Transport phenomena in metallic nanostructures

Peter Zahn

Vortrag im Rahmen des Habilitationsverfahrens an der TU Dresden

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Outline

Introduction

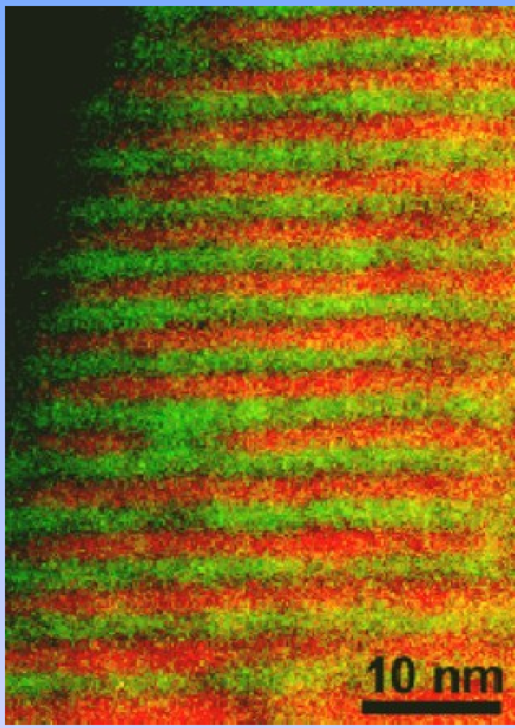
Electronic Structure and Transport Theory

Applications

- Transport properties of ultrathin films: Cu
- Conductance of Fe/V and Mo/V multilayers: H loading
- Tunneling MagnetoResistance: Interface structure

Summary

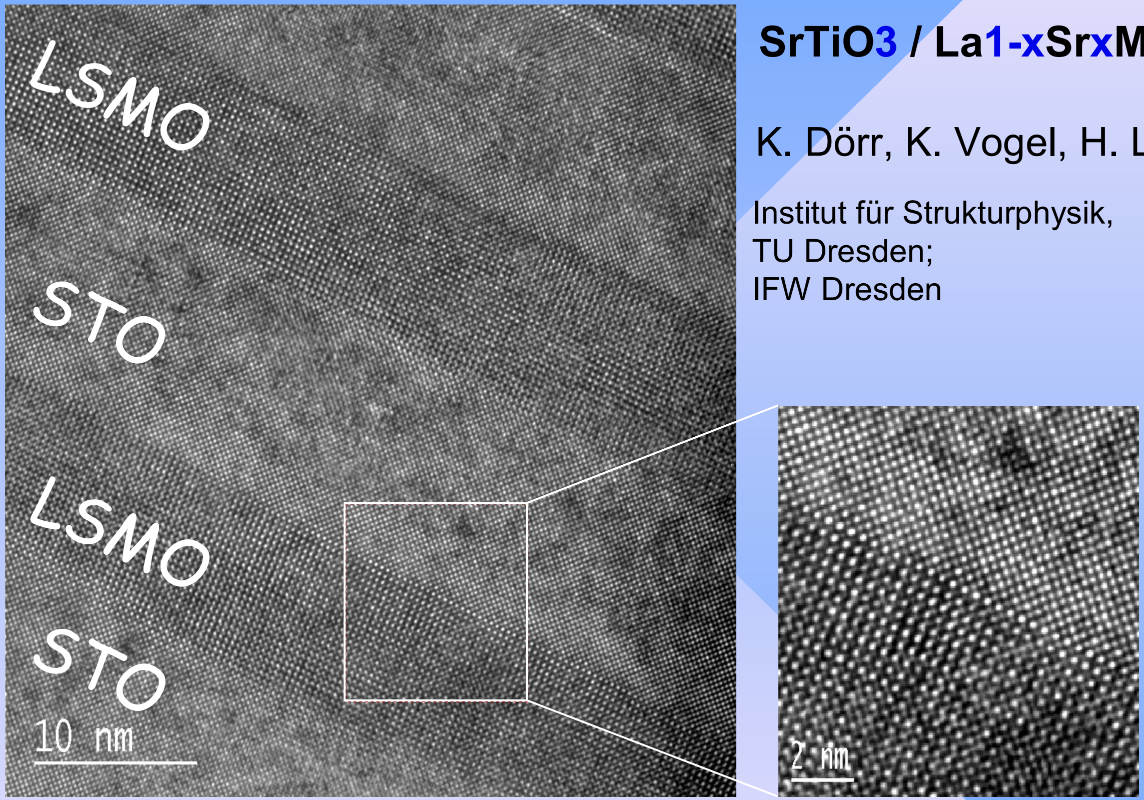
Material design on the atomic scale



Co/Cu

W. Brückner et al.

IFW Dresden



$SrTiO_3$ / $La_{1-x}Sr_xMnO_3$

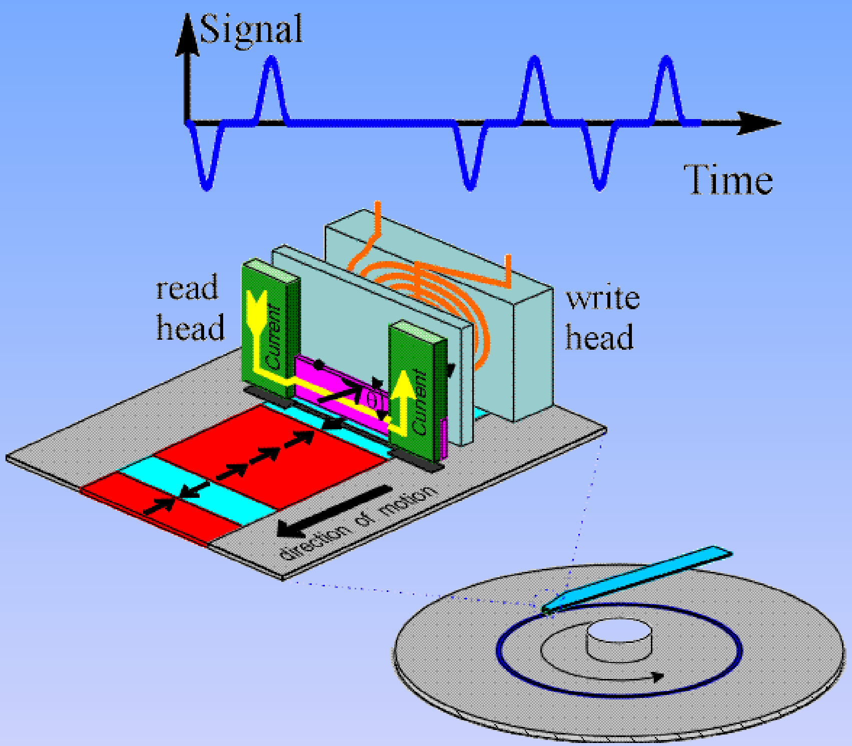
K. Dörr, K. Vogel, H. Lichte

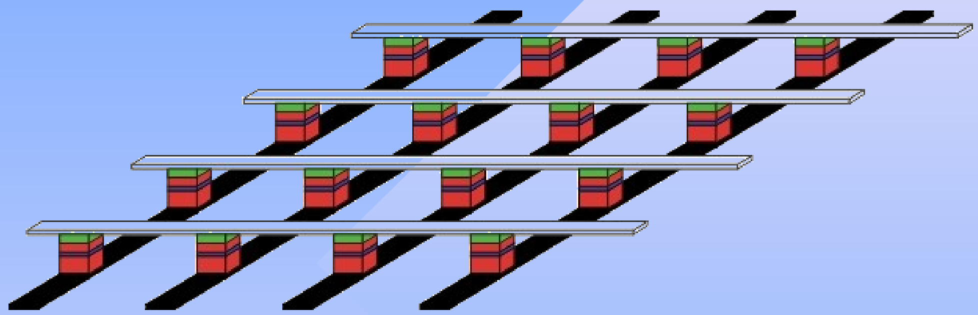
Institut für Strukturphysik,
TU Dresden;
IFW Dresden

Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden

IAPD

Applications of magneto-resistive elements





Hard disk read head

Magnetic **R**andom **A**ccess **M**emory (MRAM)

(IBM)

(VDI-Verlag)

