Including Effects of Band Structure and Disorder in Spin Transport Calculations

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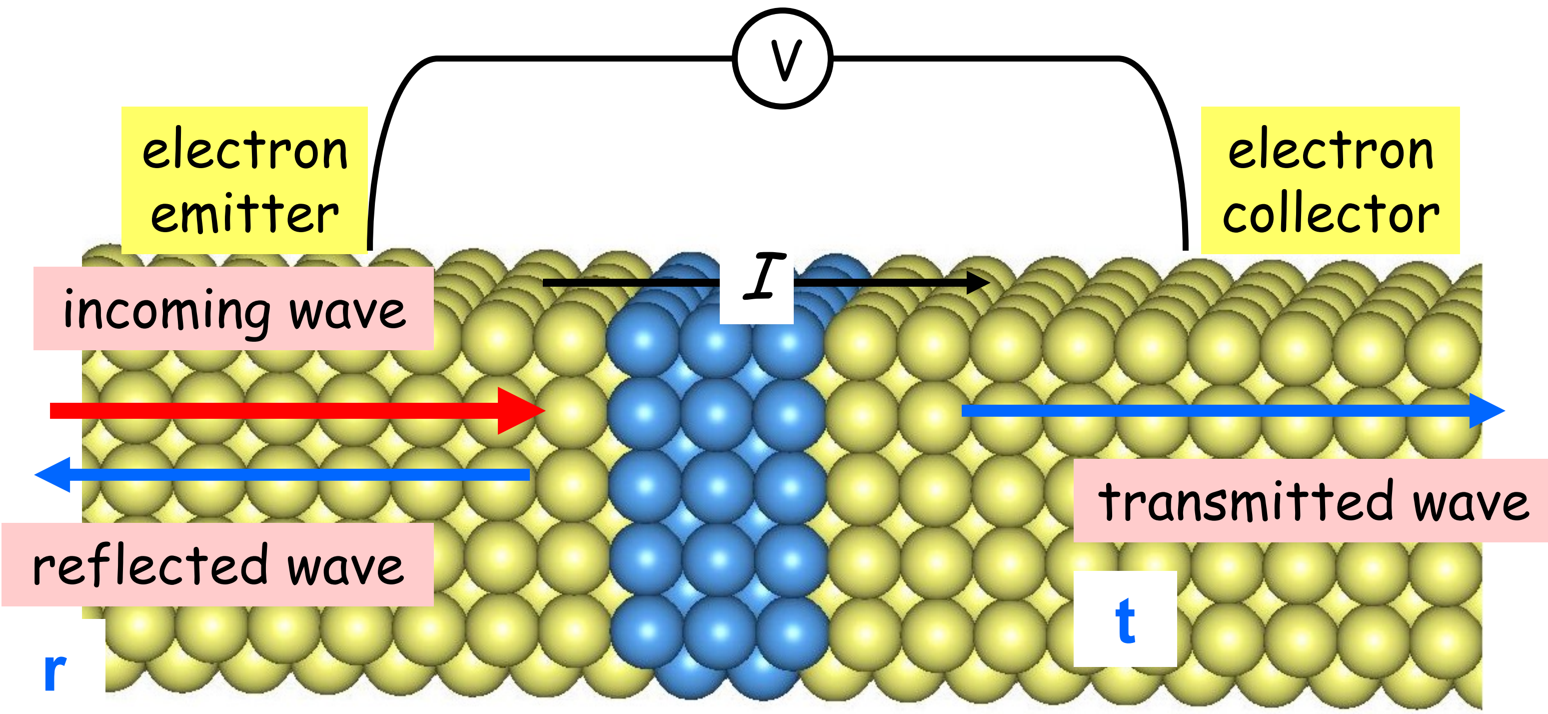
Landauer-Büttiker Formulation of Electron Transport



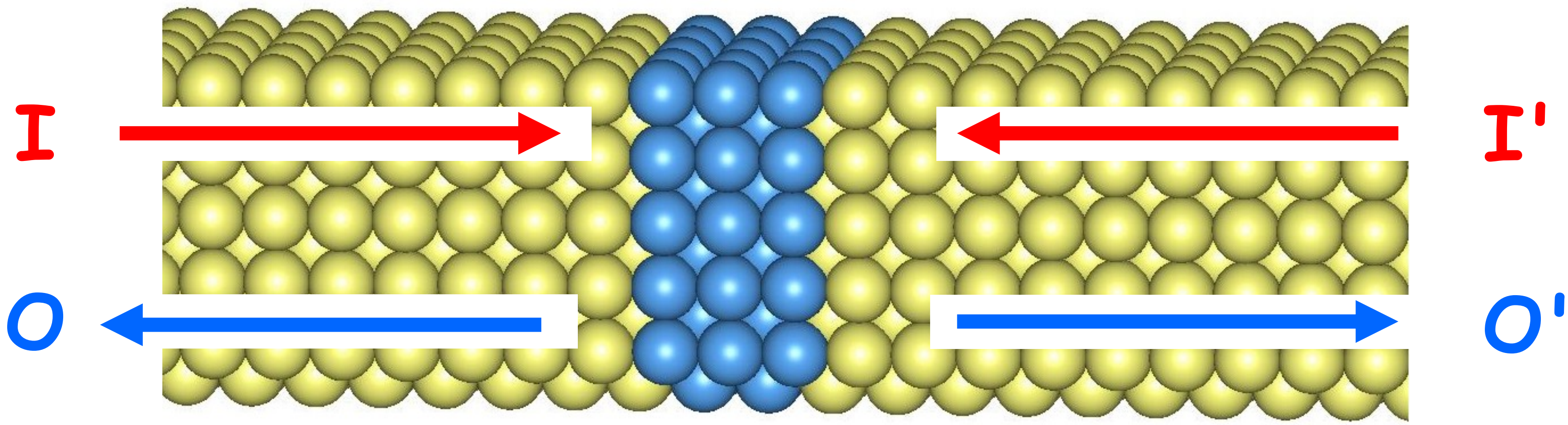
conductance:

$$G = \frac{dI}{dV} = \frac{2e^2}{h}\mathrm{Tr}\{\mathbf{t}\,\mathbf{t}^\dagger\}$$

transmission

Scattering Theory of Electron Transport

on the atomic scale electrons are wavelike

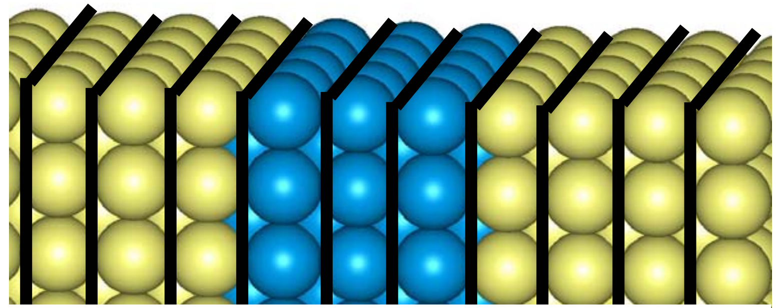


$$\begin{pmatrix} O \\ O' \end{pmatrix} = \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} I \\ I' \end{pmatrix}$$

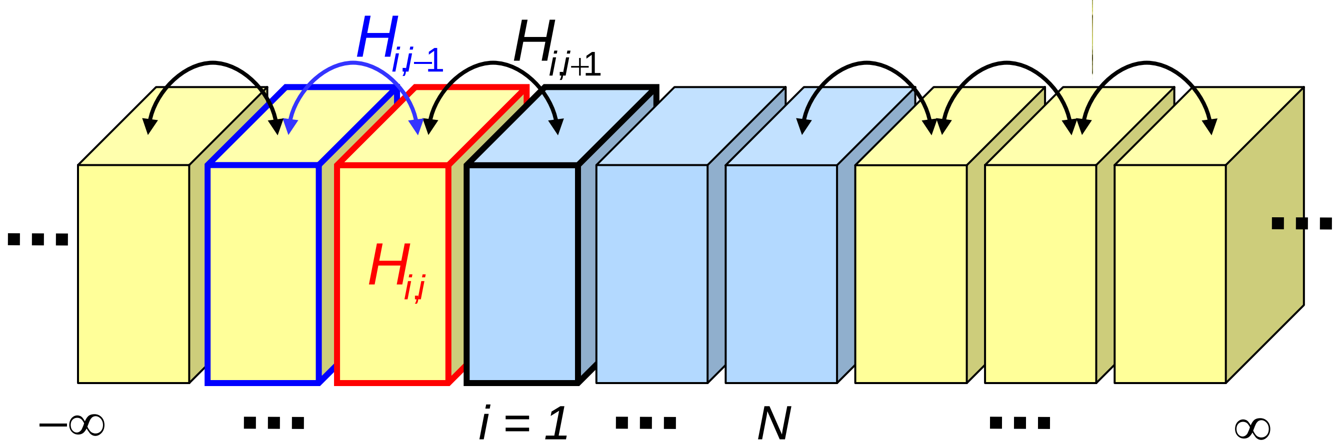
Scattering
Matrix

Approach: DFT first principles calculations

- use layers
- atomic orbital basis or real space grid



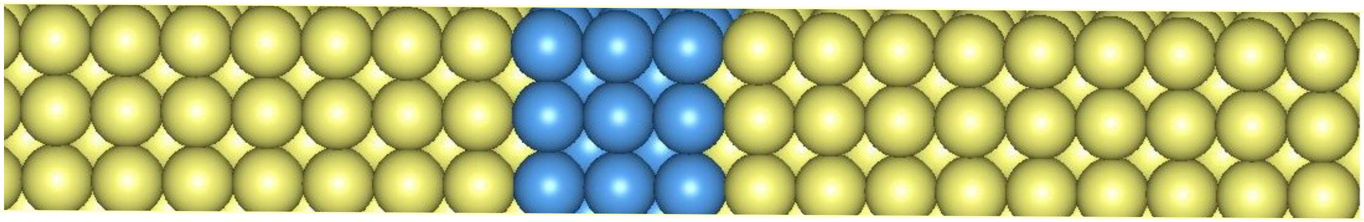
Hamiltonian matrix

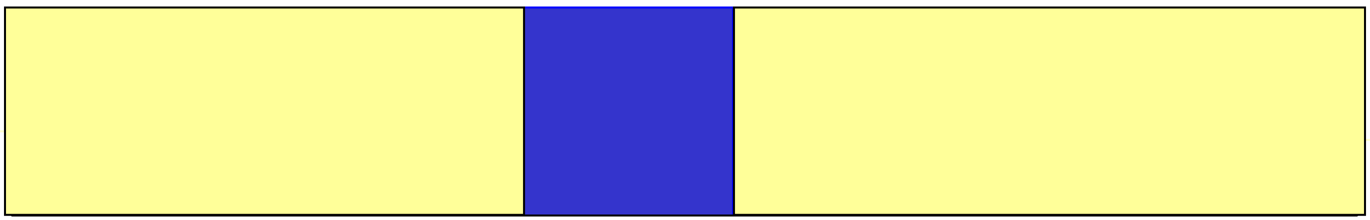


Kohn-Sham equation

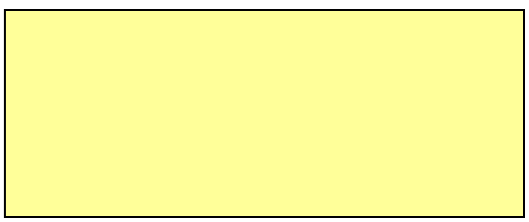
$$-H_{i,i-1}\psi_{i-1} + (E - H_{i,i})\psi_i - H_{i,i+1}\psi_{i+1} = 0\,; \quad i = -\infty, \infty$$

