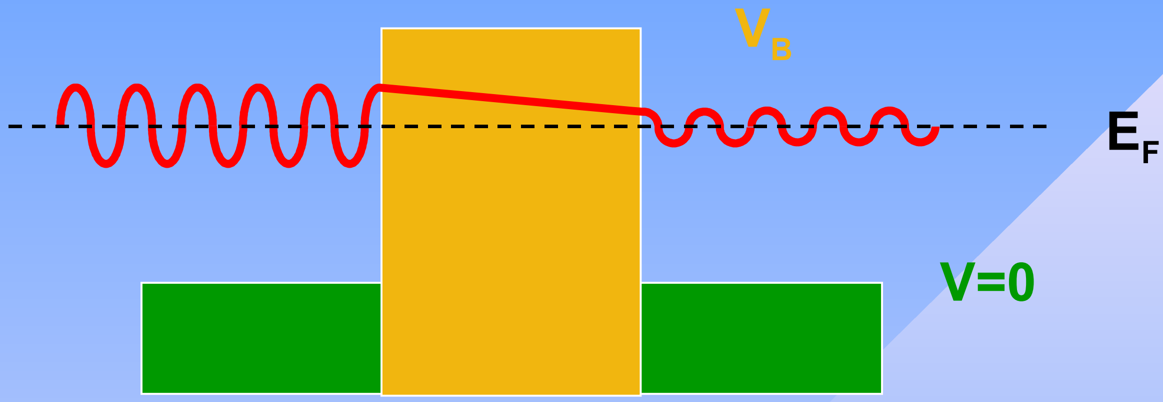
J. S. Moodera et al., PRL **74**, 3273 (1995)

A simple Model



Julliere: $TMR=2P_L P_R(1-P_L P_R)$

Coherent tunneling



Wave function matching:

$$\psi(x) = \begin{cases} e^{ikx} + re^{-ikx} & (x < -d/2) \\ Ce^{-\kappa x} + De^{\kappa x} & (-a < x < a) \\ te^{ikx} & (d/2 < x) \end{cases}$$

atomic units $\kappa = \sqrt{(V_B - E_F)}$

Transmitted wave

Transmitted wave:

$$t = \frac{e^{-ikd}}{cosh\kappa d + i(\varepsilon/2) sinh\kappa d} \qquad \varepsilon = \frac{\kappa}{k} - \frac{k}{\kappa}$$

Transmission coefficient:

$$T = |t|^2 \approx e^{-2\kappa d}\left(\frac{4k\kappa}{k^2+\kappa^2}\right)^2 \qquad \kappa d \gg 1$$

3-dimensional case

Complex band structure

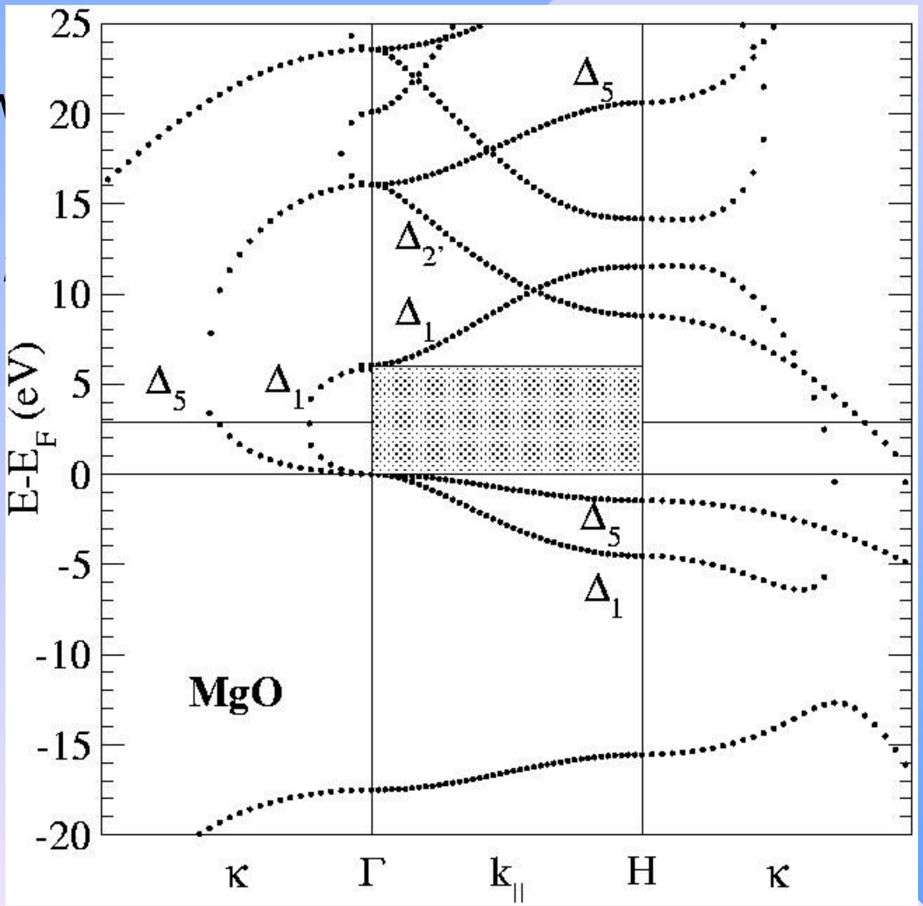
Bloch waves: periodic eigensolutions for a periodic potenial

$$\psi(\mathbf{r}) = e^{\imath \mathbf{k}\mathbf{r}} u_{\mathbf{k}\nu}(\mathbf{r})$$

Evanescent waves: eigensolutions w

$$\psi(\mathbf{r}) = e^{\imath \mathbf{k}'\mathbf{r}} e^{\imath \kappa \mathbf{r}}\; u_{\mathbf{k}}$$

- expoenentially decaying or decreasing,
- but important for surfaces, interfaces, defects
- Bulk property



Ab initio Transport Calculation

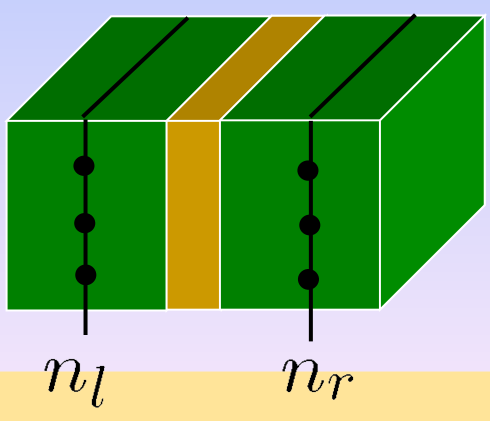
- Conductance: Landauer Formula

$$g = \textstyle\sum_{\mathbf{k}_{||}\,\sigma} T^{\sigma}_{\mathbf{k}_{||}}$$

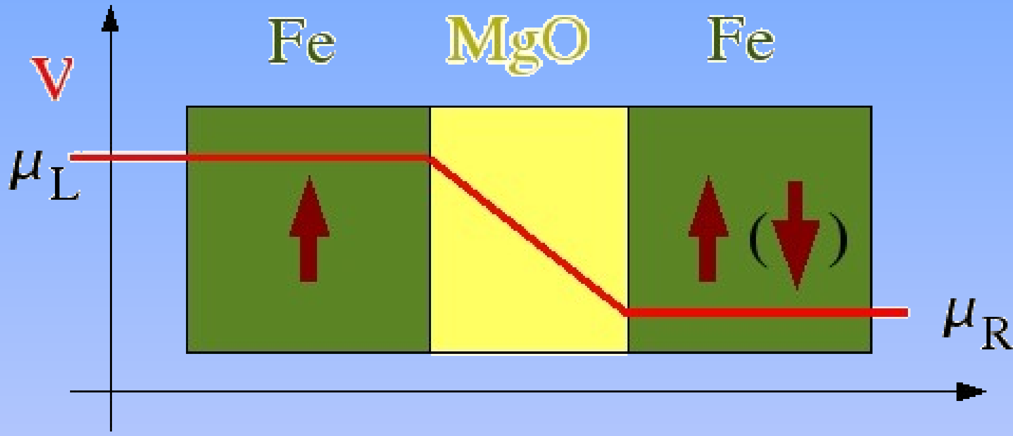
- Green's Function formulation (Baranger&Stone 1989)