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Electronic structure

- Kohn-Sham equation

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

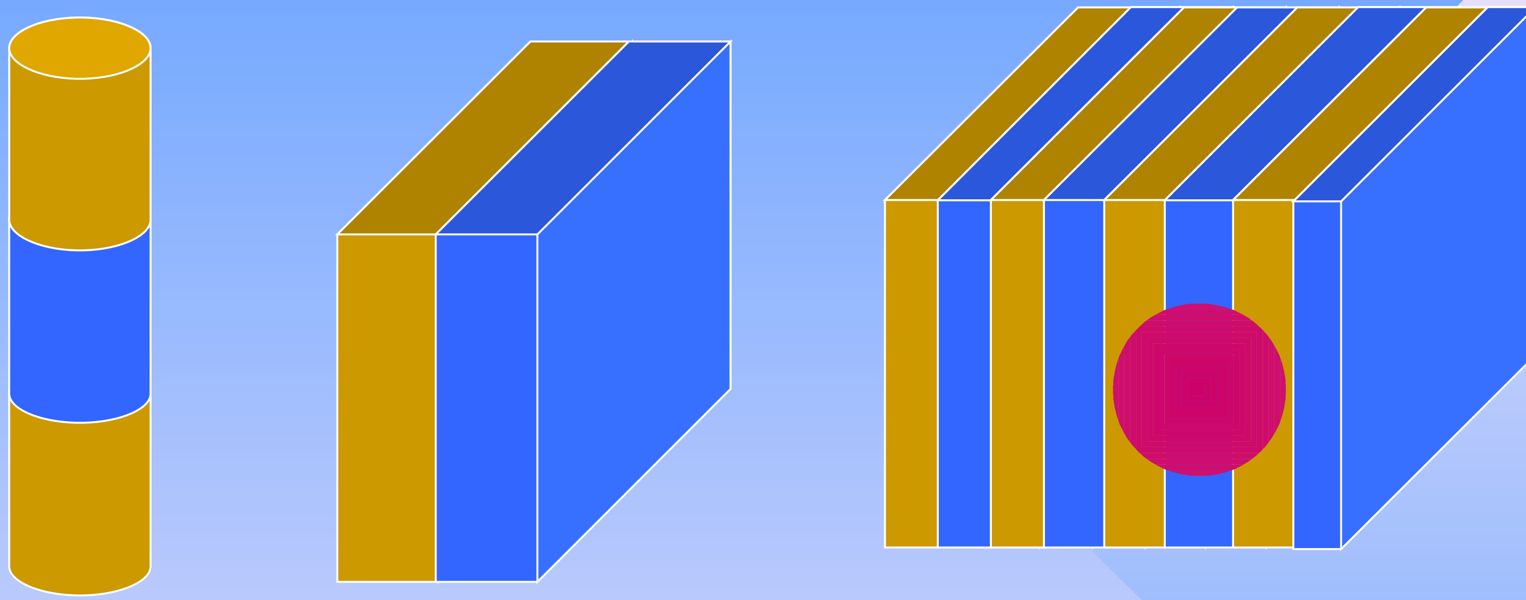
- Green's function

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

- Dyson equation

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

Screened KKR



1D 2D 3D

- Linear scaling of computational effort
- Systems of different dimensionality
- Treatment of defects: $\mathcal{G} = \mathring{\mathcal{G}} + \mathring{\mathcal{G}}\, \Delta V\, \mathcal{G}$

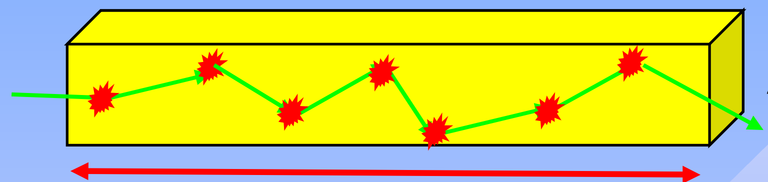
Transport theory

Resistance

Diffusive

Conductance

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



A

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

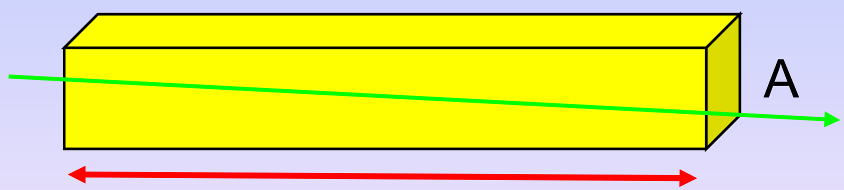
$$\lambda \ll L$$

Resistivity ρ

Conductivity σ

Ballistic

$$R \not\propto L$$



A

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

$$\lambda > L$$

Diffusive transport: Boltzmann equation

- One-particle distribution function

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\frac{\partial f_k}{\partial \mathbf{r}} + \frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t}\frac{\partial f_k}{\partial \mathbf{k}} - \left.\frac{\partial f_k}{\partial t}\right|_{scatt} = 0$$

- Scattering term

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

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

- Linearized Boltzmann equation

$$\mathbf{\Lambda}_k = \tau_k^B\left[\mathbf{v}_k + \sum_{k'} P_{kk'}\mathbf{\Lambda}_{k'}\right] \quad \text{with} \quad \tau_k^B = \left[\sum_{k'} P_{kk'}\right]^{-1}$$

! Iterative solution

! Relaxation time approximation

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

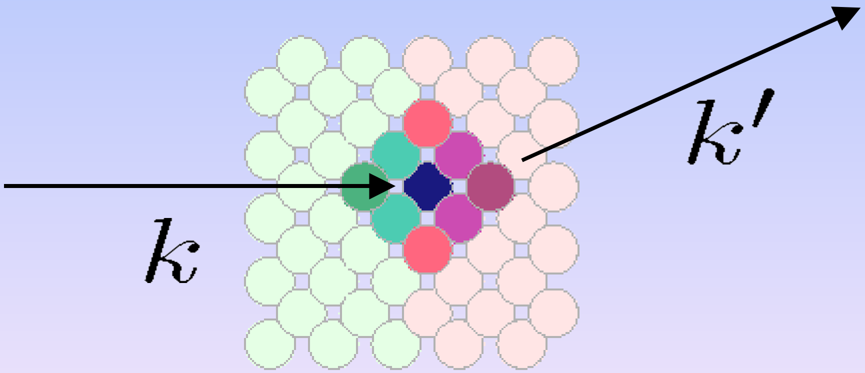
Transition probability

- Microscopic transition matrix

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

- Transition probability

$$P_{kk'} = 2\pi c N \,|T_{kk'}|^2$$



Transport coefficients

- Residual conductivity

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

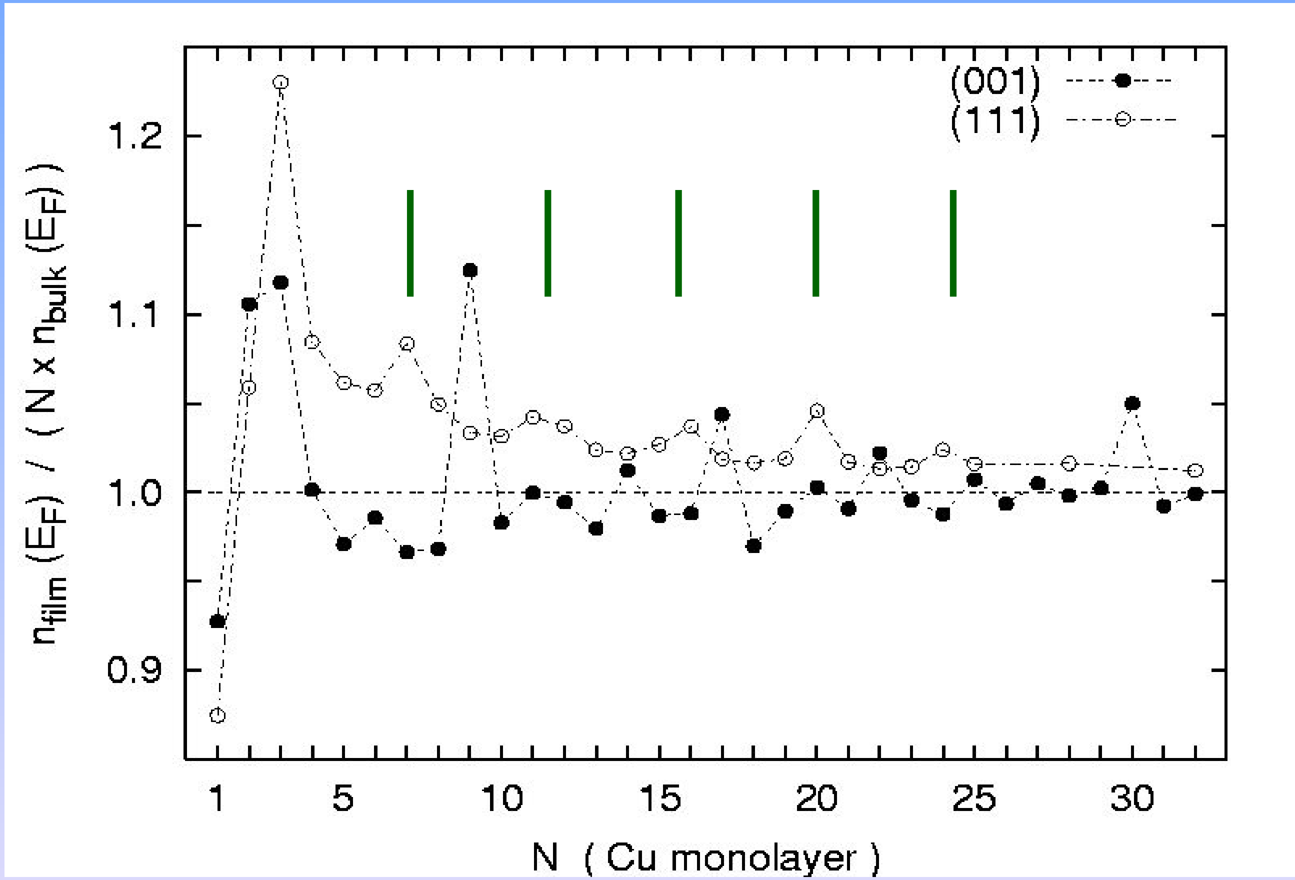
$$= \frac{e^2}{(2\pi)^3} \oint_{E_k=E_F} \frac{\mathrm{d}S}{v_k} v_k^i v_k^j \tau_k^B$$