solve scattering problem at fixed energy $E = E_F$



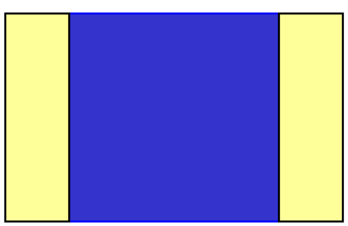


Ideal lead Scattering region Ideal lead



Ideal lead

Part I: solve ideal lead



Scattering region

Part II: solve scattering region

Wave Function Matching: Ando PRB**44** (1991)
Khomyakov et al. PRB**72** (2005)

2 Implementations

1. Tight-Binding Muffin Tin Orbitals (TB-MTO)
   - minimal basis (1xs,1xp,1xd orbital per atom)
   - suitable for transition metals (magnetism)
   - close-packed solids (Atomic Spheres Approx.)

Spin Transport

Xia et al. PRB**63** (2001)
PRB**73** (2006)

2. Real-space grid + Pseudopotentials
   - full potential
   - open structures

Molecular Electronics

Khomyakov et al. PRB**70** (2004)

Spin Transport: Applications

- GMR
  - CPP - Interface resistances
  - CIP
- Transport through domain walls
- Magnetization Switching
- Andreev reflection at F/S interfaces
- Enhancement of Gilbert damping
- Spin injection in F/SC (Reflection): DFP
- Spin Valve Transistor
- Tunneling MR
- Spin injection in F/SC (Transmission)

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M. Zwierzycki (Twente)
M. Talanana (Twente)
I. Turek (Brno)
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P.X. Xu (Beijing)
A. Brataas (Trondheim)
G.E.W. Bauer (Delft)
K.M. Schep (Philips)
J.B.A.N. van Hoof (Philips)

Review: A. Brataas, G.E.W. Bauer and P.J. Kelly, Physics Reports **427** (2006)

Spin Transport: Applications

- GMR
    - **CPP - Interface resistances**
    - CIP
- Transport through domain walls
- Magnetization Switching
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- Spin injection in F/SC (Reflection): DFP
- Spin Valve Transistor
- **Tunneling MR**
- **Spin injection in F/SC (Transmission)**

Spin-dependent Transmission

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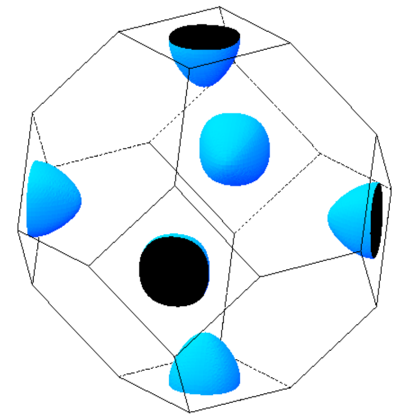
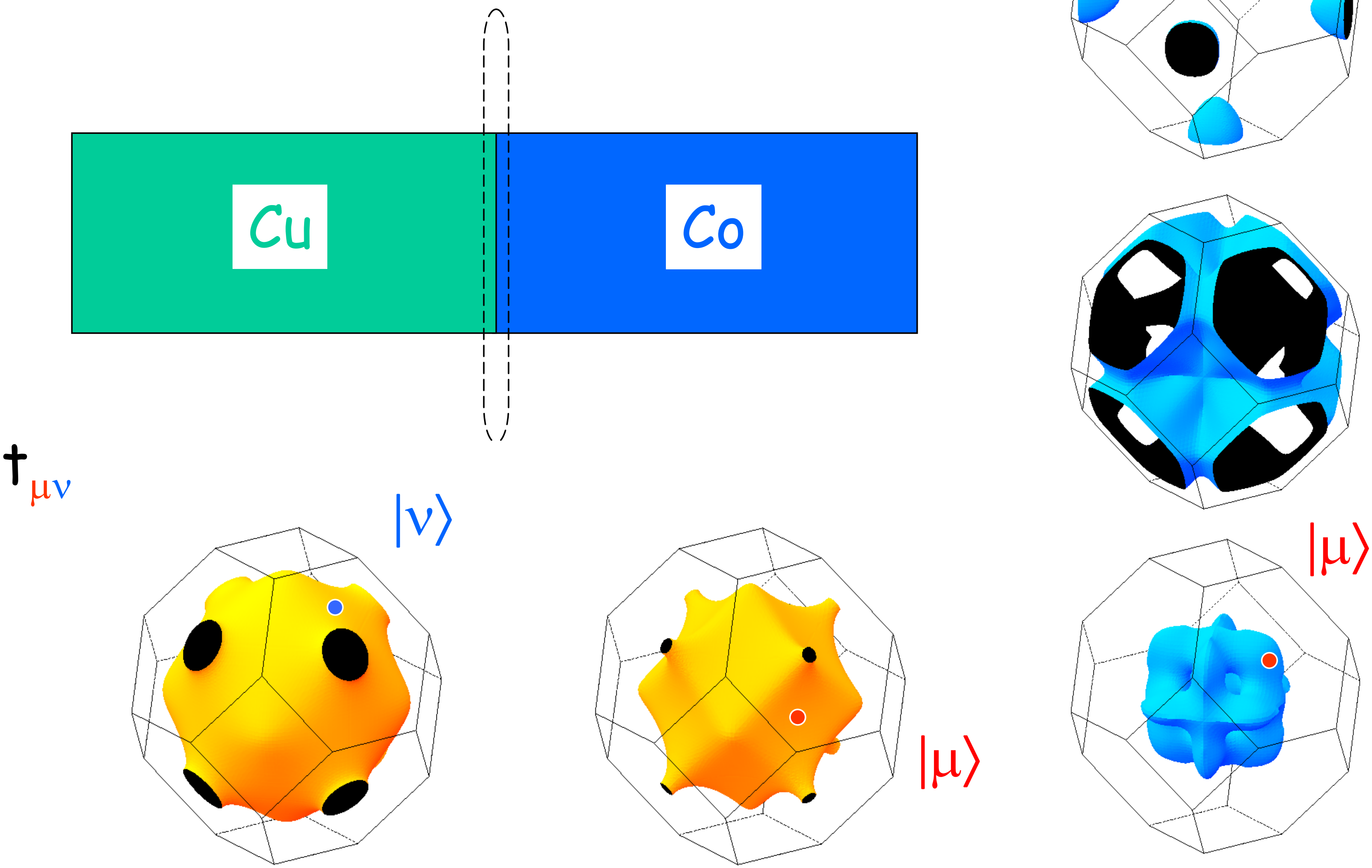
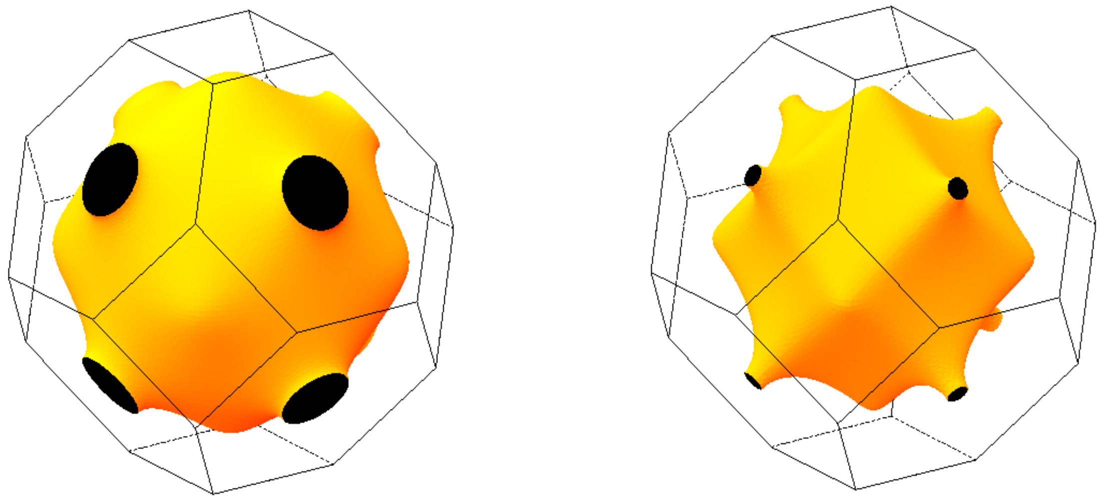
[2] *Institute of Physics, Beijing, China*
[3] *Max-Planck Institute for Solid State Research, Stuttgart, Germany*
[4] *Kavli Institute of NanoScience, Delft University of Technology, The Netherlands*