$$g \propto \sum_{\sigma} \left[\int d^2\mathbf{k}_{||} \sum_{n_l n_r} \sum_{L L' L'' L'''} \tilde{J}^{T\,n_l}_{L''' L}\, G^{n_l n_r}_{L L'}\, \tilde{J}^{n_r}_{L' L''}\, G^{+\,n_r n_l}_{L'' L'''} \right]^{\sigma}$$

$$\tilde{J}^{n}_{L L'} = \textstyle\int_{V_n} d^3\mathbf{r} \left[R^n_L(\mathbf{r}) \partial_z R^{*\,n}_{L'}(\mathbf{r}) - R^{*\,n}_{L'}(\mathbf{r}) \partial_z R^n_L(\mathbf{r}) \right]$$



Applying bias: Potential construction



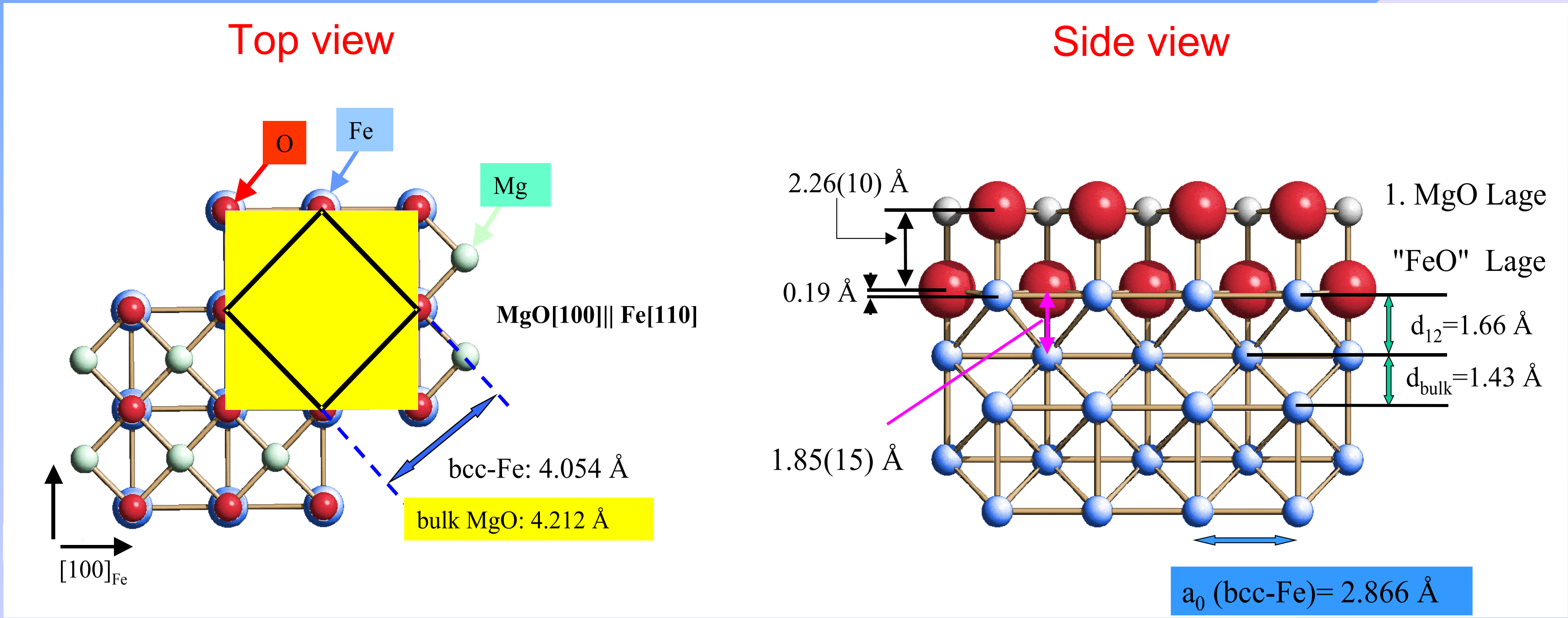
$$\mu_L = \mu_R + eV_B$$

- Integrated Transmission

$$\bar{T}^{\sigma}_{\mathbf{k}_{||}} = \frac{1}{\mu_L - \mu_R} \int_{\mu_R}^{\mu_L} dE\, T(E, \mathbf{k}_{||})$$

$$g = \sum_{\mathbf{k}_{||}\,\sigma} \bar{T}^{\sigma}_{\mathbf{k}_{||}}$$

Interface Structure: mixed FeO layer



H.L. Meyerheim et al., PRL **80**, 076102 (2001)

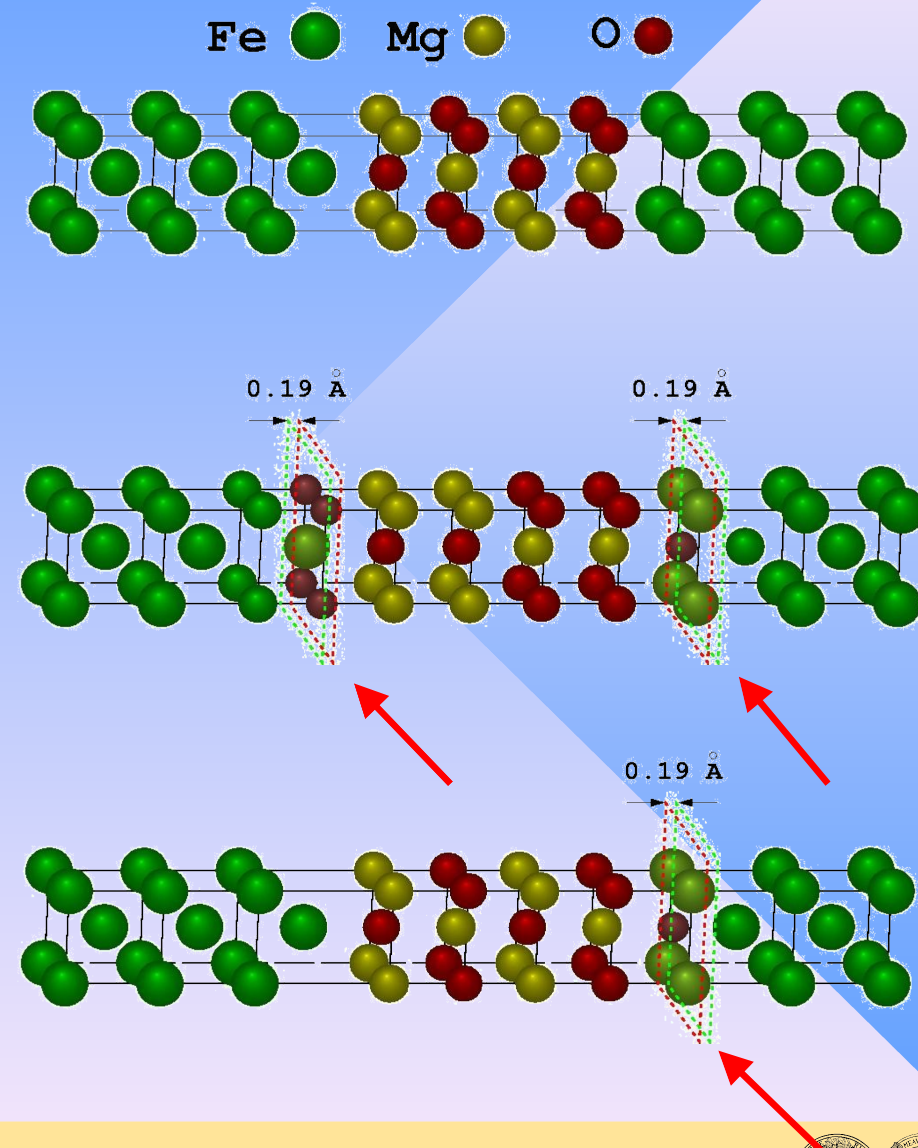
H.L. Meyerheim et al., PRB **65**, 144433 (2002)