Relaxation time approximation

- Plasma frequency

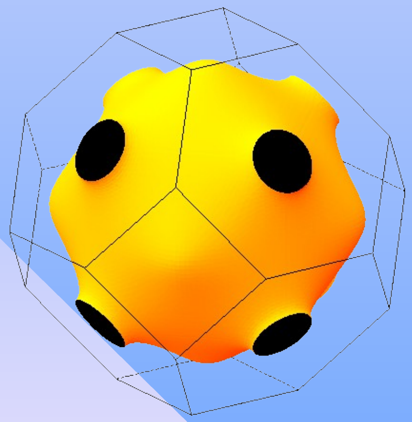
$$\omega_P^2 \propto \oint_{E_k=E_F} \frac{\mathrm{d}S}{v_k} \mathbf{v}_k^2$$

Ultrathin films: Density of states oscillations



Cu(001)

Cu(111)

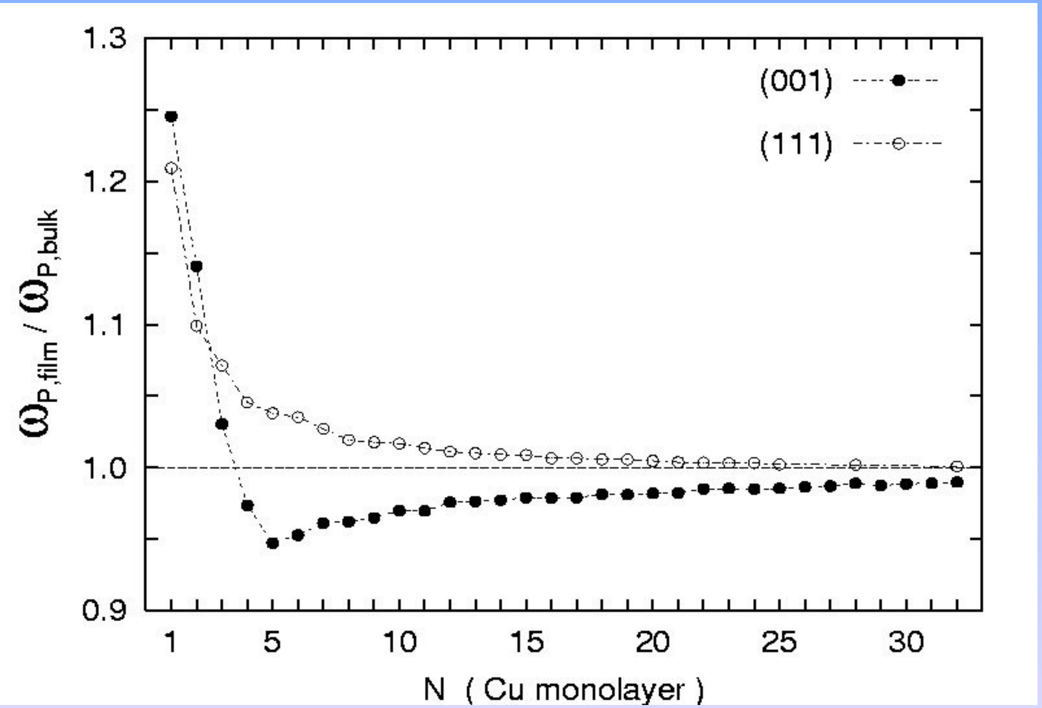


$$\lambda_{(001)} = 2.56ML \quad 5.88ML$$
$$\lambda_{(111)} = 4.33ML$$

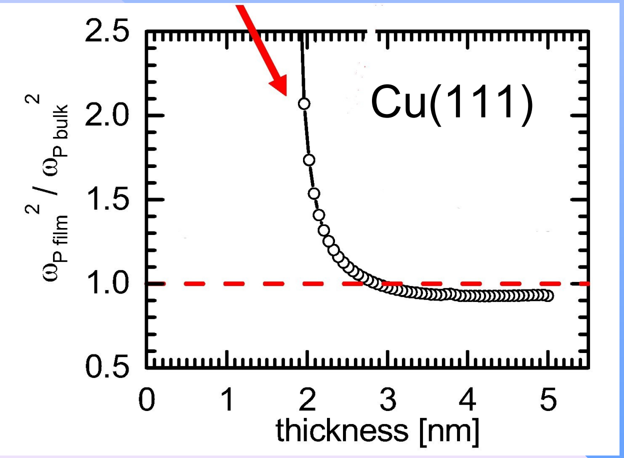
Transport properties of ultrathin films

Plasma frequency

Cu(001) Cu(111)



D. Fedorov et al., Thin Solid Films **473**, 346 (2005)

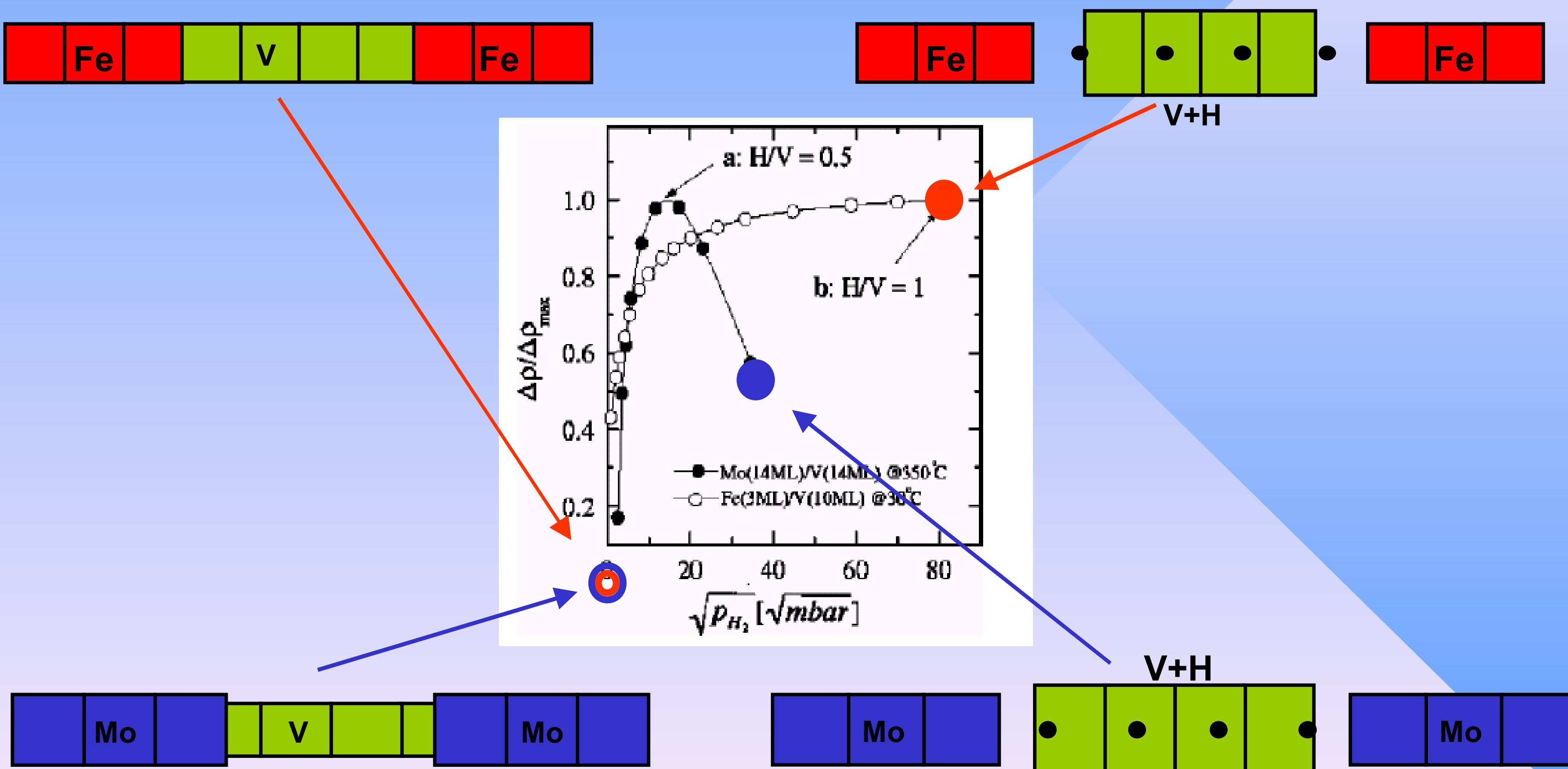


Experiment:

G. Fahsold, priv. Comm. (2005)

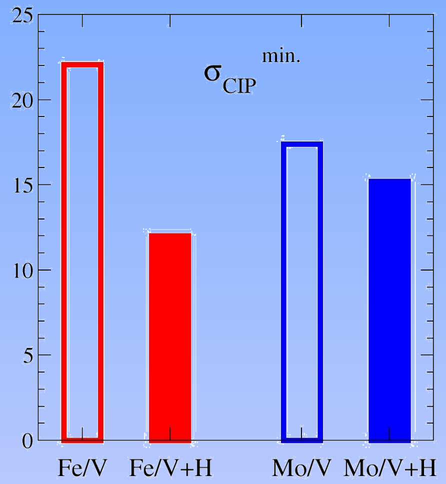
Transport properties of multilayers

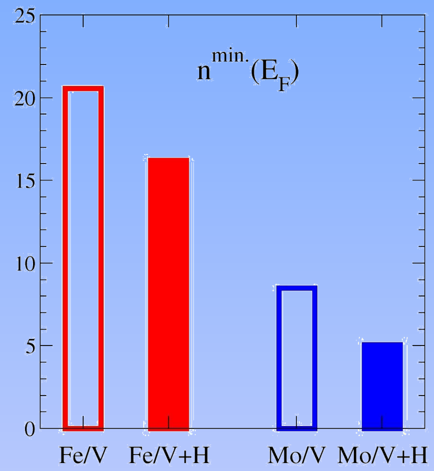
Fe/V and Mo/V(001) under H loading

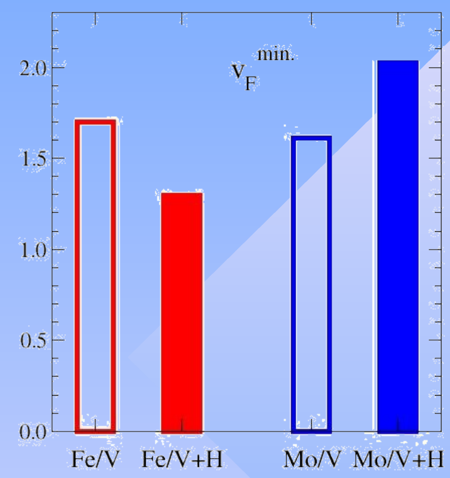


Fe/V and Mo/V(100) under H loading

The role of V expansion

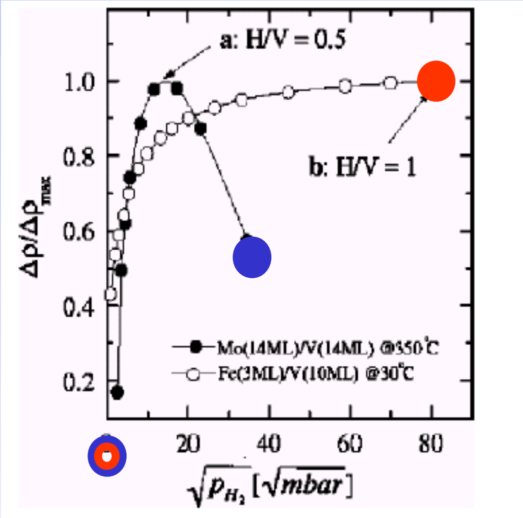






Fe/V

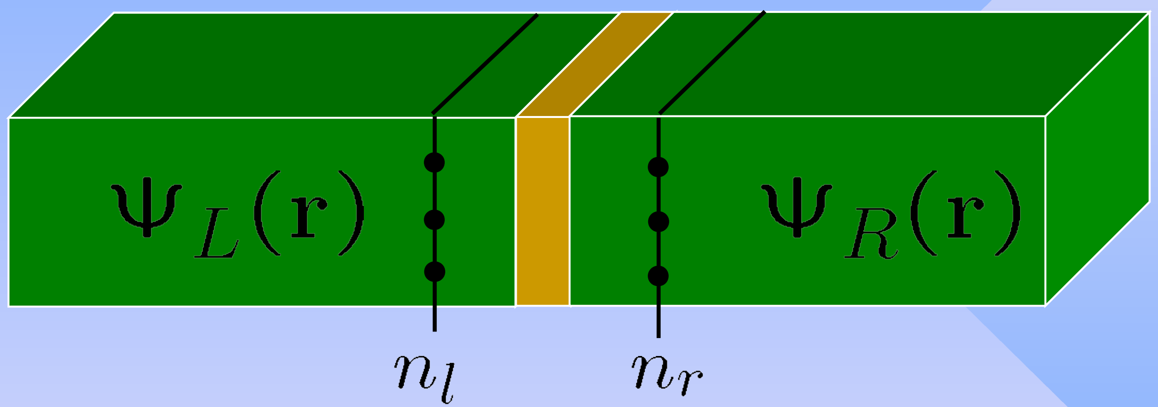
Mo/V



V. Meded et al.,
PRB **69**, 205409 (2004)

Coherent transport: Landauer conductance

$$g = g_0 \sum_{L,R} T_{LR}(E_F) = g_0 \sum_{\sigma} \int d\mathbf{k}_{||} T^{\sigma}_{\mathbf{k}_{||}}(E_F)$$



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

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

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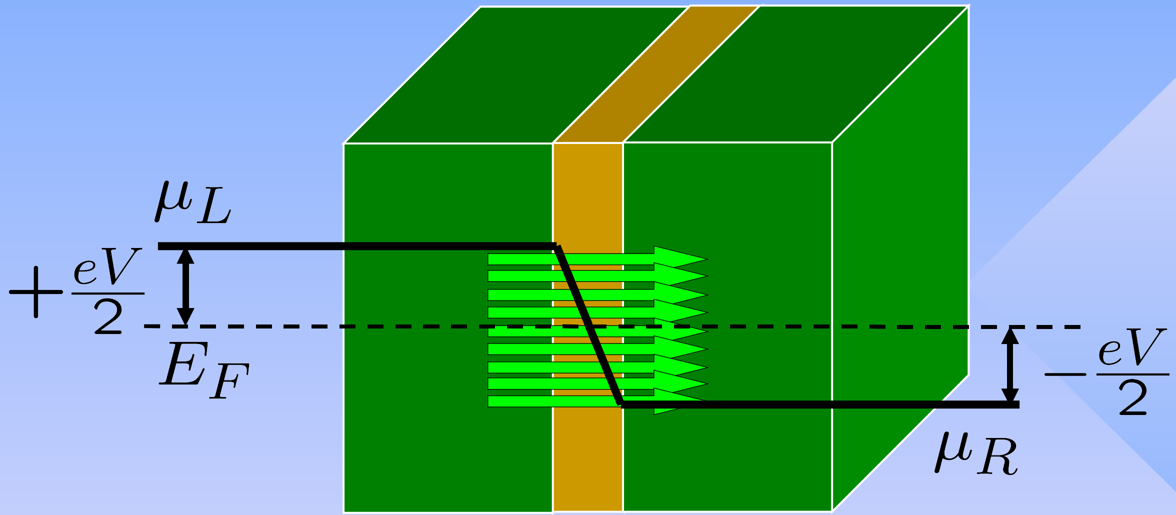
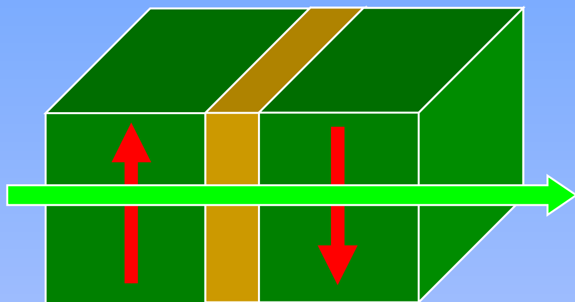
Applying a bias voltage

Rigid-band model



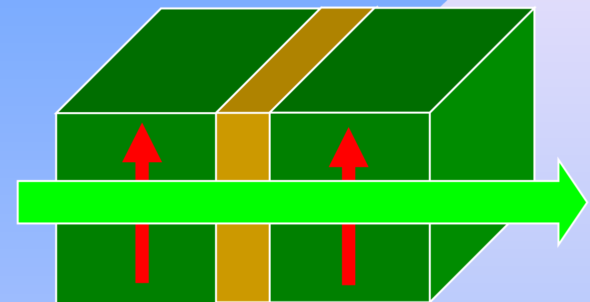
$$I(V) = g_0 \frac{1}{e} \int_{\mu_R}^{\mu_L} dE\; T(E,V)$$