Single interface between (almost) perfectly lattice matched Cu and Co

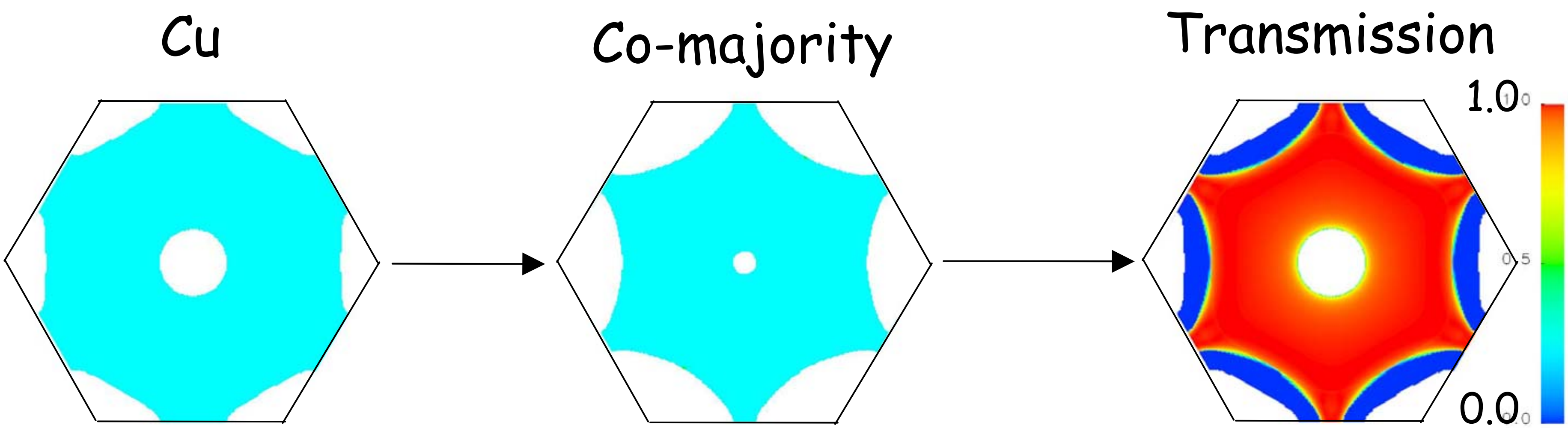




Cu/Co(111): specular interface - $k_{||}$ conserved

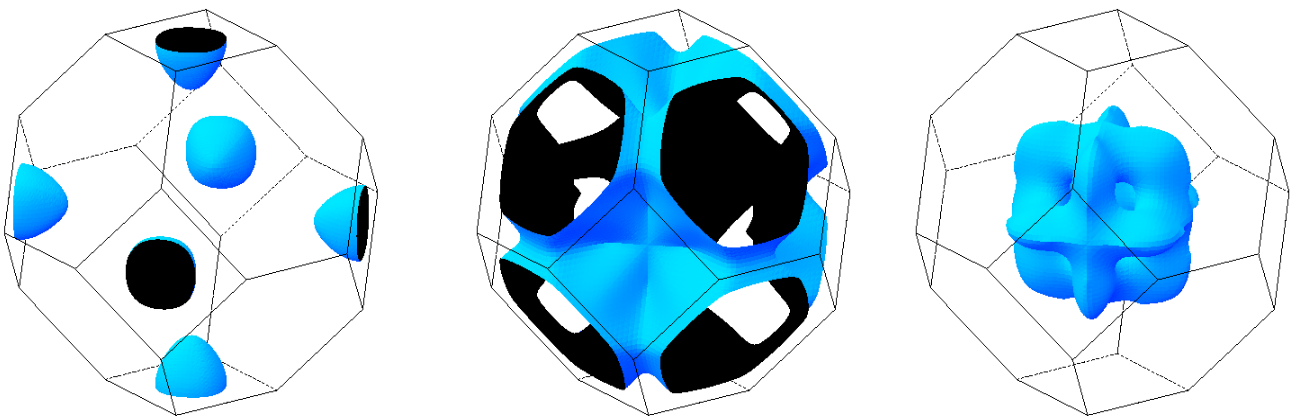


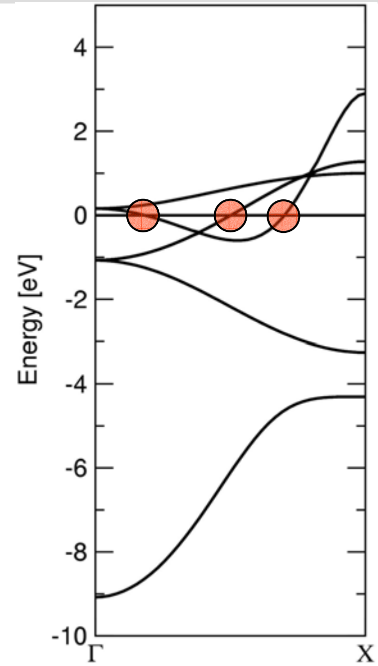
Majority Spin



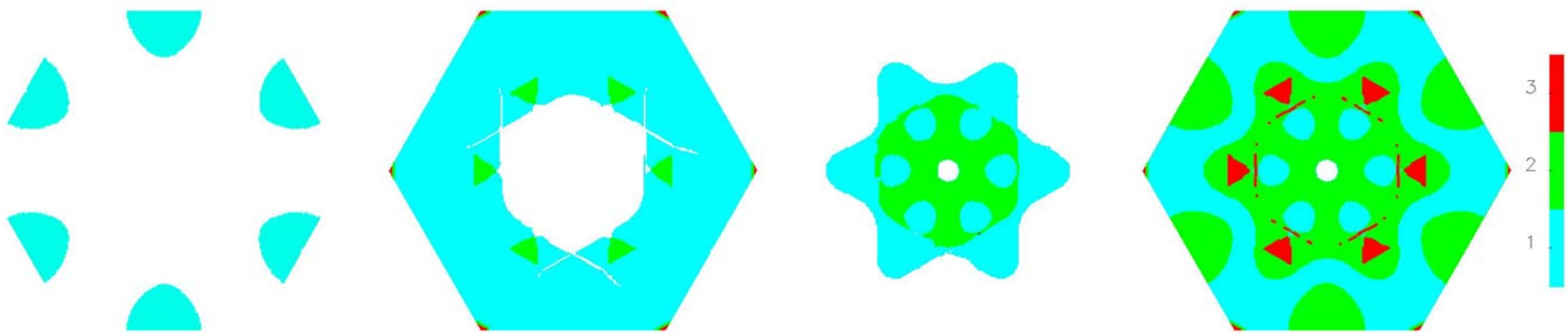
Cu/Co(111): specular case - $k_{||}$ conserved