Investigated Systems

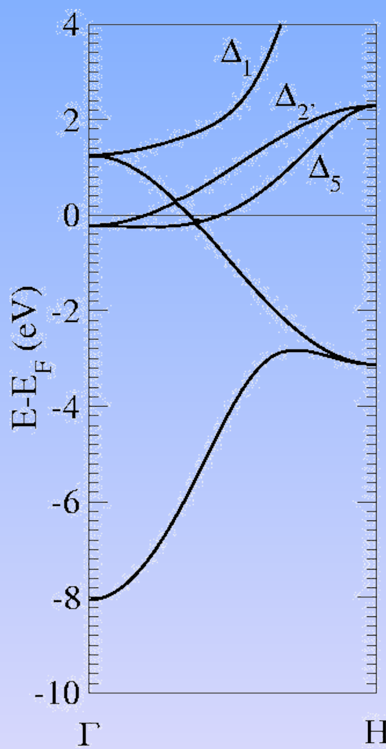
Ideal Interfaces:

Two FeO interfaces: symmetric

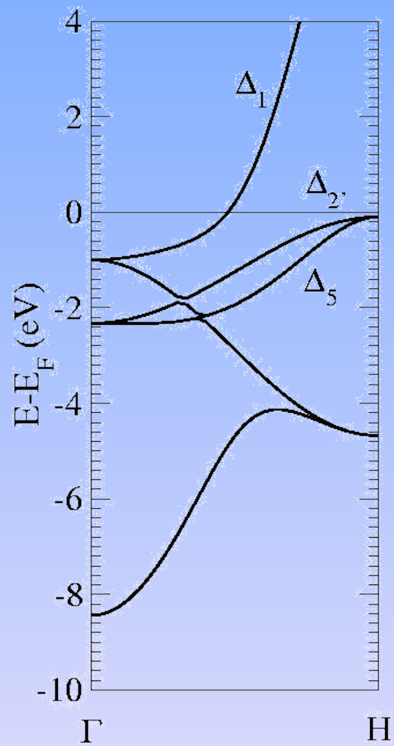
Single FeO interface: asymmetric



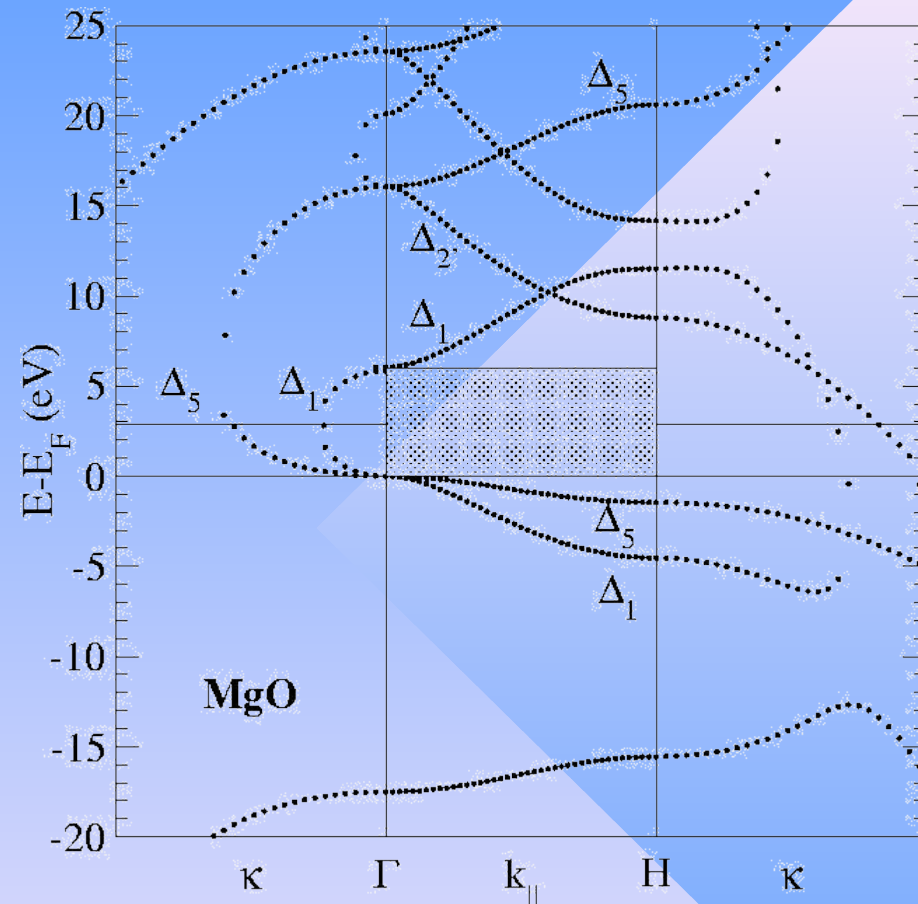
Fe/MgO/Fe(100)



Fe Min.



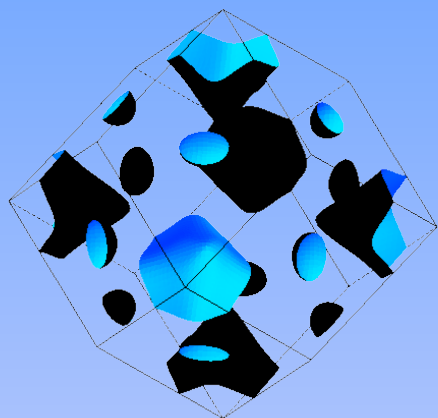
Maj.

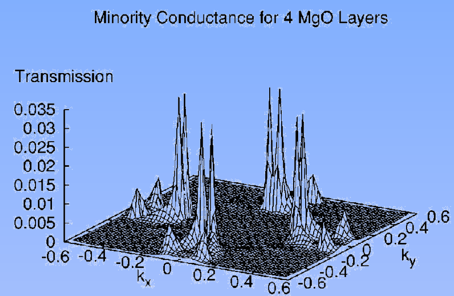


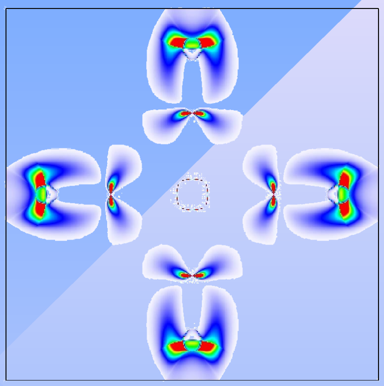
MgO

Fe/MgO/Fe(100)

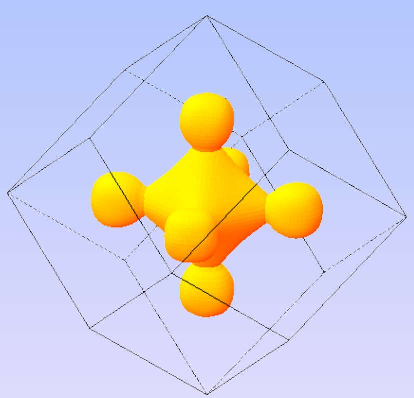
Min.