Tunneling MagnetoResistance



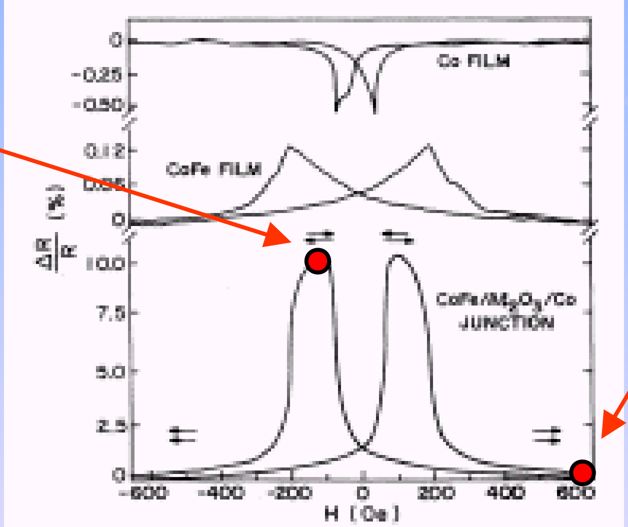
AP

g



P

g



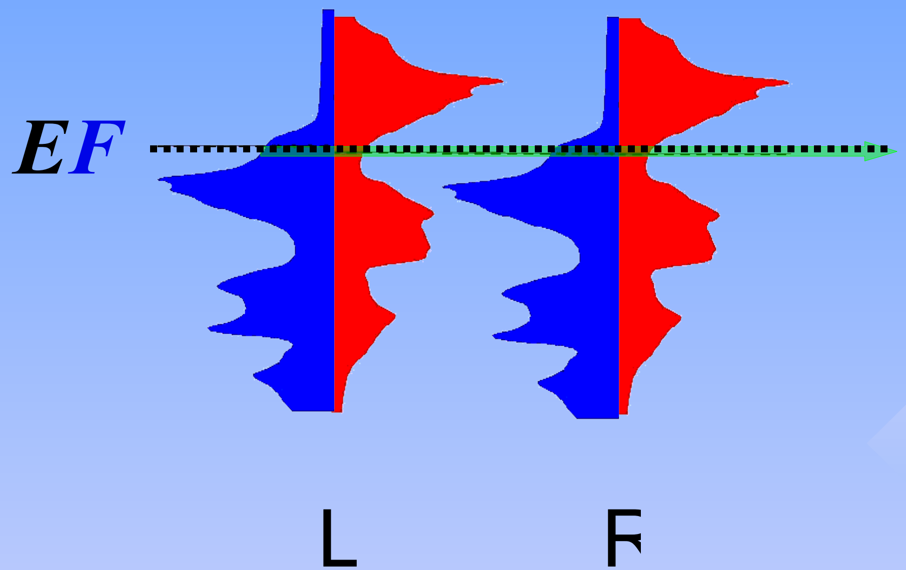
J. Moodera et al.,
PRL 74, 3273 (1995)

$$TMR_1 = \frac{g^P - g^{AP}}{g^{AP}}$$

$$TMR_2 = \frac{g^P - g^{AP}}{g^P + g^{AP}}$$

The Julliere model

Phys. Lett. **54A**, 225 (1975)

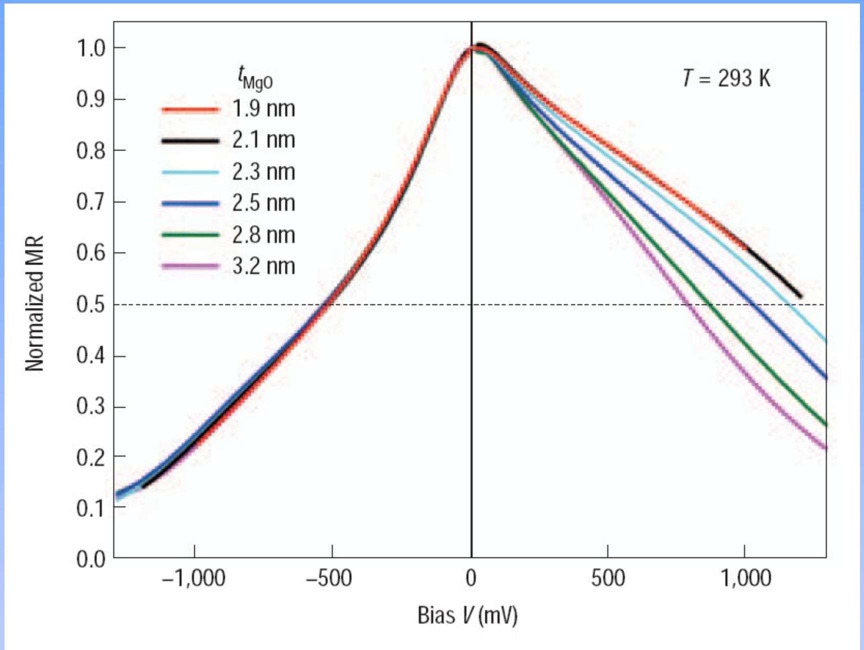


$$TMR_1 = \frac{2P_L P_R}{1-P_L P_R} \qquad P_{L,R} = \frac{n^\uparrow - n^\downarrow}{n^\uparrow + n^\downarrow}$$

	Fe	Co	Ni
P	44 %	34 %	11 %
TMR_1	48 %	26 %	1 %

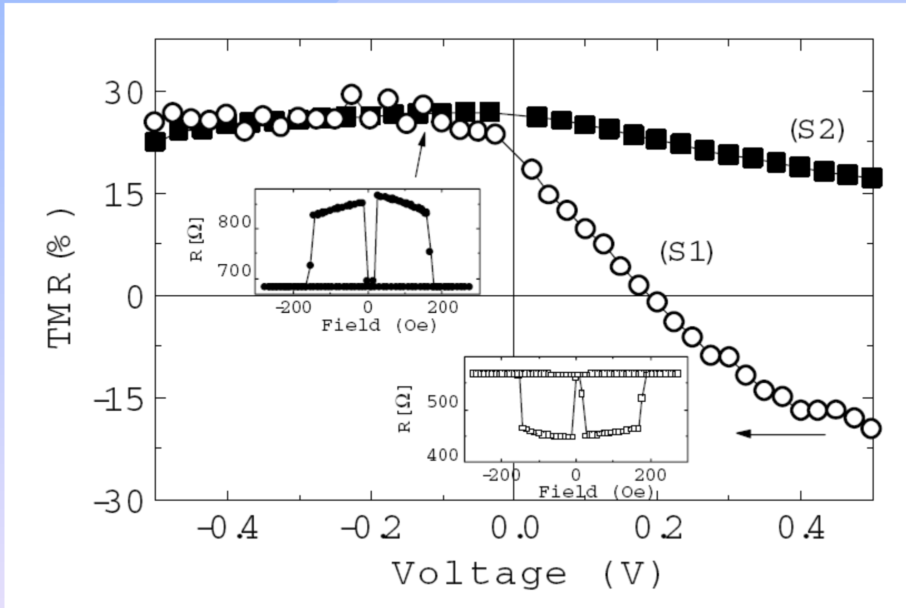
P.M. Tedrow and R. Meservey, PRB **7**, 318 (1973)

New experimental results: Fe/MgO/Fe



S. Yuasa et al.
Nature Materials **3**, 868 (2004)
S. Parkin et al.
Nature Materials **3**, 862 (2004)

TMR1 > 180 %



Tiusan et al.
PRL **93**, 106602 (2004)