3rd band 4th band 5th band

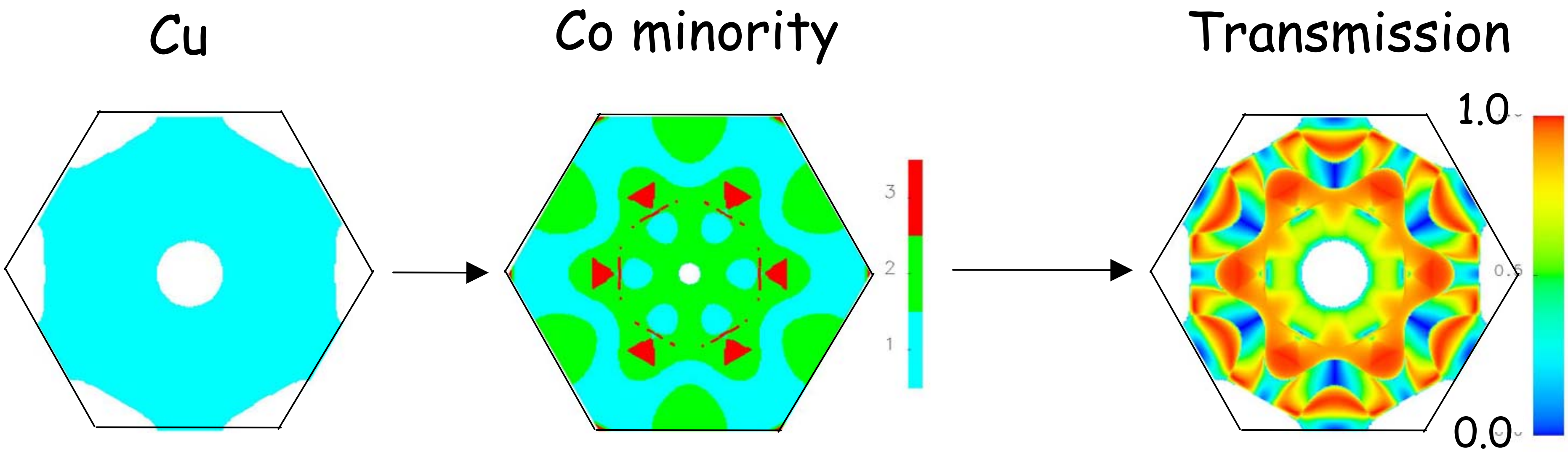




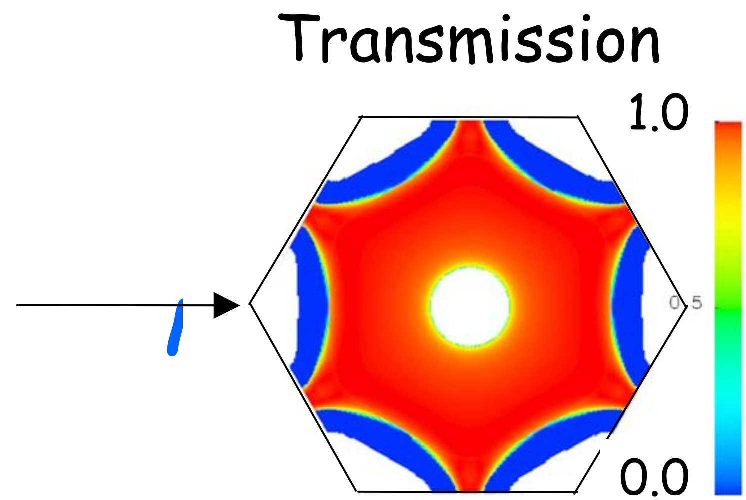
Minority Spin



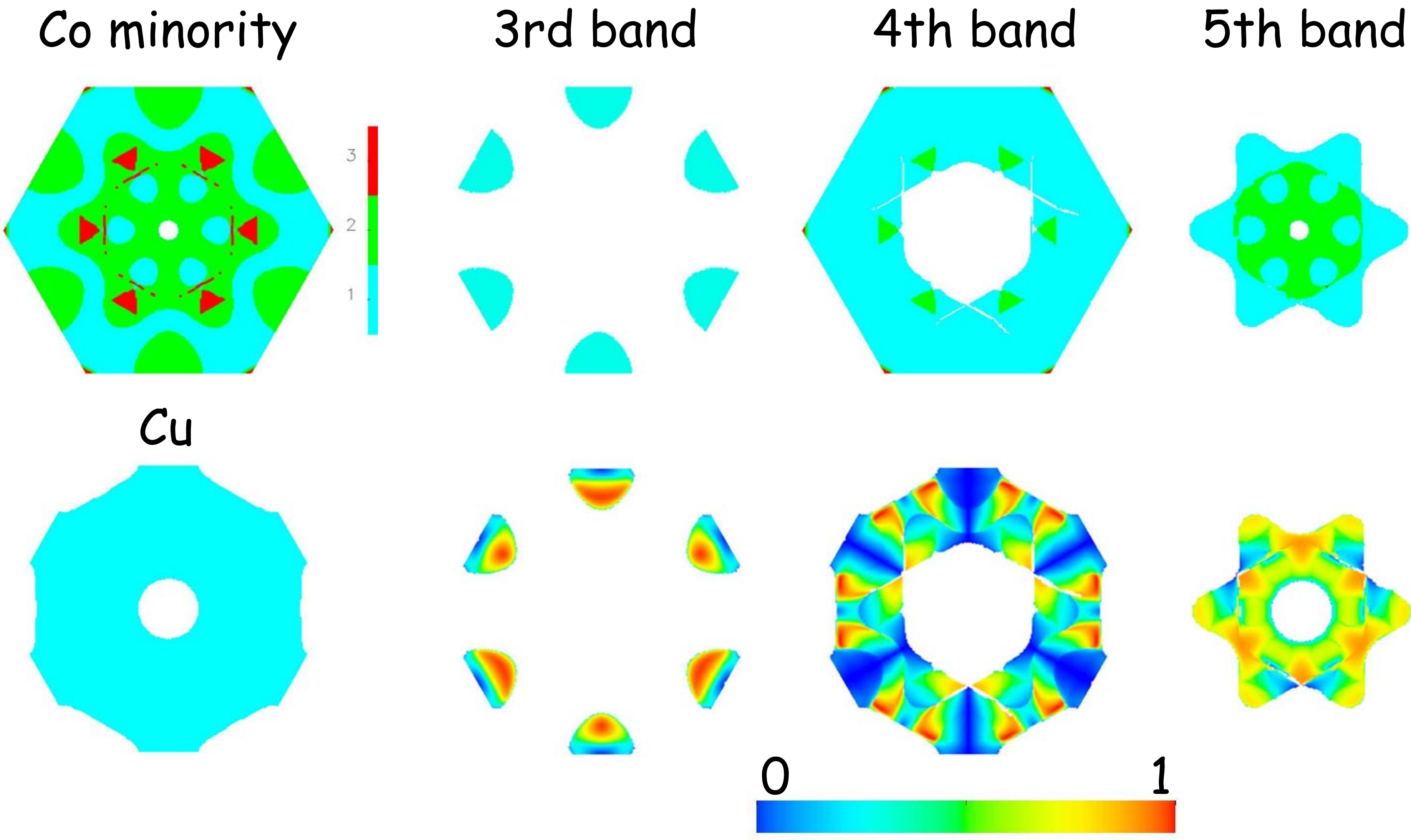
Cu/Co(111): specular case - $k_{||}$ conserved



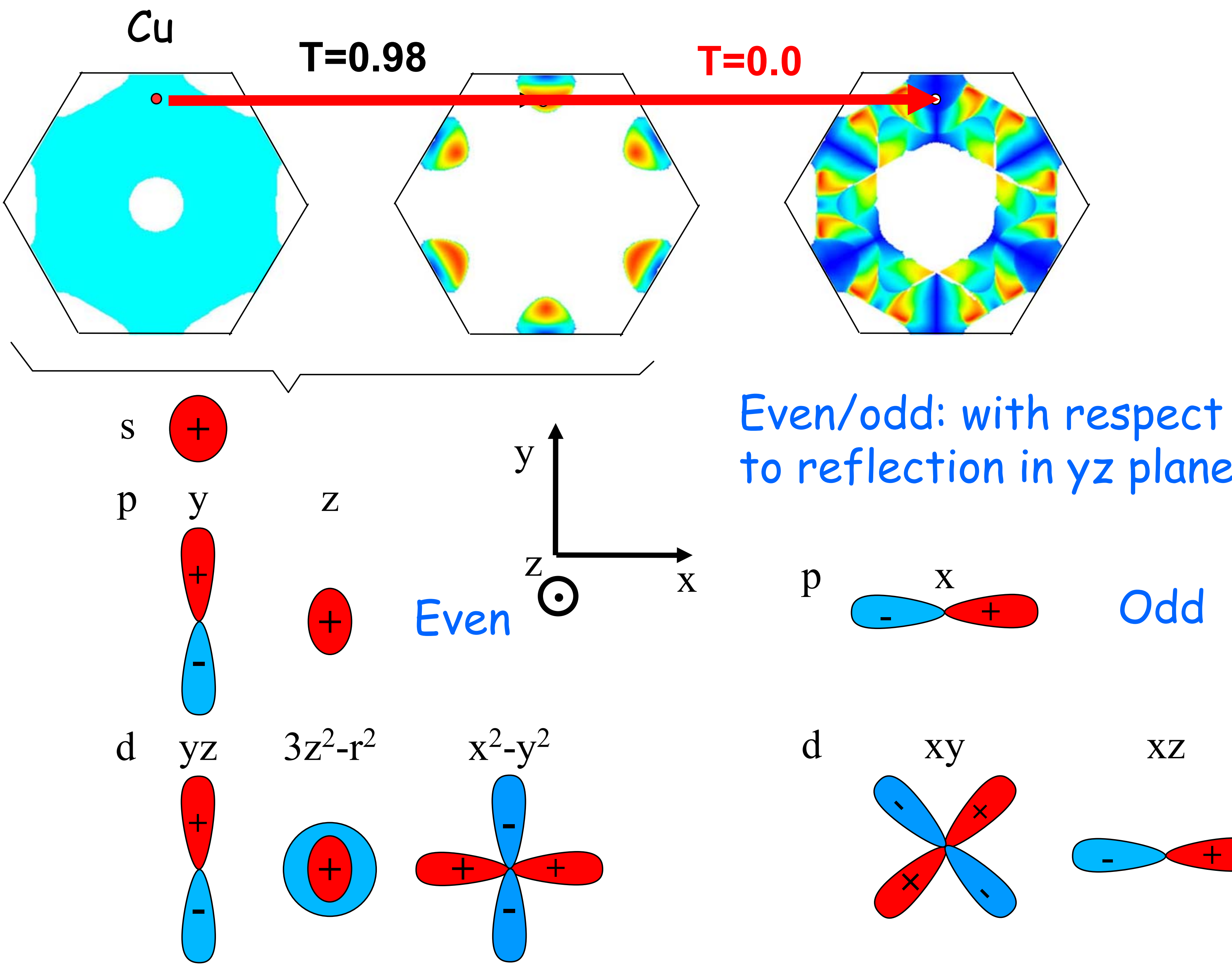
This spin dependence of the transmission/reflection is the origin of OEC, GMR, JMR, CIMS etc.