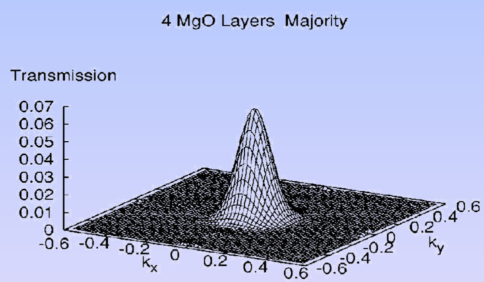


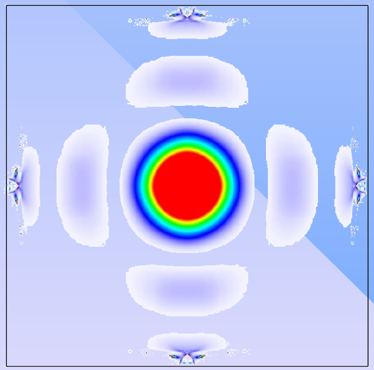


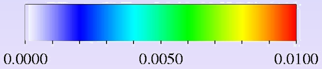


Maj.



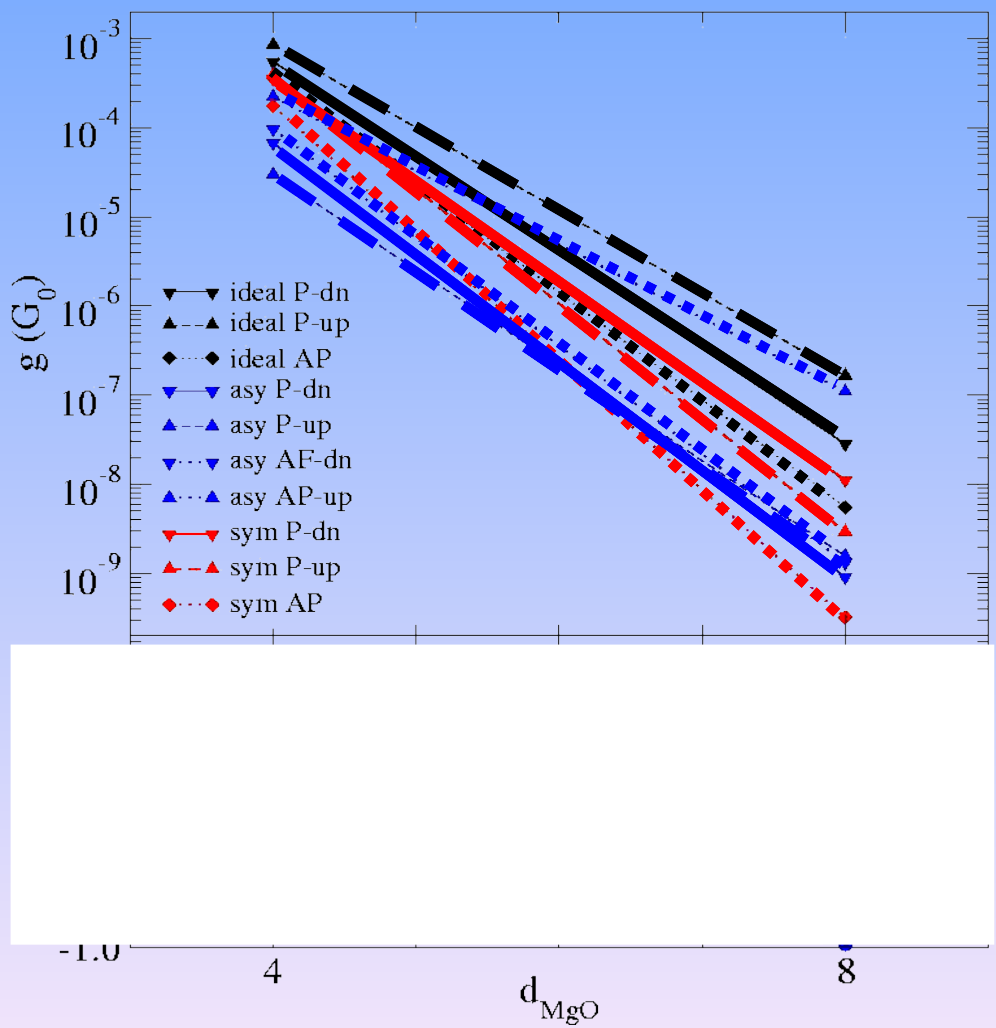




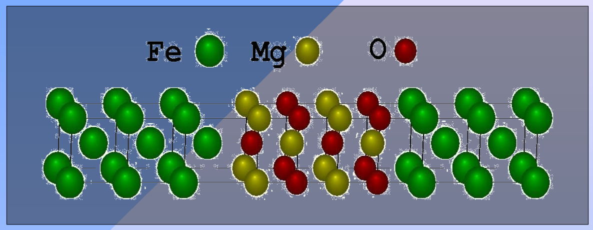


Butler et al. PRB (2001)