contradiction to Julliere‘s model

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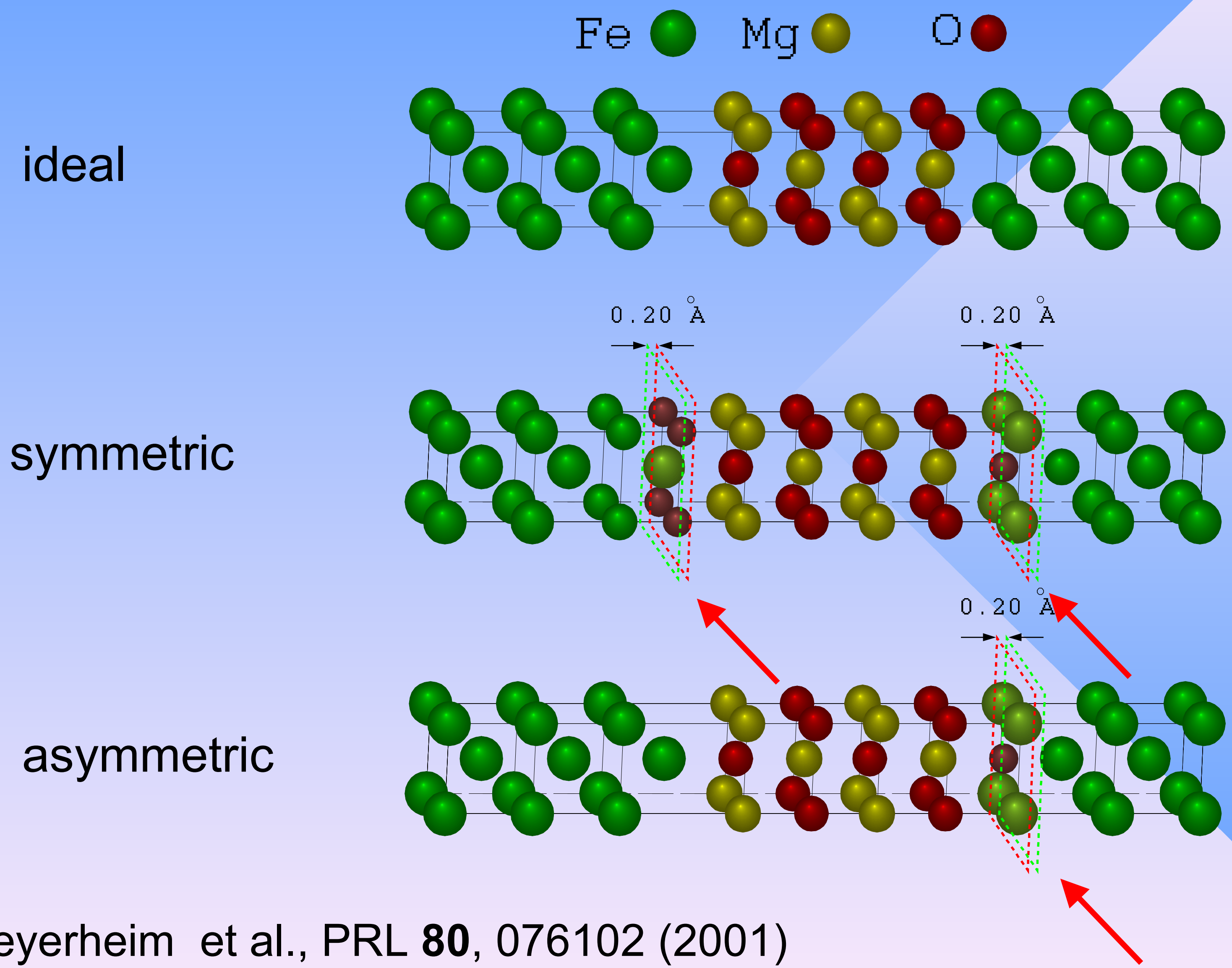
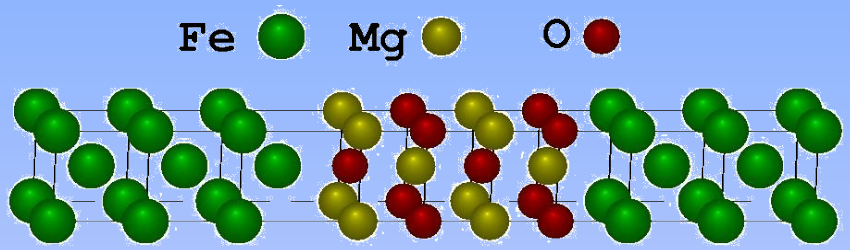
Investigated systems

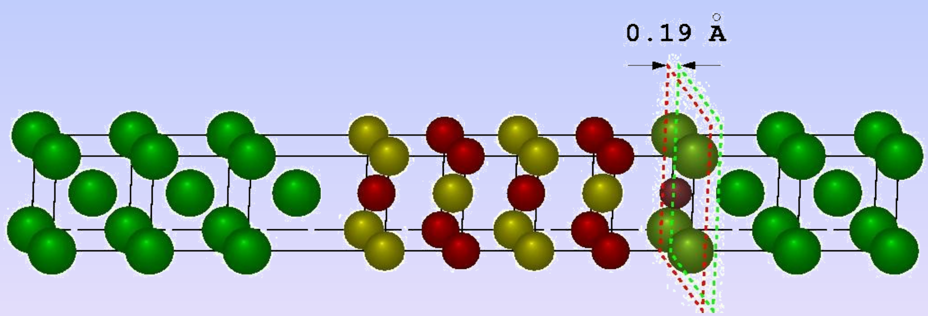


H.L. Meyerheim et al., PRL **80**, 076102 (2001)