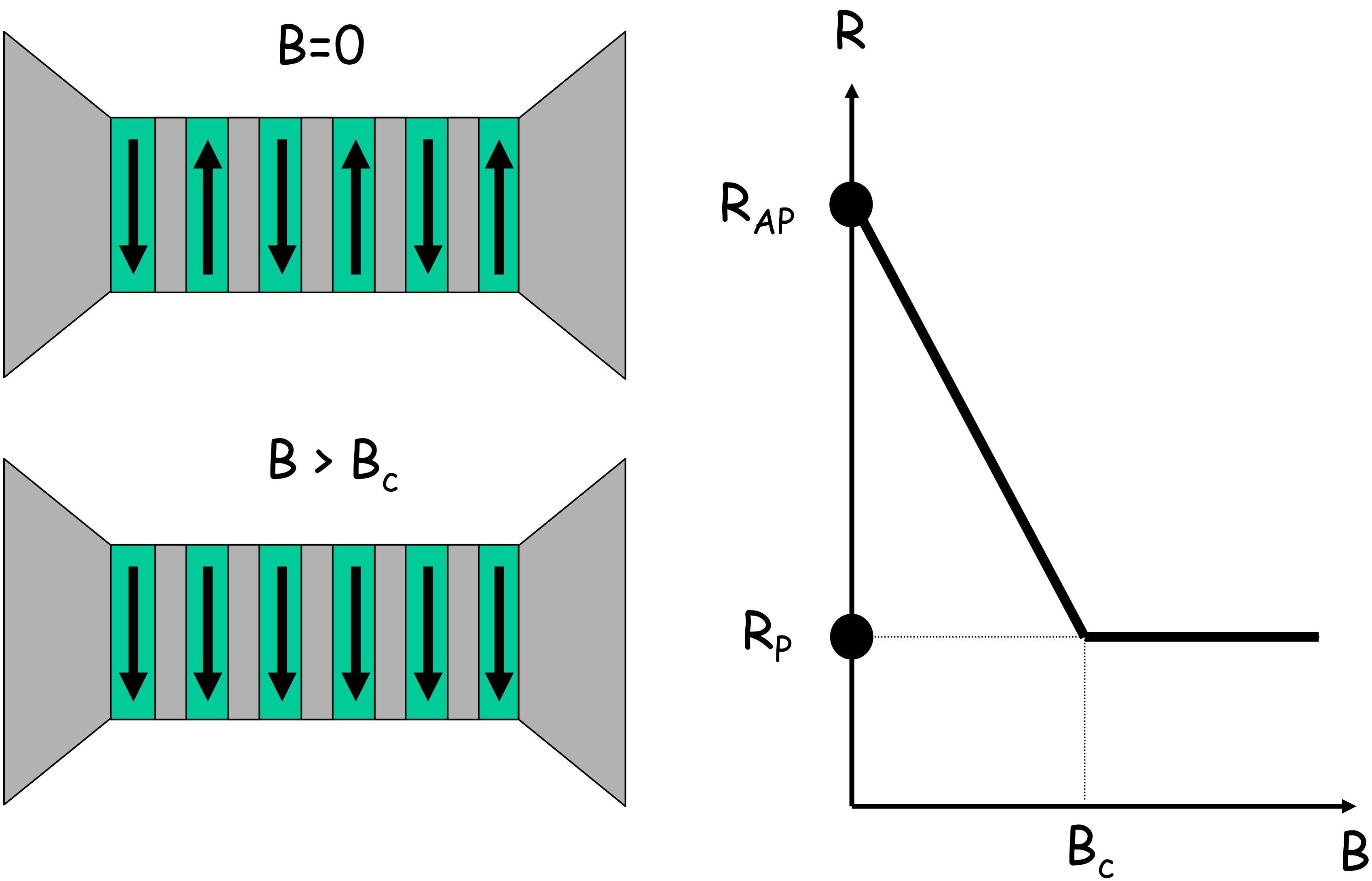
Sheet decomposition of transmission



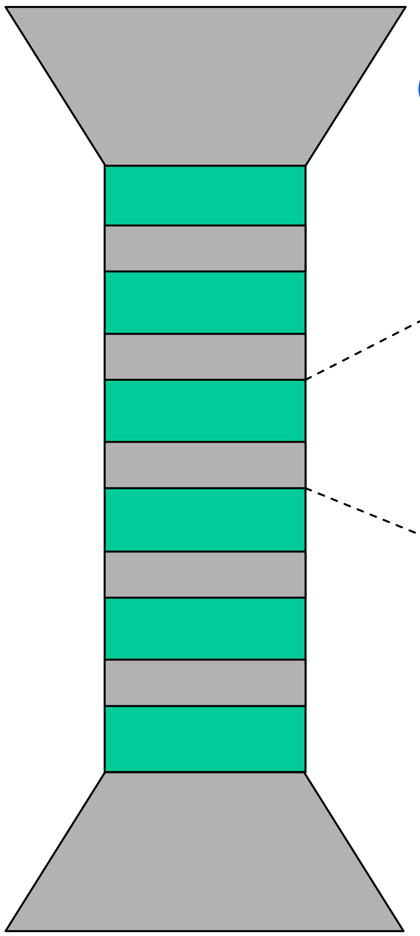
→ matrix element effects are important

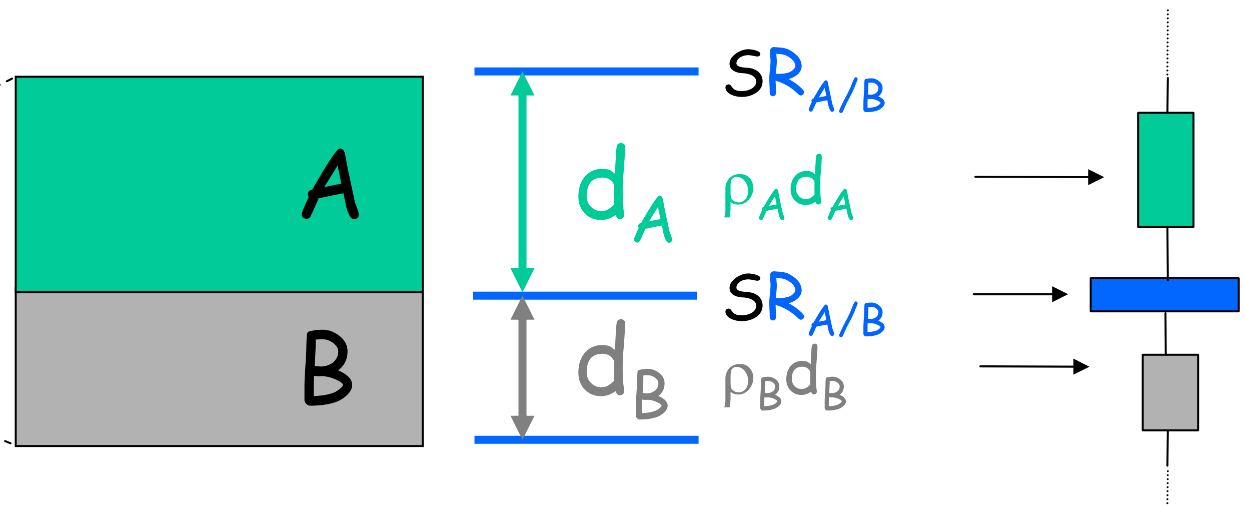

Cu
T=0.98
T=0.0
s
+
p y z
+
-
+
Even
y
z
x
Even/odd: with respect
to reflection in yz plane
p x
-
+
Odd
d yz 3z²-r² x²-y²
d xy xz

Giant MagnetoResistance (GMR)



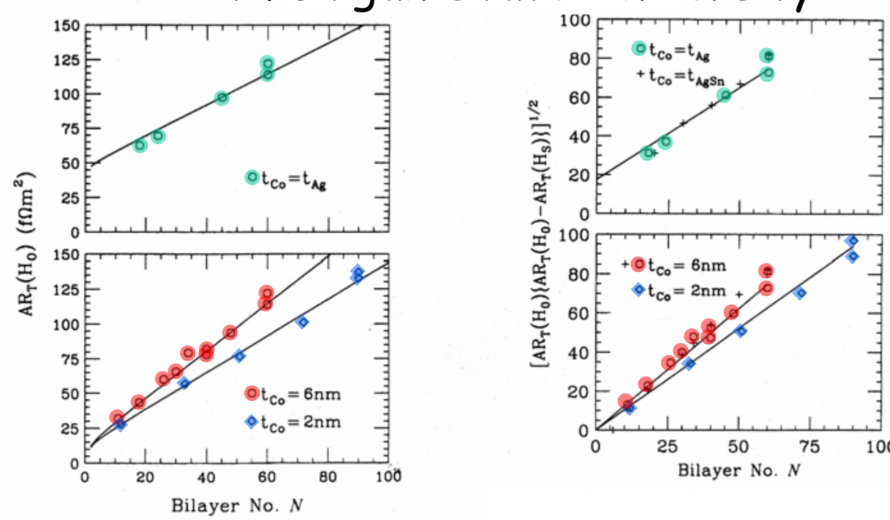
CPP-GMR: Series Resistor Model





$$SR_T = N(SR_{A/B} + \rho_A d_A + SR_{A/B} + \rho_B d_B)$$

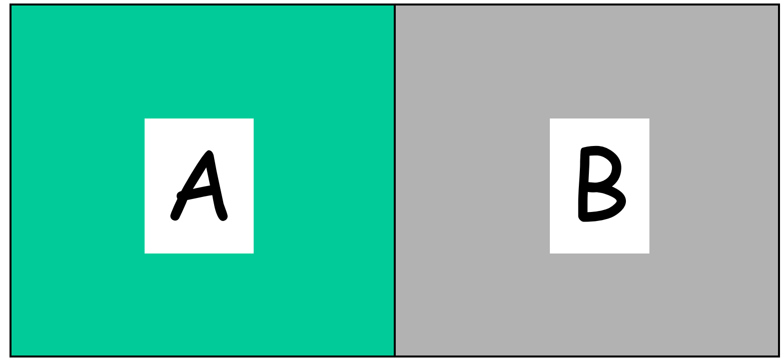
Michigan State University



For typical values of d_A and d_B GMR is mainly determined by the spin-dependence of $R_{A/B}$ - relate this to transmission t

Interface Resistances

$$\frac{1}{R} = G = \frac{e^2}{h} \mathrm{Tr}\{t\, t^+\}$$



But suppose A=B; then R≠0 ?

Correction for Sharvin resistance

$$SR_{A/B} = \frac{Sh}{e^2}\left[\frac{1}{\mathrm{tr}\{t\, t^+\}} - \frac{1}{2}\left(\frac{1}{N_A} + \frac{1}{N_B}\right)\right]$$

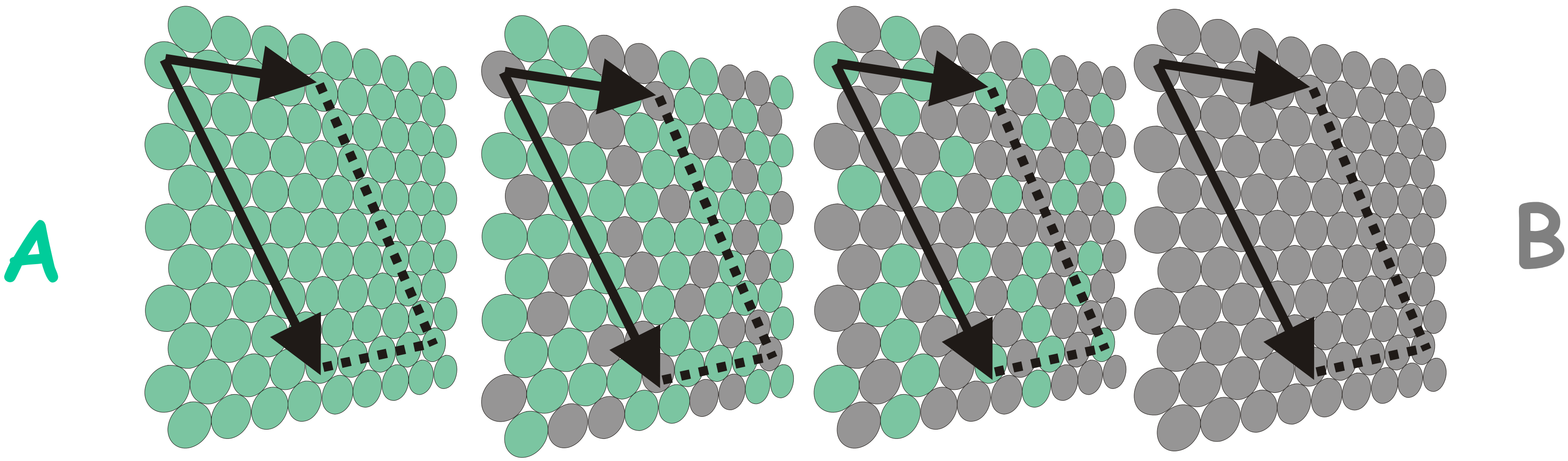
Co/Cu

fΩm^2	Orientation	majority	minority
calculation	(111)	0.39	1.46
expt (MSU)	(111)	0.26±0.06	1.84±0.14

Schep et al. PRB**56** (1997)