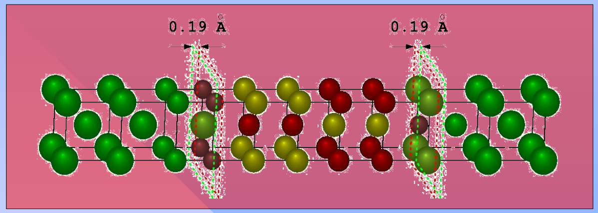
Conductance and TMR: zero bias



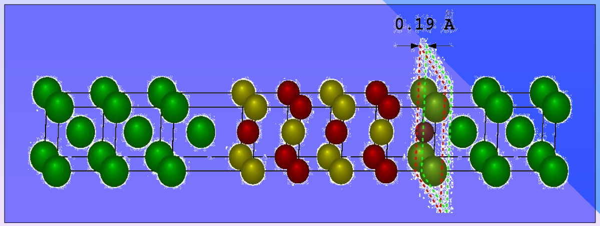
Ideal interface



Two FeO interfaces

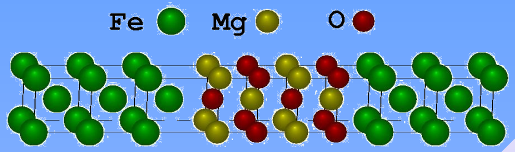


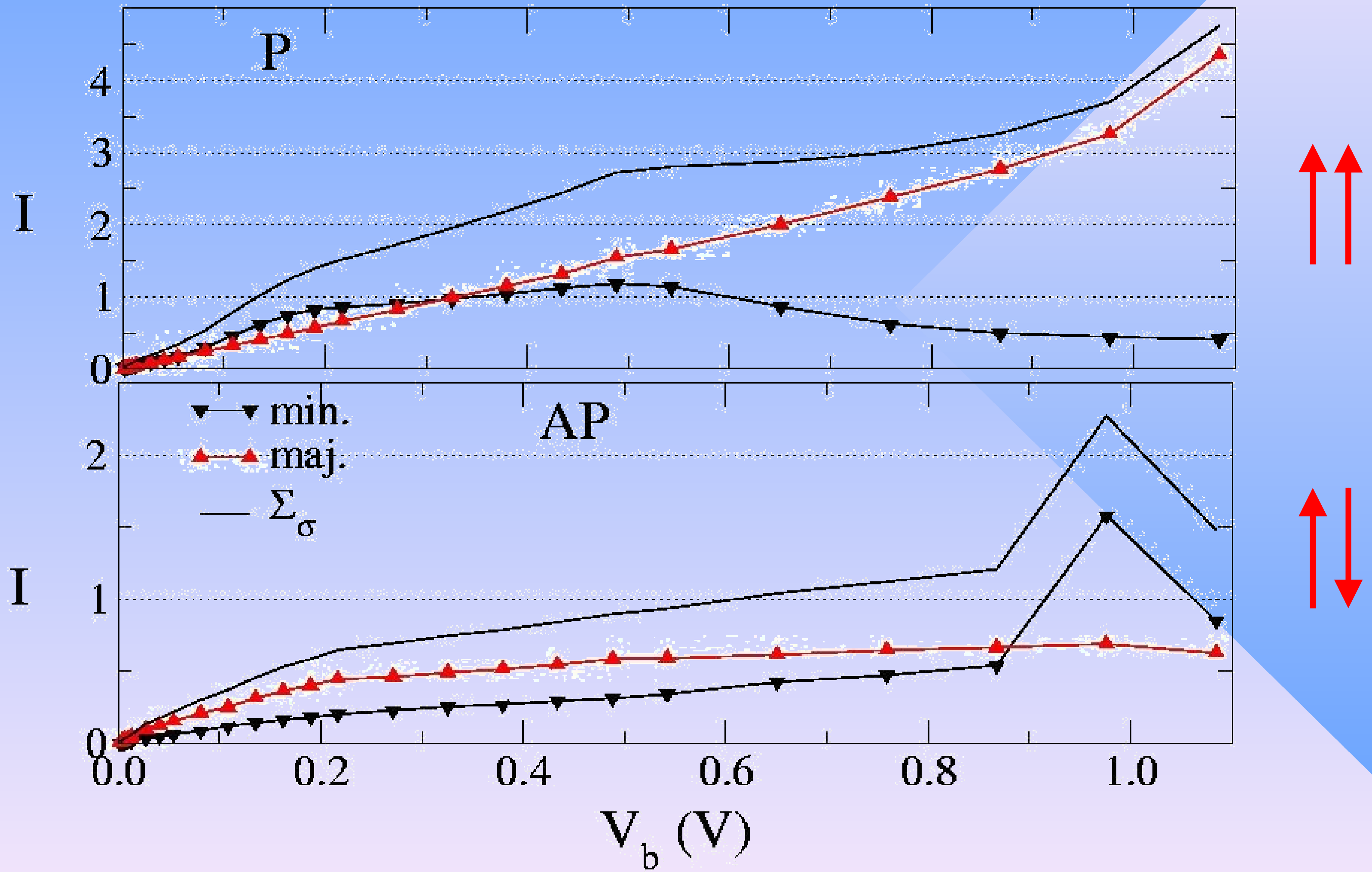
Single FeO interface



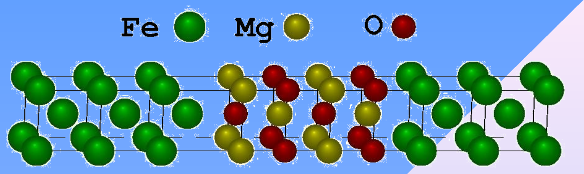
Bias dependence: P/AP configuration

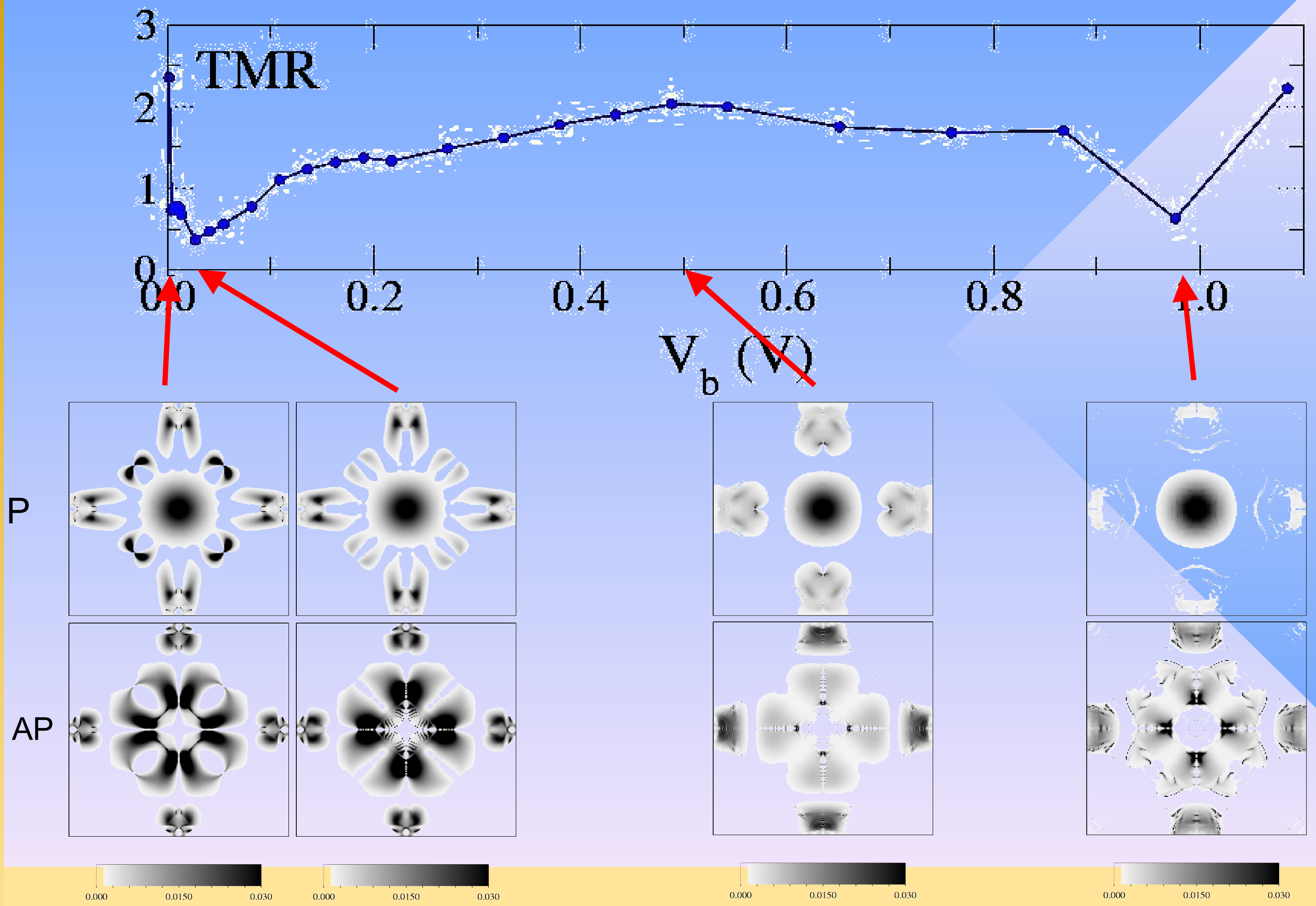