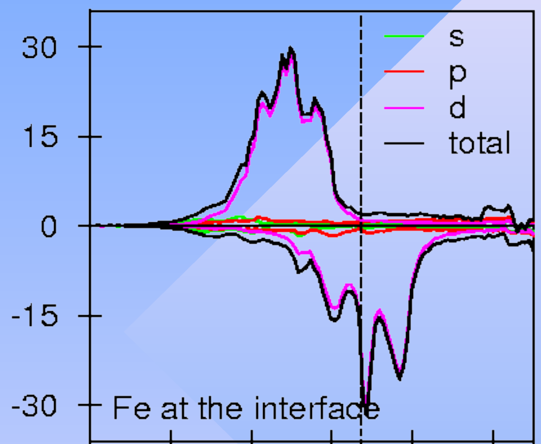
Charge self consistency

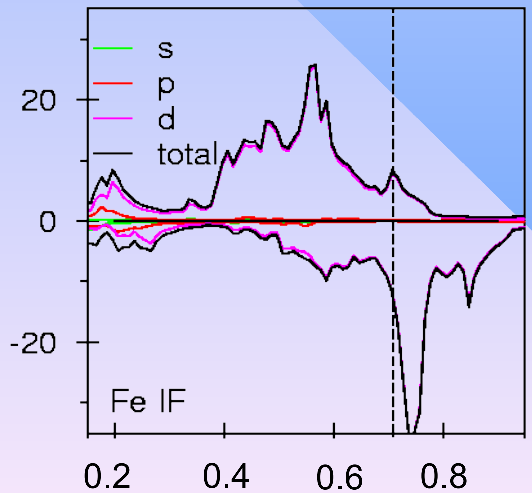
- Supercell calculation



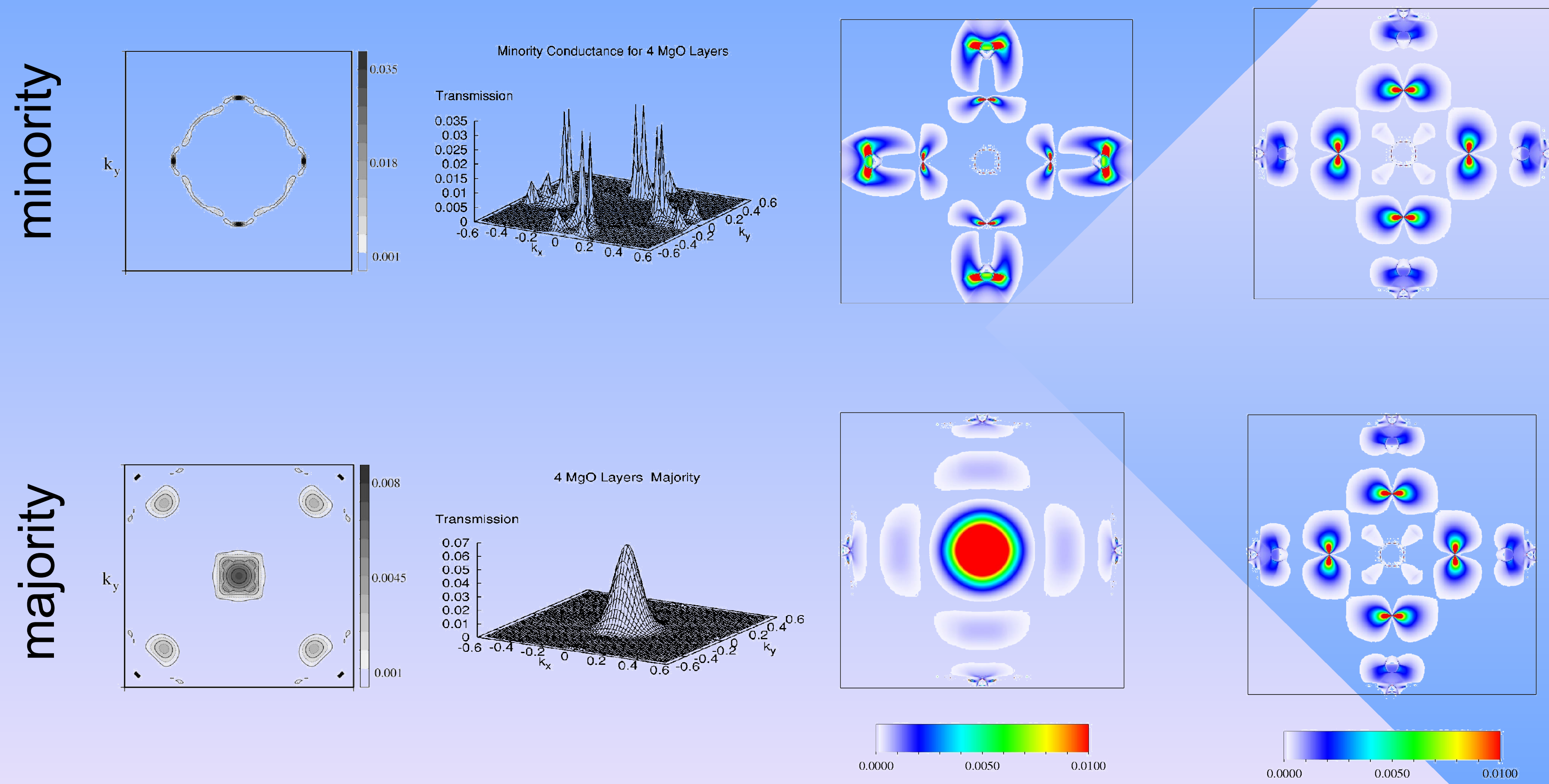


- Density of States



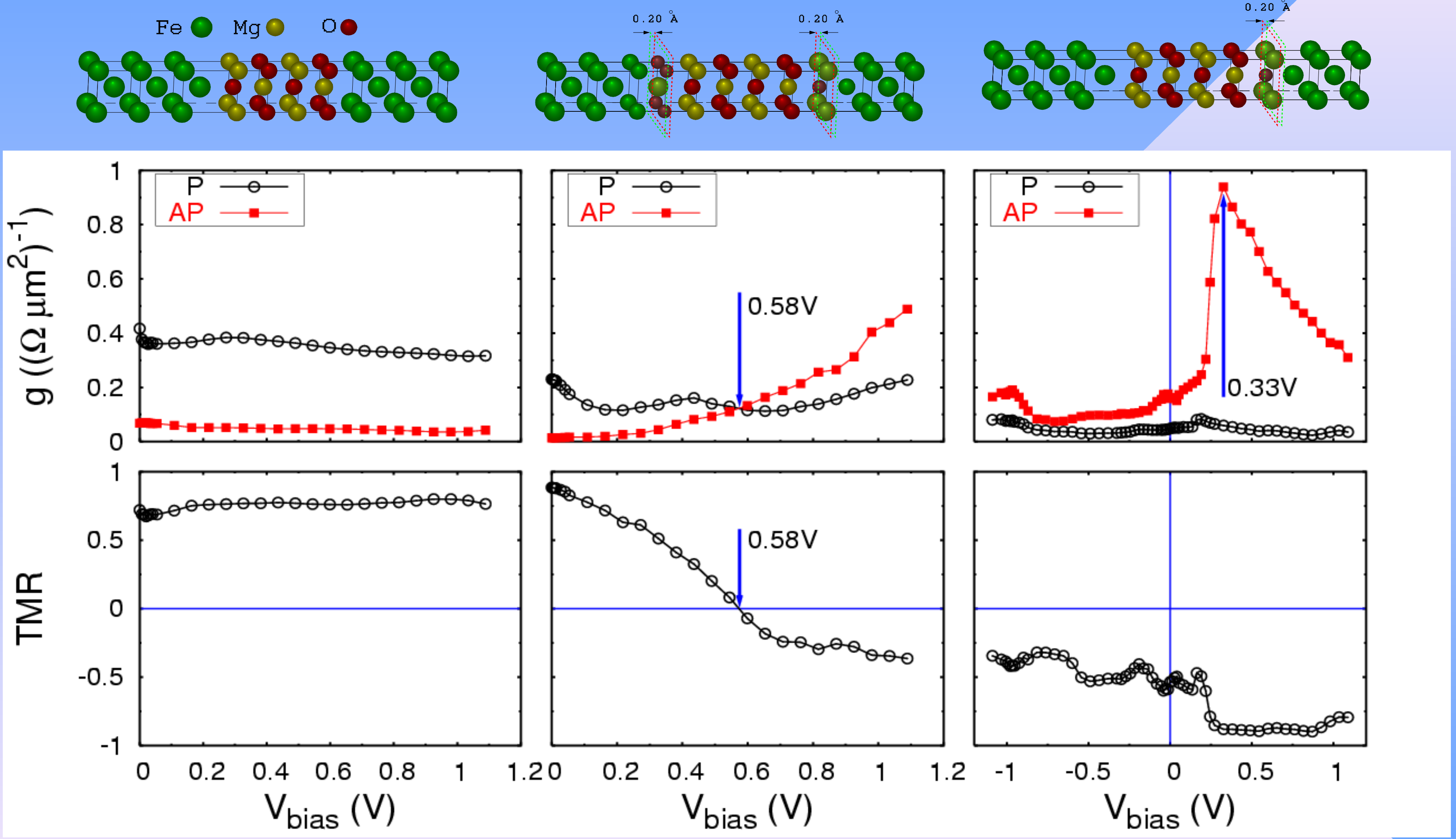


Transmission $T(\mathbf{k}_k, E_F)$: Fe/4MgO/Fe



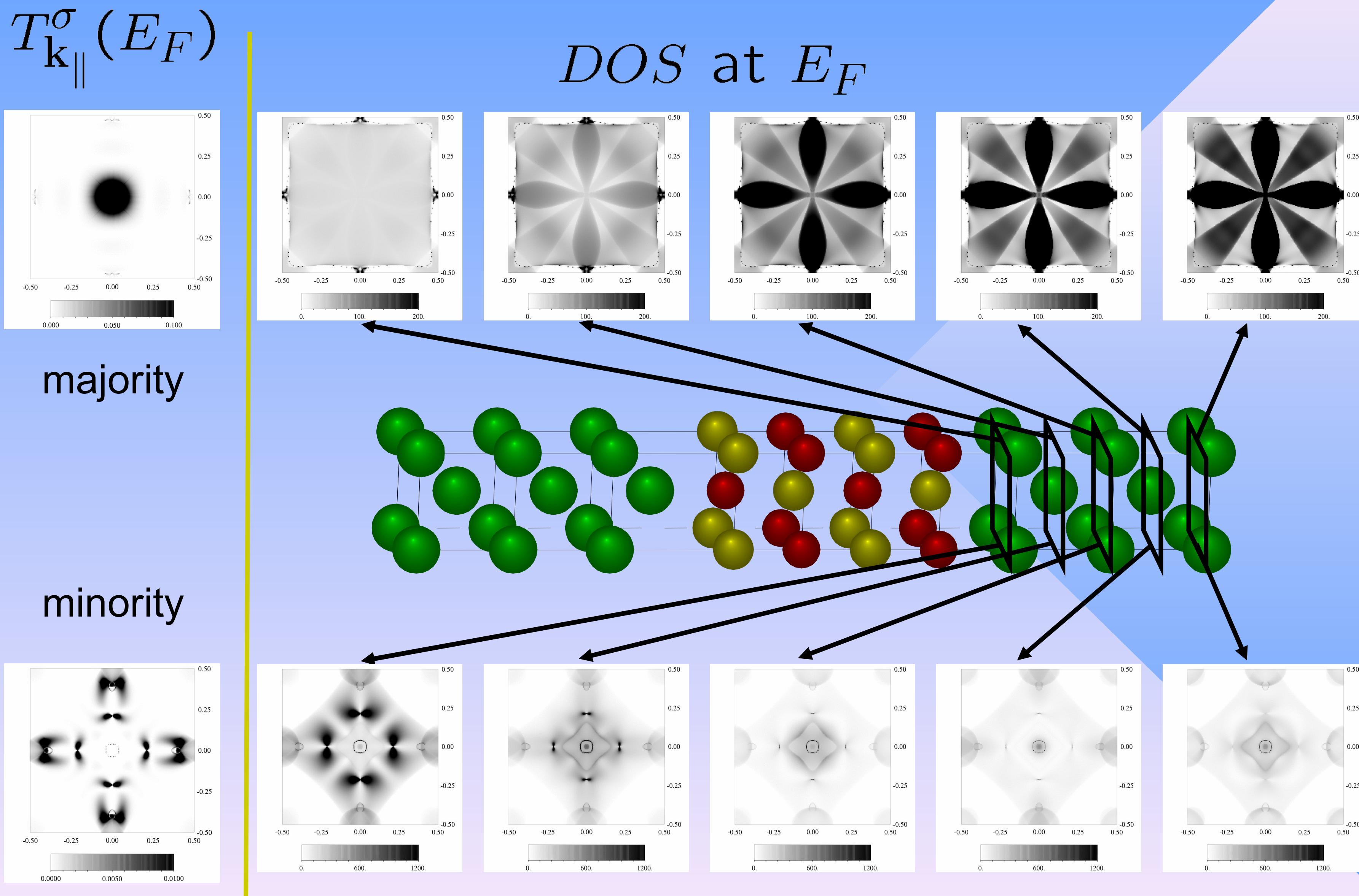
Mathon et al. 2001 Butler et al. 2001 P configuration AP configuration