Interface Disorder

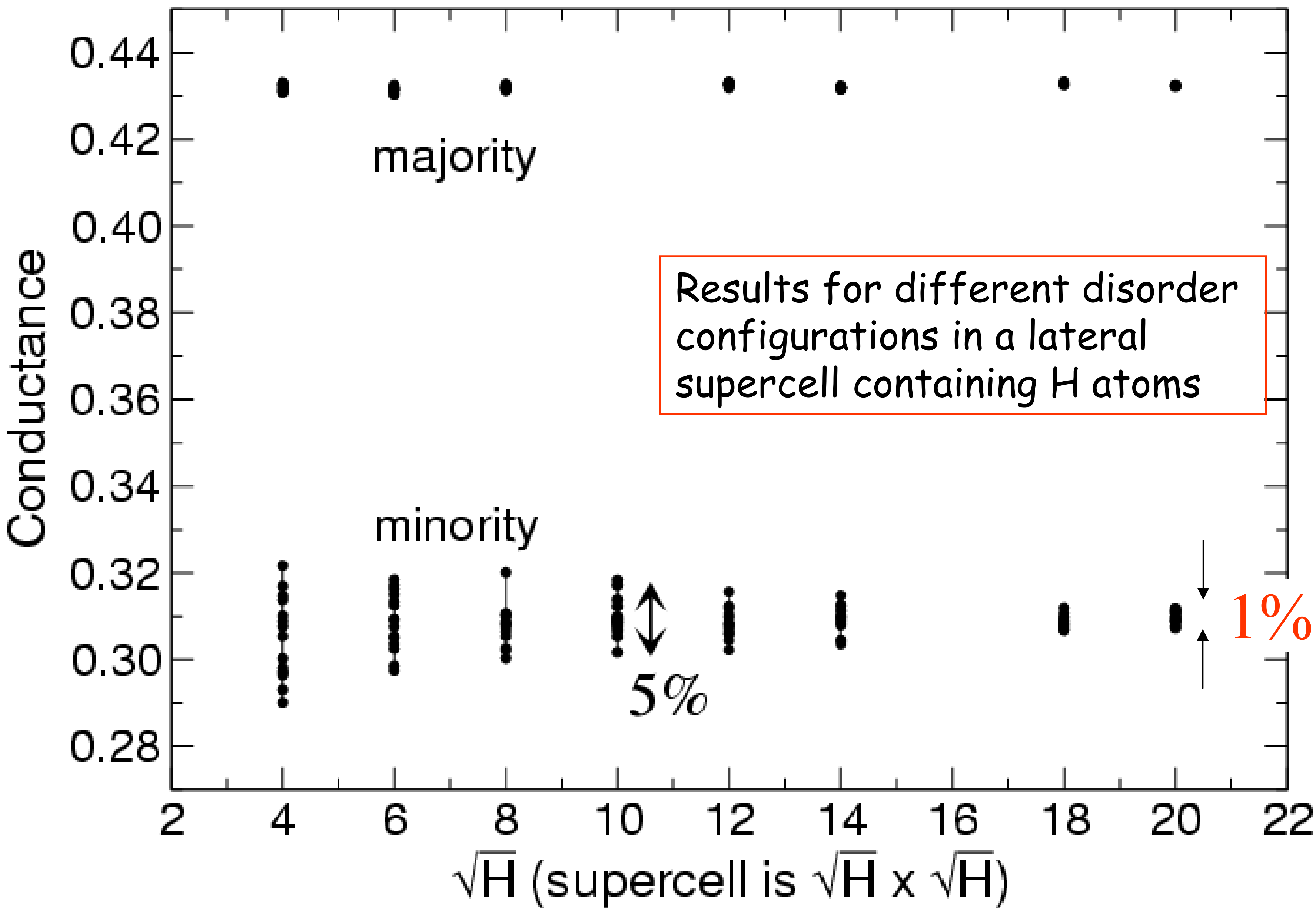
Model disorder in lateral supercells as two layers of alloy.



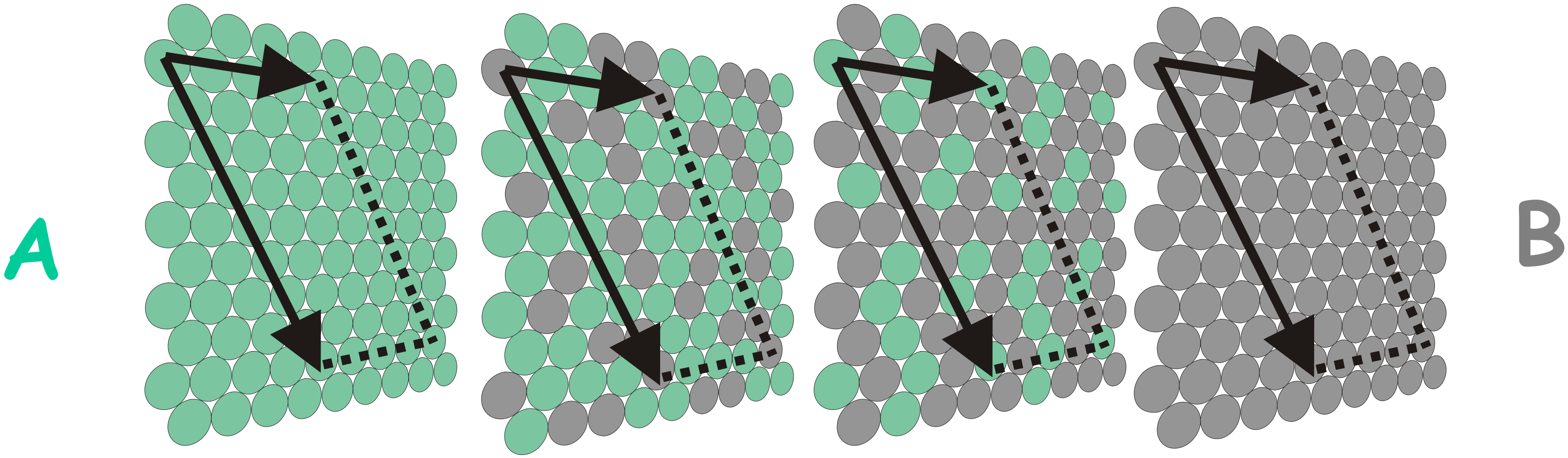
AS potentials calculated self-consistently using layer CPA

Xia et al. PRB**63** (2001)
PRB**73** (2006)

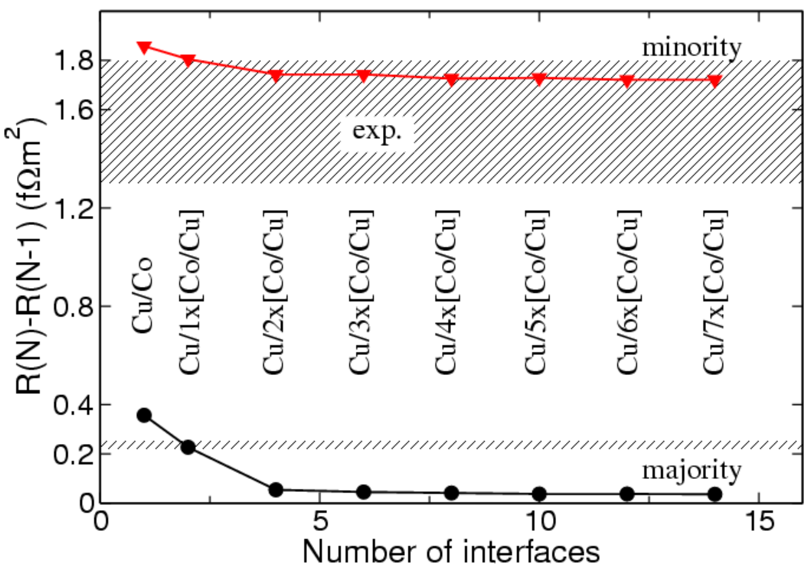
Convergence for Cu/Co(111) interface



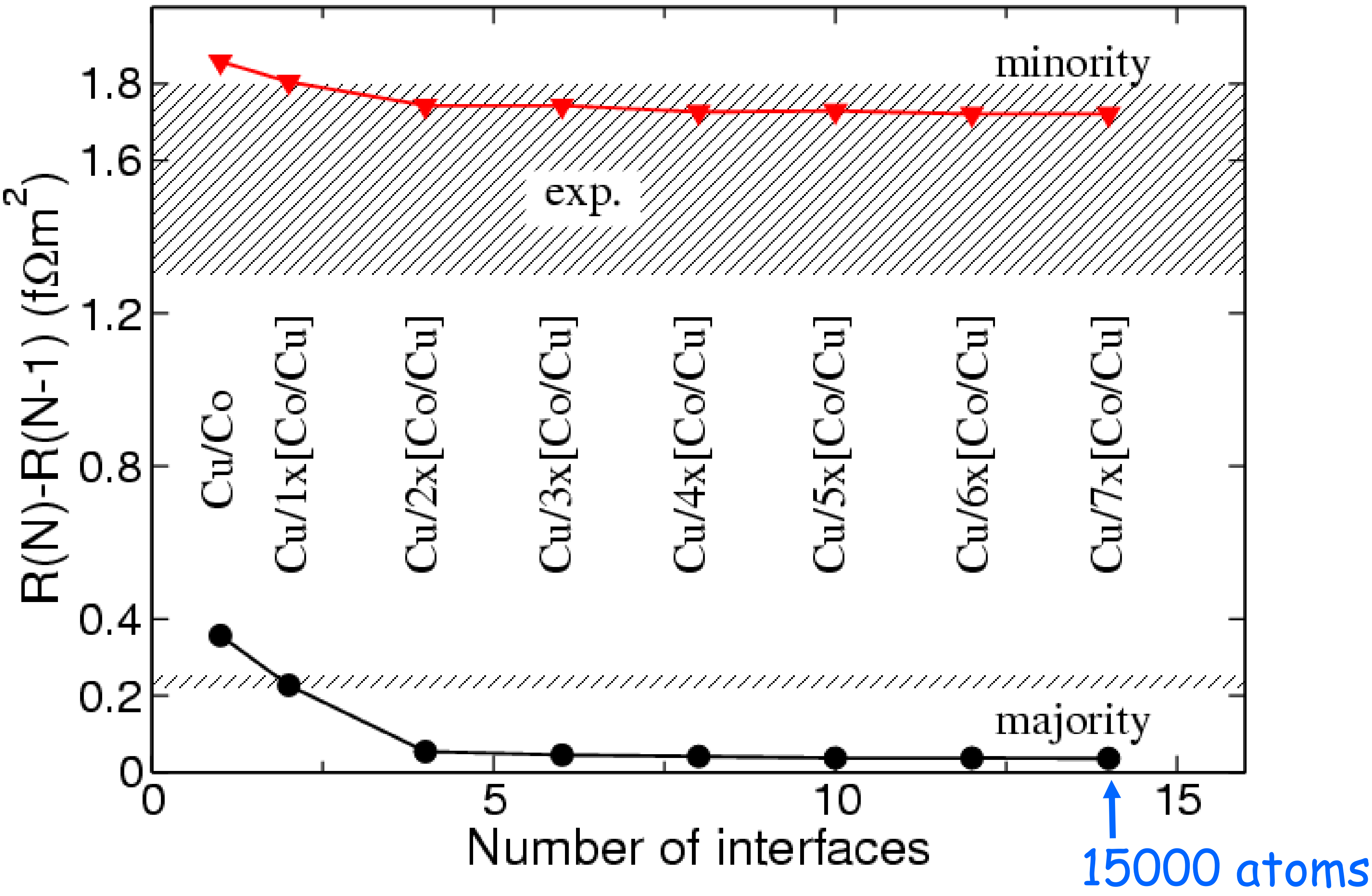
Interface Disorder



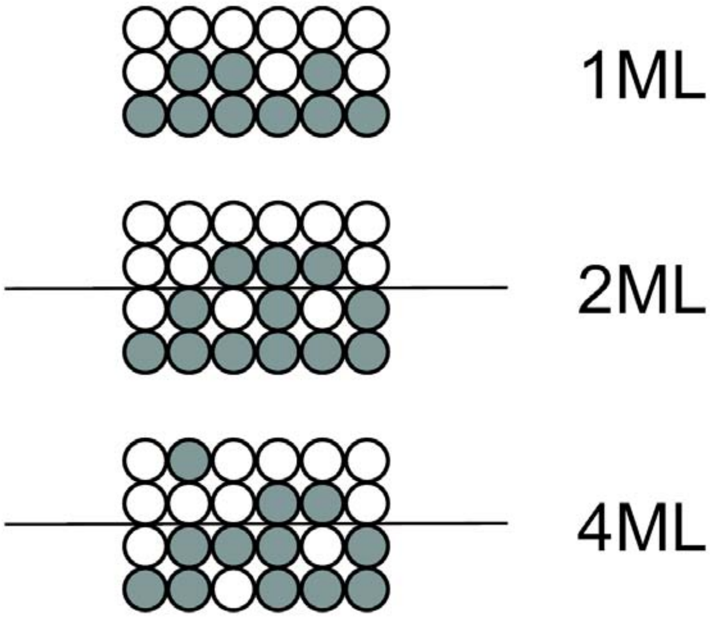
Cu/Co fcc(111)	R↑ $f\Omega m^2$	R↓ $f\Omega m^2$
Clean	0.39	1.46
2x50-50 alloy	0.41	1.82
Expt (MSU)	0.26±0.06	1.84±0.14