ideal System



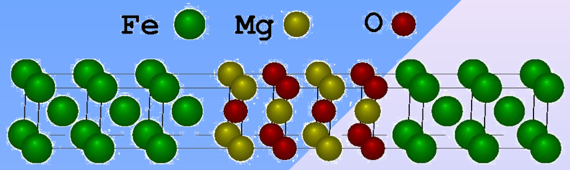


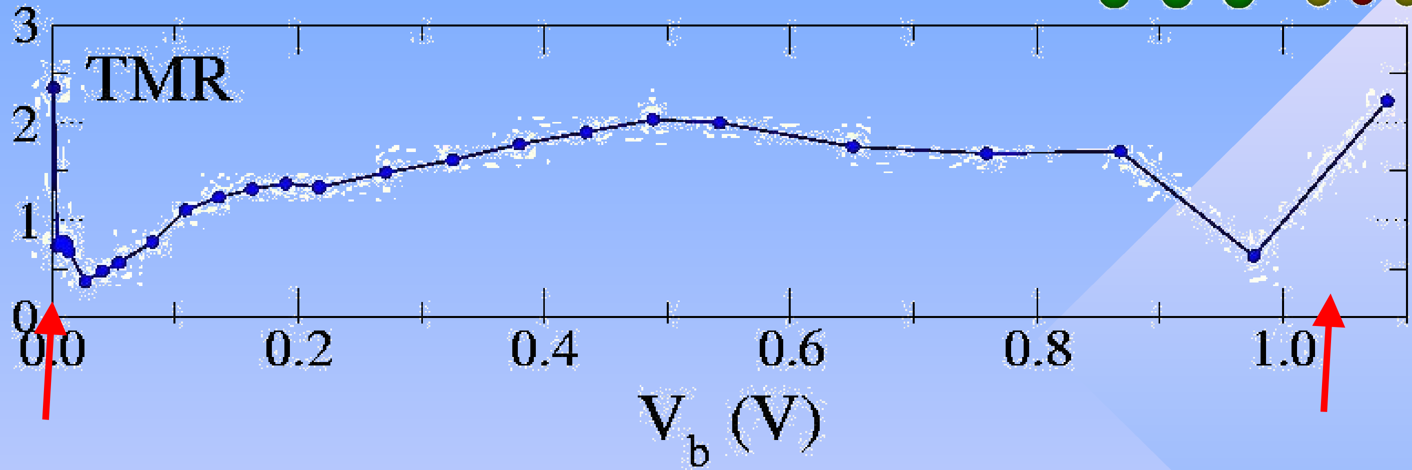
Bias dependence: TMR

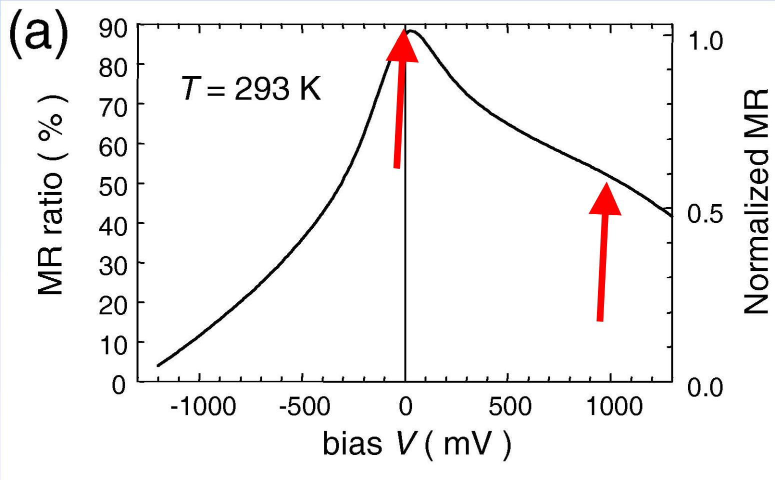




Bias dependence: comparison with experiment

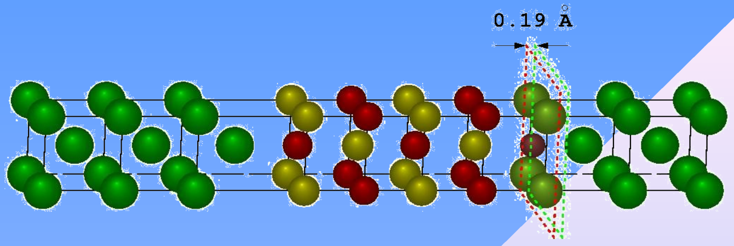


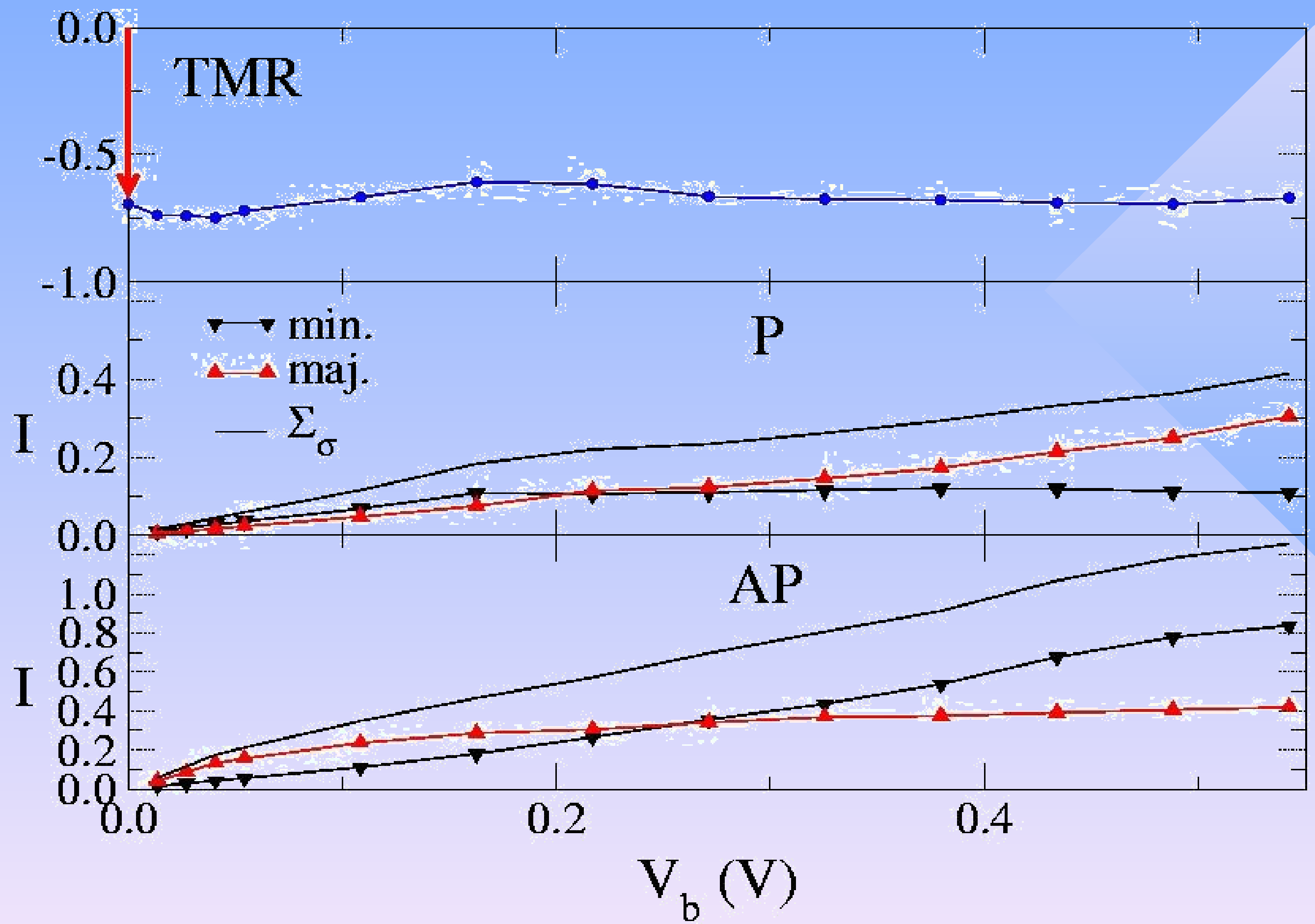




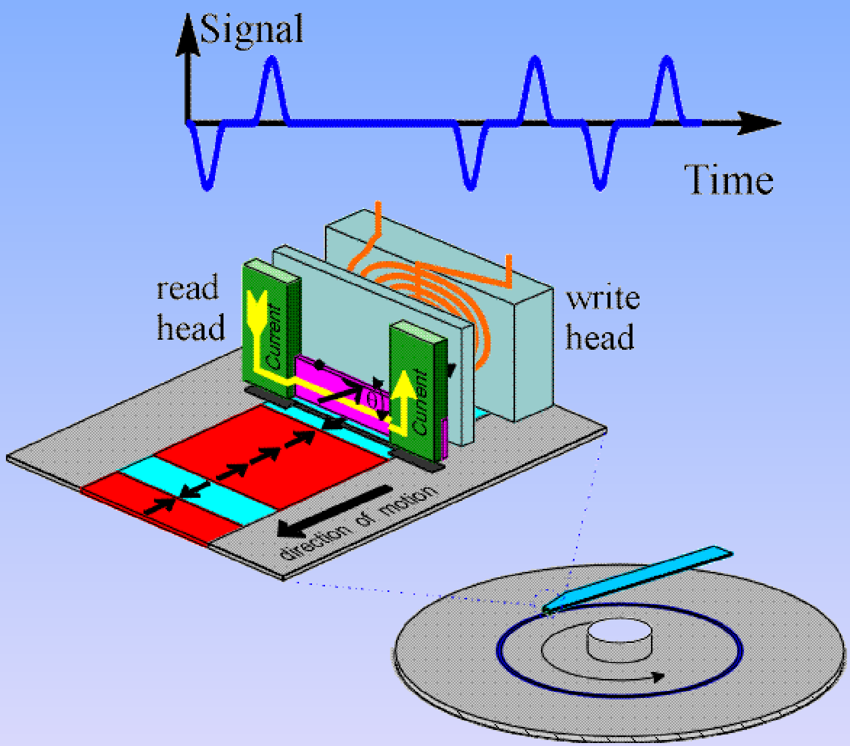
S. Yuasa et al. (2004)