Bias dependence: TMR

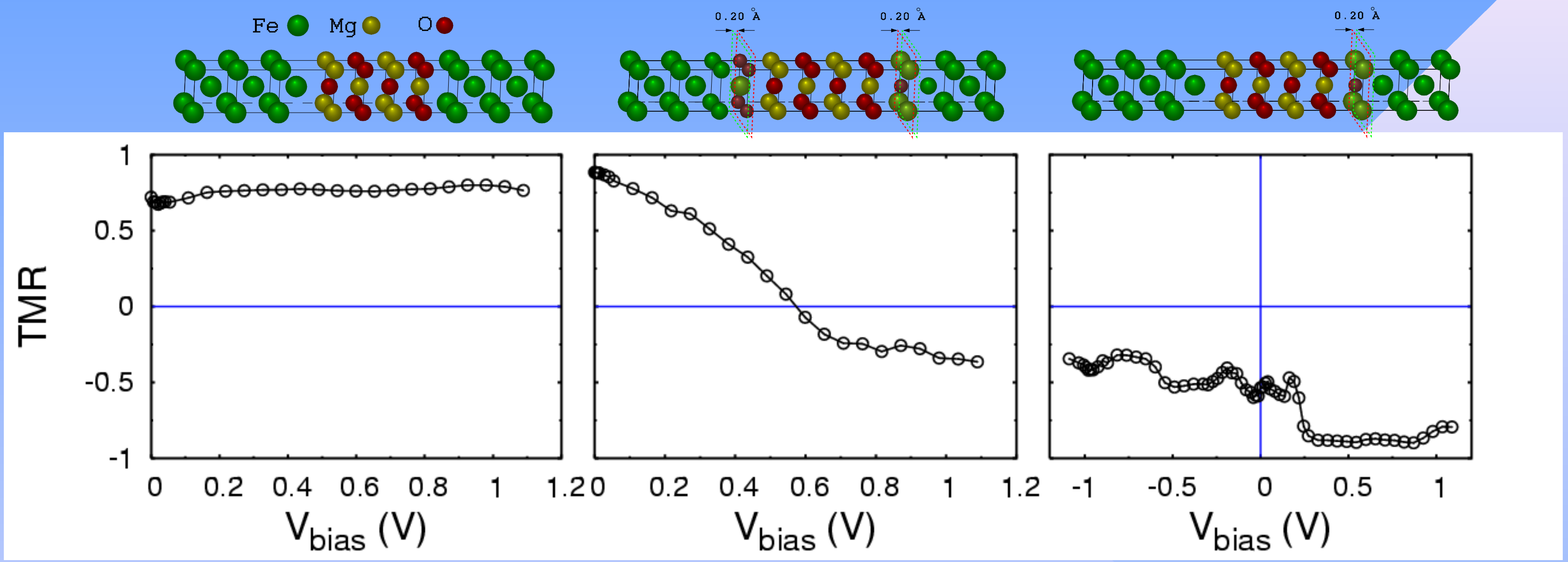


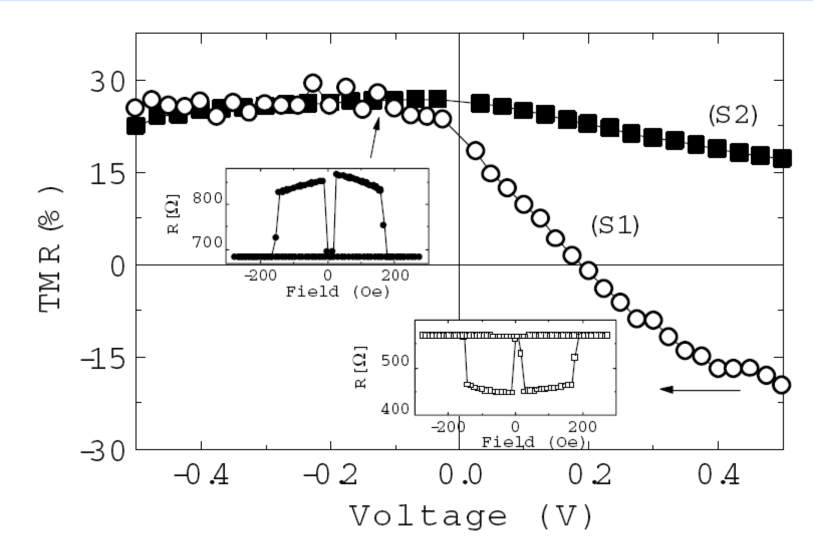
Ch. Heiliger et al., subm. to PRL (2005)

Transmission and local DOS



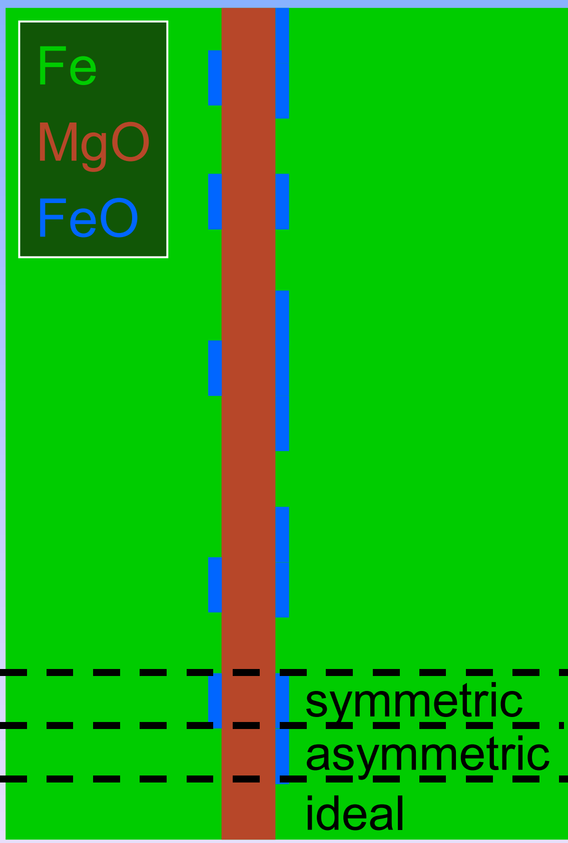
Comparison with experiment

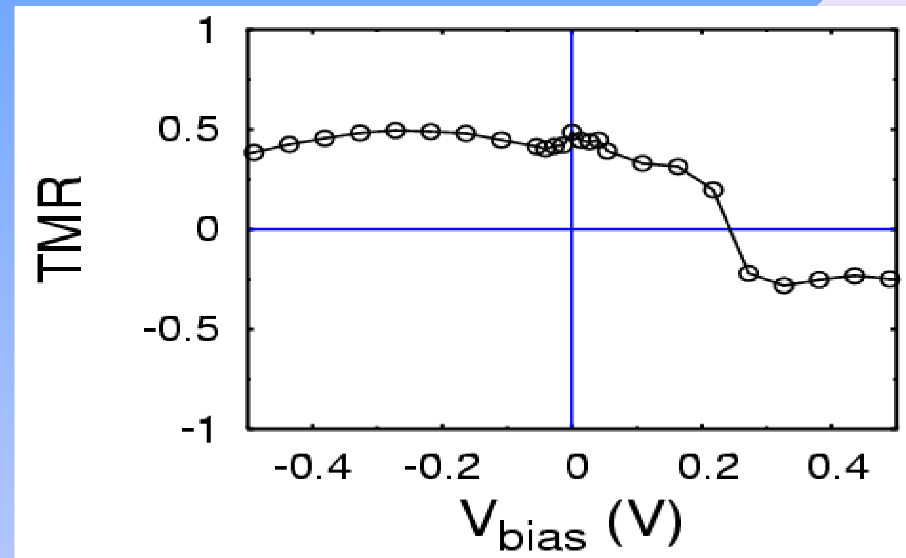


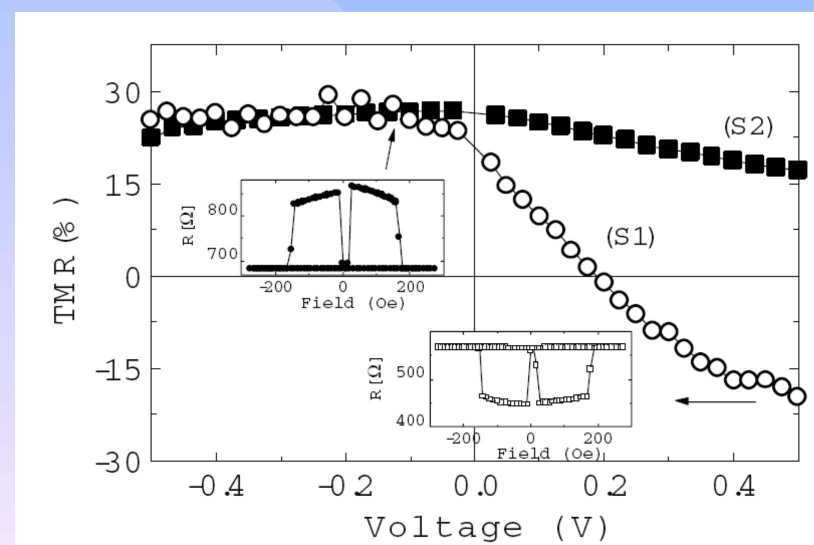


Tiusan et al.,
PRL 93, 106602 (2004)

Variation of interface structure







Tiusan et al., PRL 93, 106602 (2004)

Summary

- Screened-KKR Green‘s function formalism allows the self consistent treatment of nanostructures of realistic dimensions
- Microscopic origin of transport phenomena can be elucidated by ab-initio theory
- Optimization of nanostructures by „Theoretical material design“

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Zusammenfassung

- Screened-KKR Greenscher Funktions-formalismus gestattet selbstkonsistente Behandlung von Nanostrukturen realistischer Dimension
- Beschreibung der mikroskopischen Prozesse durch ab-initio Transporttheorie
- Optimierung von Nanostrukturen durch „Theoretisches Material Design“

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