Differential Interface Resistance

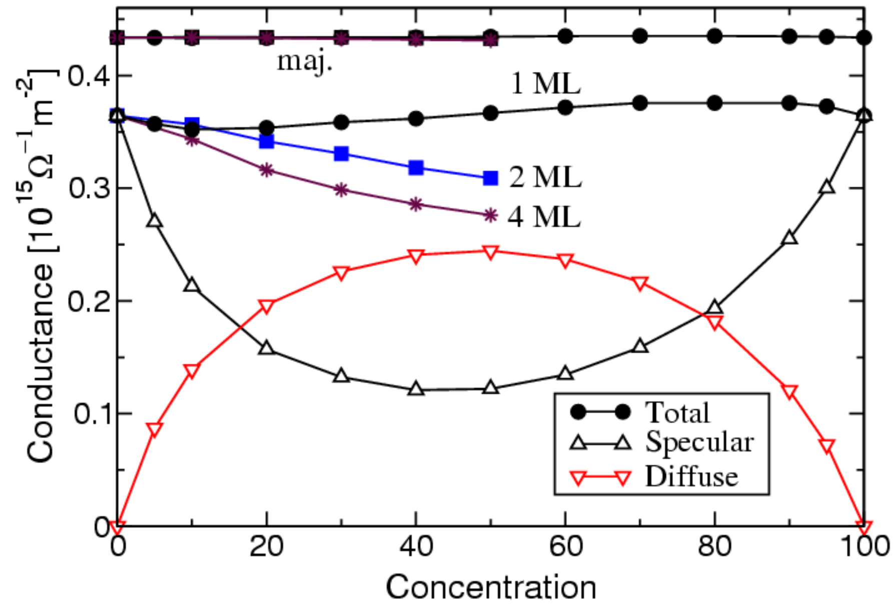


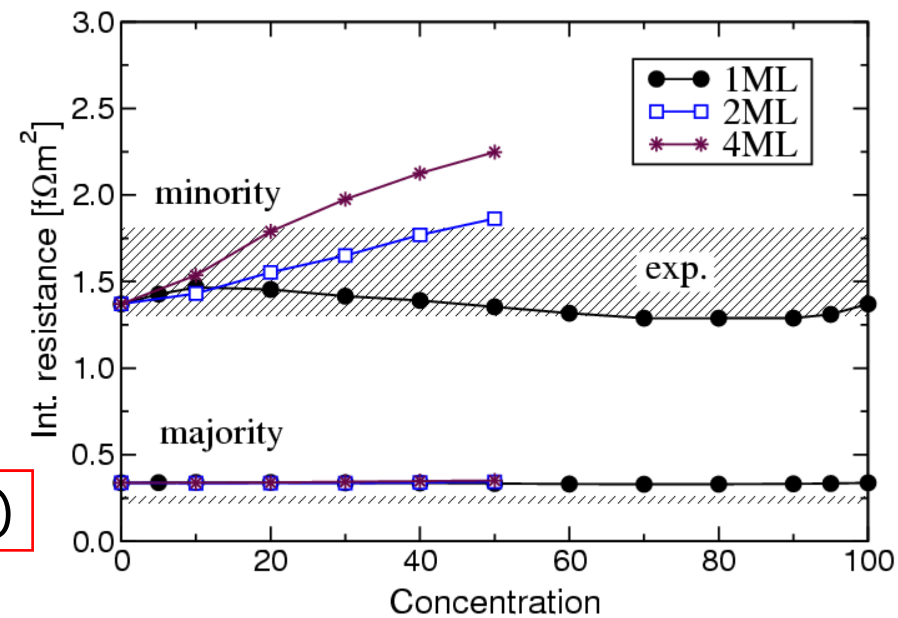
Modelling Interface Disorder



$$R_{A/B} = \frac{1}{G_{A/B}} - \frac{1}{2}\left(\frac{1}{G_A} + \frac{1}{G_B}\right)$$

Expt: Bass & Pratt JMMM **200** (1999)





Orientation-dependent interface transparency

P.X.Xu[1,2], K.Xia[1,2], M.Zwierzycki[1,3], M. Talanana[1]
P.J.Kelly[1]

[1] *University of Twente, Enschede, The Netherlands*
[2] *Institute of Physics, Beijing, China*
[3] *Max-Planck Institute for Solid State Research, Stuttgart, Germany*

Identify a suitable system to confront theory and experiment

→ Study pairs of lattice-matched metals

A/B		G_A	G_B	$G_{A/B}$
Al/Ag a_{fcc}=4.05 Å	(111) (110) (001)	0.69 0.68 0.73	0.45 0.47 0.45	0.41 0.30 0.22
Al/Au a_{fcc}=4.05 Å	(111) (001)	0.69 0.73	0.44 0.46	0.41 0.24
Pd/Pt a_{fcc}=3.89 Å	(111) (001)	0.62 0.58	0.71 0.70	0.55 0.52
W/Mo a_{bcc}=3.16 Å	(001) (110)	0.45 0.40	0.59 0.54	0.42 0.37
Cu/Co Majority a_{fcc}=3.61 Å	(111)* (001) (110)	0.56 0.55 0.59	0.47 0.49 0.50	0.43 0.46 0.46
Cu/Co Minority a_{fcc}=3.61 Å	(111)* (001) (110)	0.56 0.55 0.59	1.05 1.11 1.04	0.36 0.32 0.31
Cr/Fe Majority a_{bcc}=2.87 Å	(111) (001) (110)*	0.61 0.64 0.59	0.82 0.82 0.78	0.27 0.11 0.22
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~13%

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~factor 2 !

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~factor 2 !

~factor $2\frac{1}{2}$?