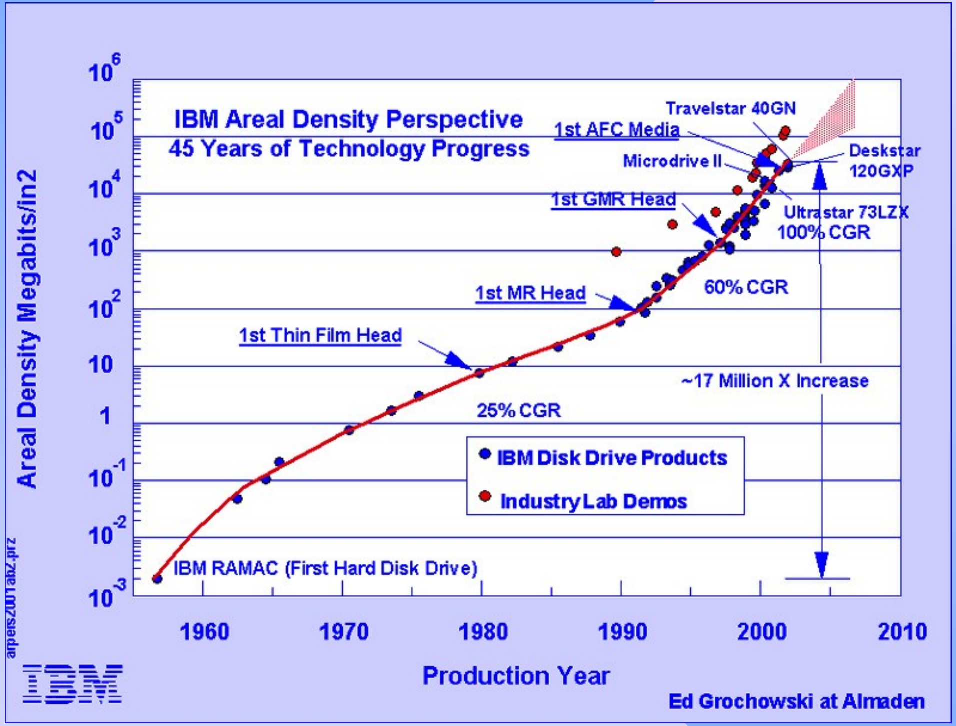
Bias dependence:
Mixed FeO interface



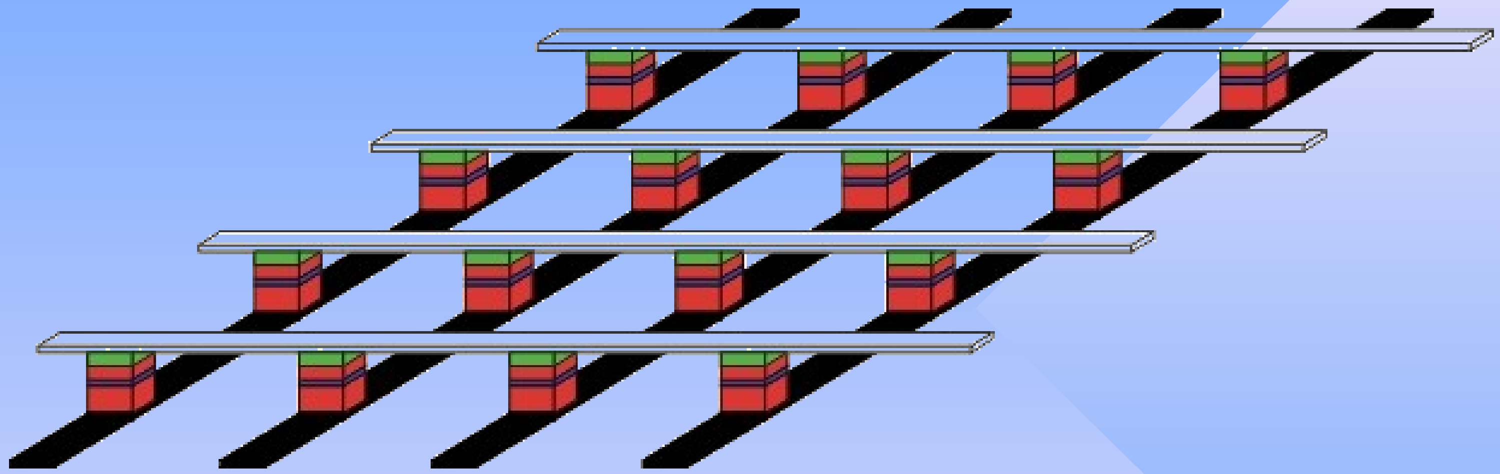


Applications of XMR elements: Read Heads



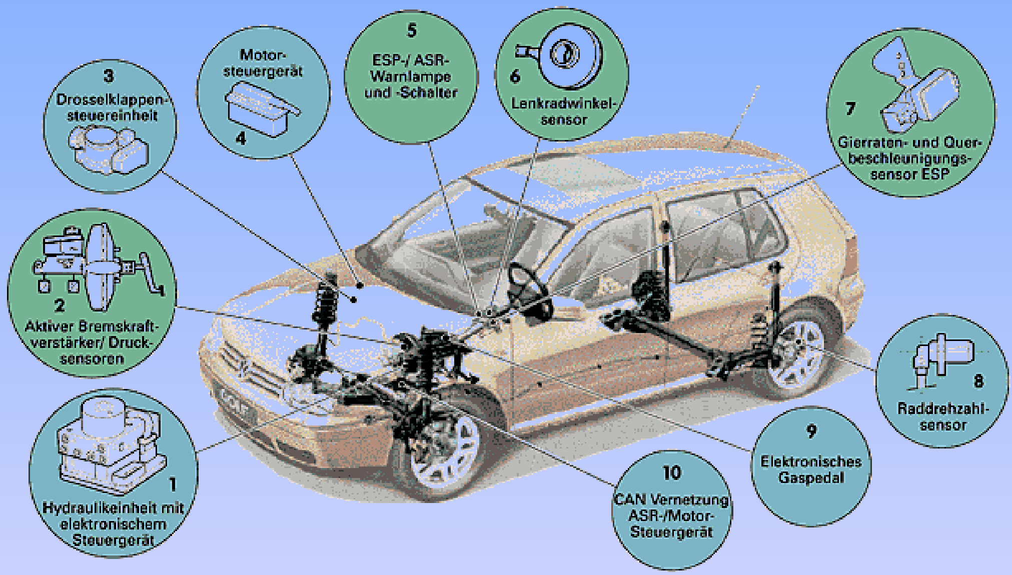


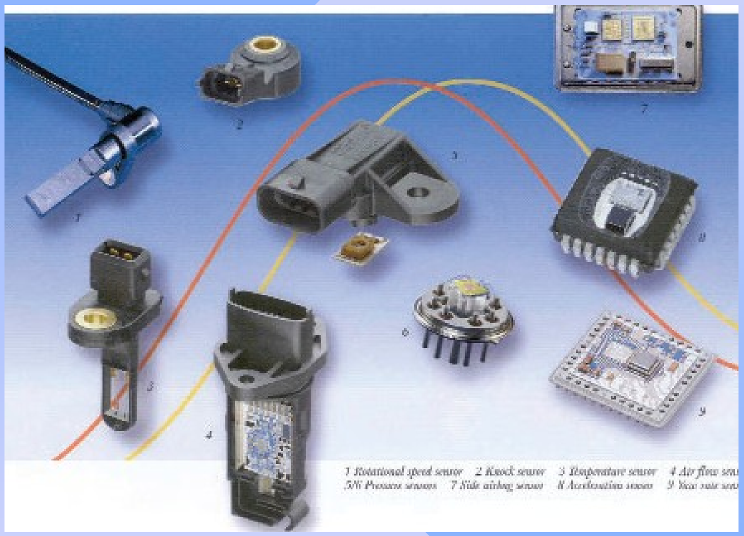
Applications of XMR elements: MRAM



Applications of XMR elements: Sensors

Elektronisches Stabilitätsprogramm (ESP)

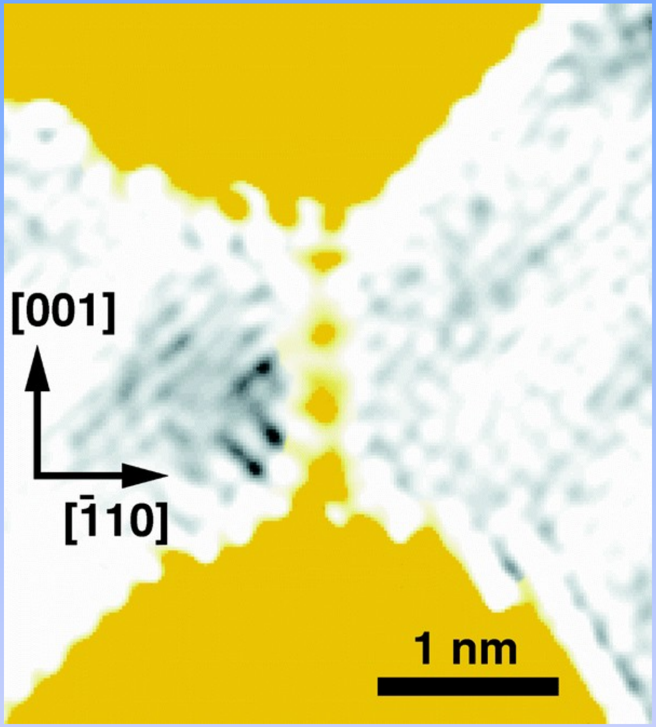




Technololgische Anforderungen

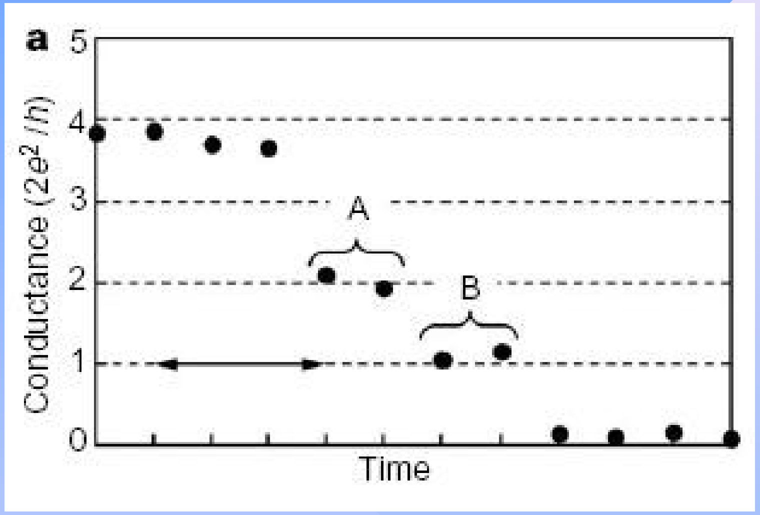
- Temperaturstabilität
  Automobil : bis 400 °C
  Back-End-Prozess: bis 250 °C
- Winkelgenauigkeit Drehsensor: 0.01 °
- Reversibilität der Ummagnetisierung:
  MRAM Schaltzyklen $\geq 10^{15}$

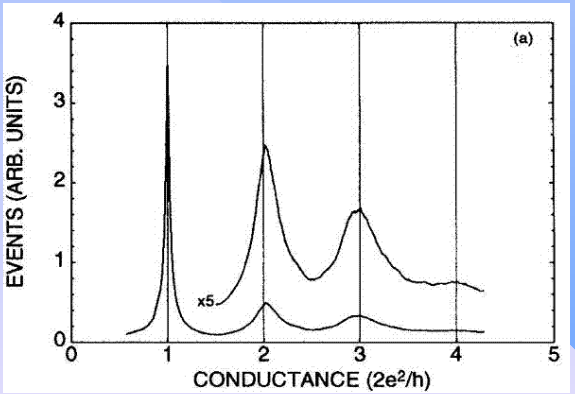
Metallic nanocontacts



H. Ohnishi, Yu. Kondo, K. Takayanagi,
Nature **395,** 780 (1998)

Conductance





M.Brandbyge, Phys.Rev. B **52**, 703 (1995)

Summary

Electronic structure

- Self-consistent treatment of structures with realistic dimensions by Screened-KKR Green's function formalism
- Microscopic processes are elucidated by ab-initio transport theory
- Nanostructure tailoring by theoretical material design

GMR

- Intrinsic GMR is caused by band matching in one spin channel
- GMR ratio can be changed, even inverted by additional defects

TMR

- Electronic structure of the leads influences conductance, I(V), and TMR
- Interface structure is decisive to tailor TMR

Summary

- Electronic structure of the leads influences conductance, I(V), and TMR
- Interface structure is decisive to tailor TMR
- Evolution of TMR with external bias reflects transmission of the lead eigenstates and resonances in the limit of coherent tunneling

Thanks to

- Ingrid Mertig
- Jörg Binder, Jörg Opitz, Frido Erler
- Rudi Zeller, Peter Dederichs and the Jülich gang
- Bogdan Yavorsky, Dima Fedorov