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Al/Ag a_{fcc}=4.05 Å	(111) (110) (001)	0.69 0.68 0.73	0.45 0.47 0.45	0.41 (**0.36**) 0.30 (**0.32**) 0.22 (**0.24**)
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A/B		G_A	G_B	$G_{A/B}$	$2SR$
Al/Ag a_{fcc}=4.05 Å	(111) (110) (001)	0.69 0.68 0.73	0.45 0.47 0.45	0.41 (**0.36**) 0.30 (**0.32**) 0.22 (**0.24**)	0.64 (**0.92**) 1.60 (**1.39**) 2.82 (**2.37**)
Al/Au a_{fcc}=4.05 Å	(111) (001)	0.69 0.73	0.44 0.46	0.41 (**0.35**) 0.24 (**0.26**)	0.60 (**0.99**) 2.37 (**2.14**)
Pd/Pt a_{fcc}=3.89 Å	(111) (001)	0.62 0.58	0.71 0.70	0.55 (**0.54**) 0.52 (**0.51**)	0.30 (**0.33**) 0.37 (**0.39**)
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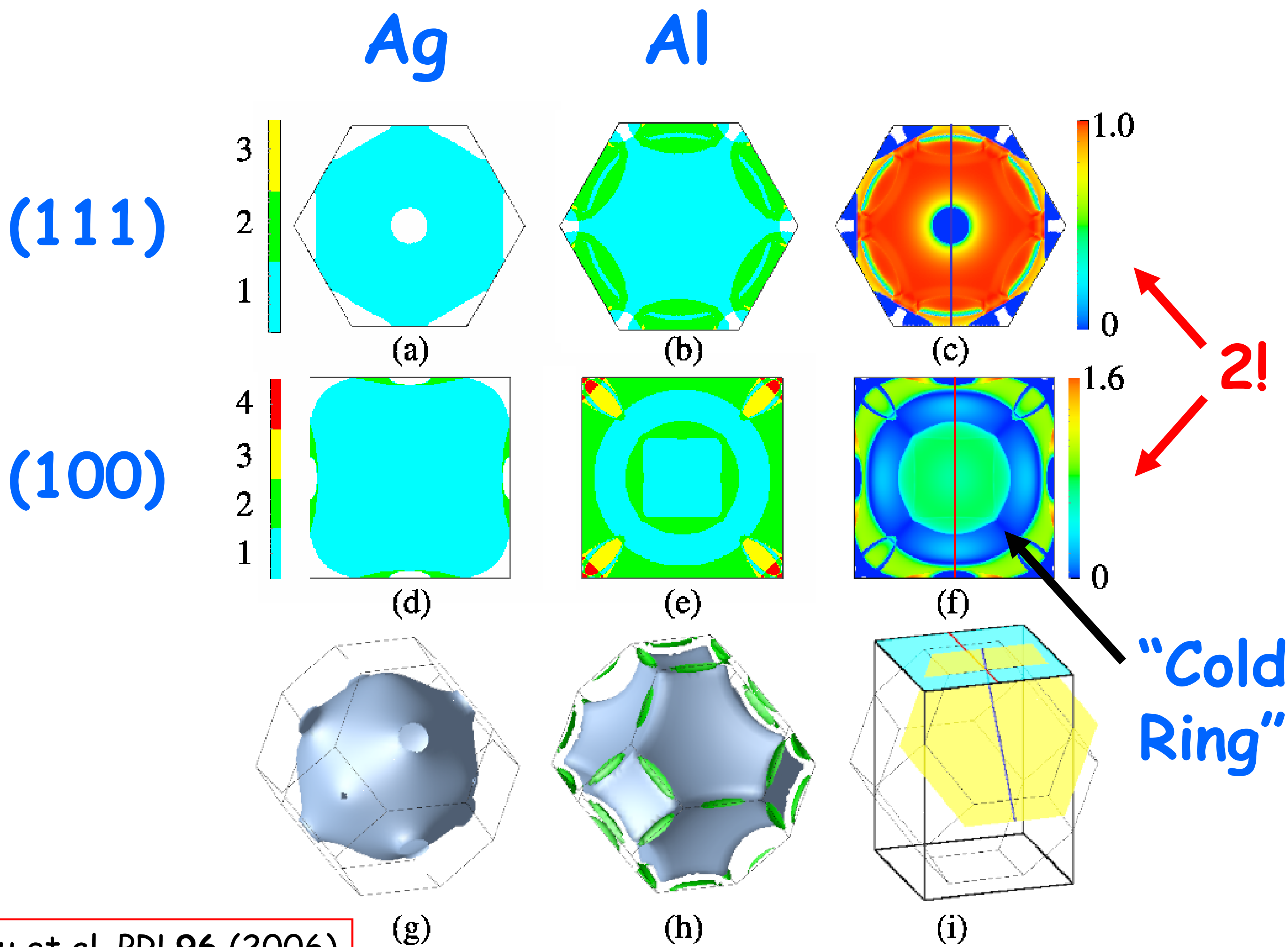
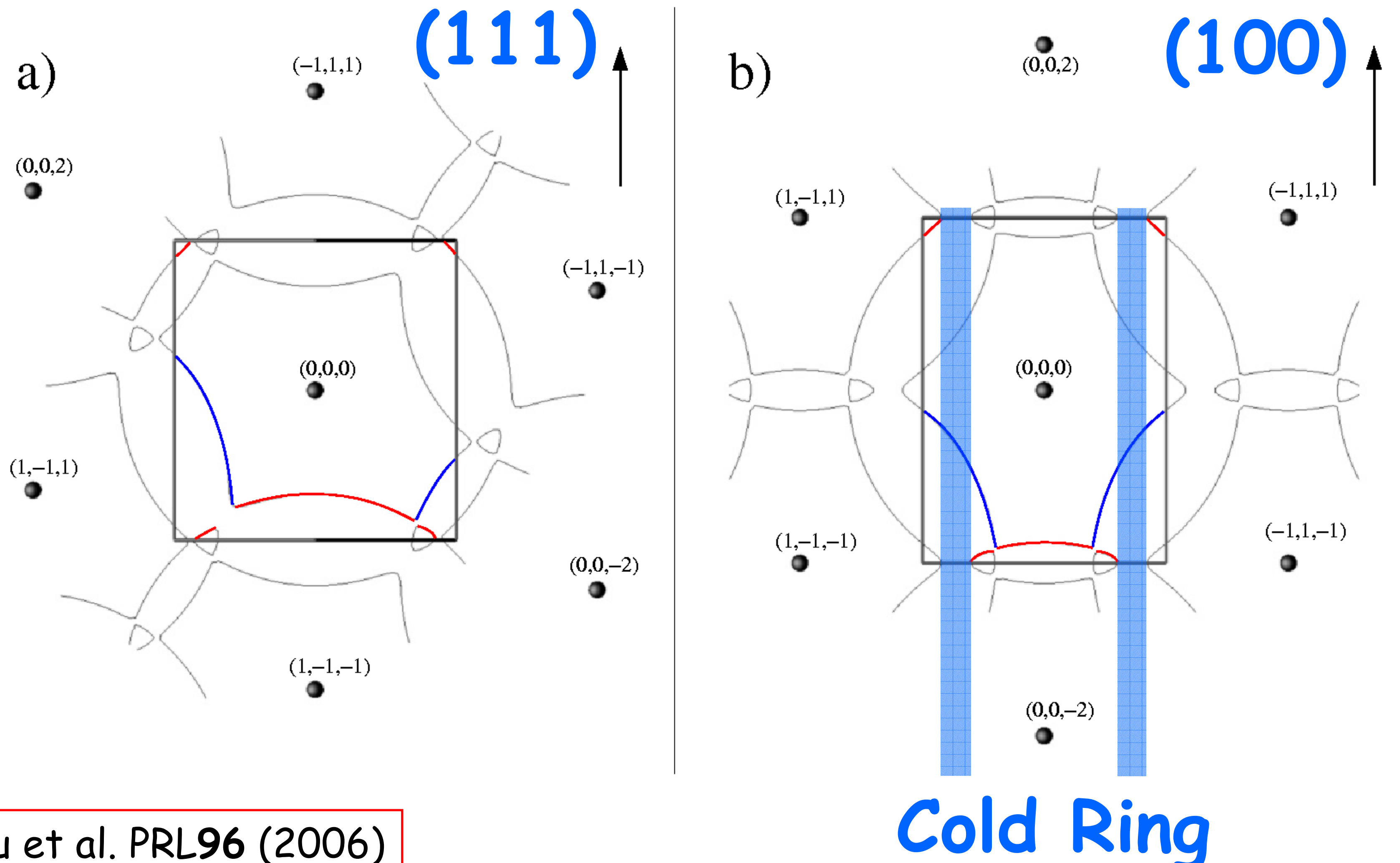
Cu/Co Minority a_{fcc}=3.61 Å	(111)* (001) (110)	0.56 0.55 0.59	1.05 1.11 1.04	0.36 (**0.31**) 0.32 (**0.32**) 0.31 **0.35**)	1.38 (**1.82**) 1.79 (**1.79**) 1.89 (**1.55**)
Cr/Fe Majority a_{bcc}=2.87 Å	(111) (001) (110)*	0.61 0.64 0.59	0.82 0.82 0.78	0.27 (**0.31**) 0.11 (**0.25**) 0.22 (**0.27**)	2.22 (**1.84**) 7.46 (**2.55**) 3.04 (**2.18**)
Cr/Fe Minority a_{bcc}=2.87Å	(111) (001) (110)*	0.61 0.64 0.59	0.41 0.46 0.40	0.34 (**0.34**) 0.35 (**0.35**) 0.32 (**0.32**)	0.93 (**0.95**) 0.98 (**0.95**) 1.03 (**1.06**)



Xu et al. PRL **96** (2006)

Even a small deviation from free-electron model can have large consequences



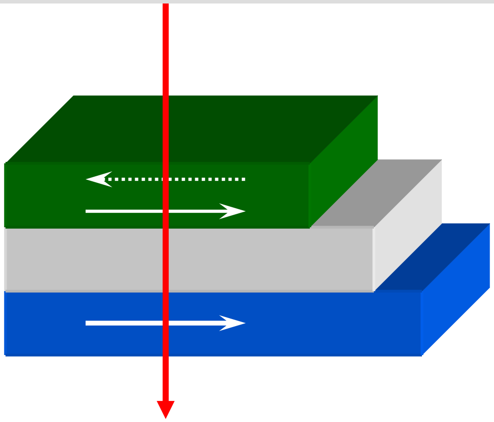
Xu et al. PRL**96** (2006)

Effect of Roughness and Disorder on Tunneling Magnetoresistance

V.M.Karpan[1], P.X.Xu[1,2], K.Xia[1,2], M.Zwierzycki[1,3], I.Marushchenko[1] and P.J.Kelly[1]

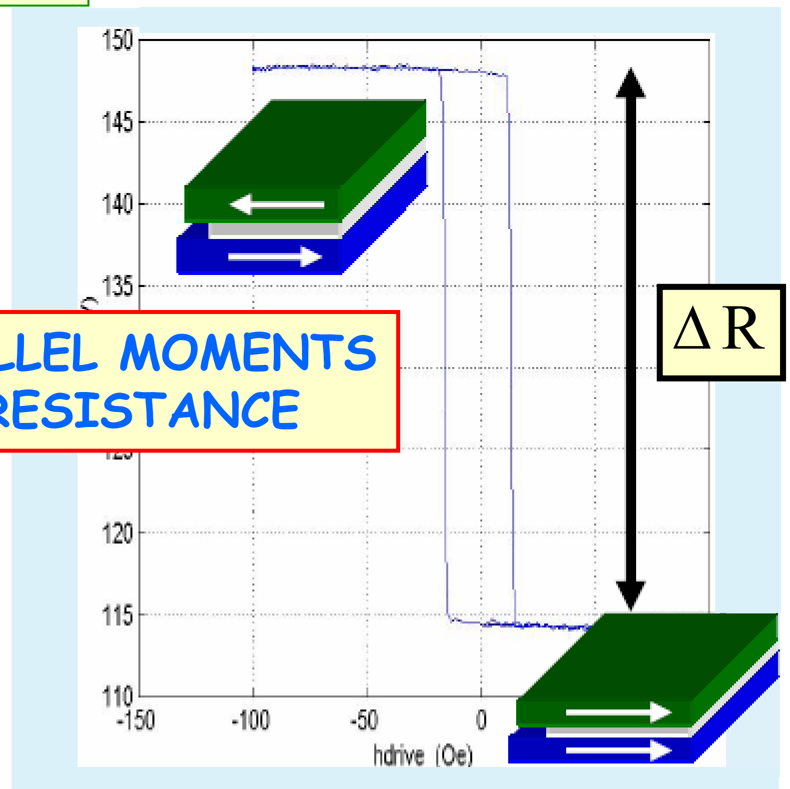
[1] *University of Twente, Enschede, The Netherlands*
[2] *Institute of Physics, Beijing, China*
[3] *Max-Planck Institute for Solid State Research, Stuttgart, Germany*

Magnetic Tunnel Junction



$$TMR = \frac{G_P - G_{AP}}{G_{AP}}$$

ANTIPARALLEL MOMENTS
HIGH RESISTANCE



$Fe Co|MgO|FeCo$: TMR ~ 353%

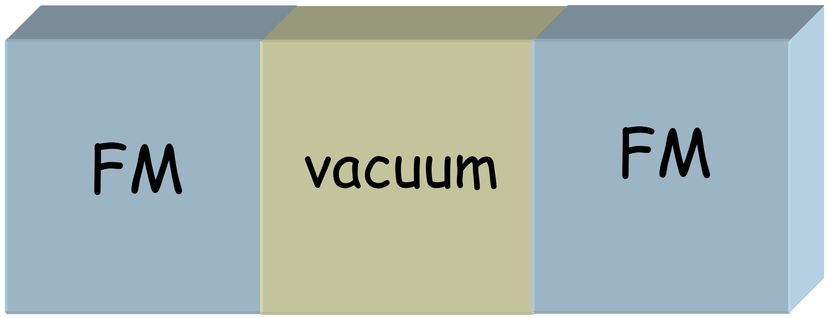
Yuasa et al. Nat.Mat.**3** (2004)
Parkin et al. Nat.Mat.**3** (2004)

Butler et al. PRB**63** (2001)
Mathon et al. PRB**63** (2001)

$Fe|MgO|Fe$:
TMR ~ 10000%

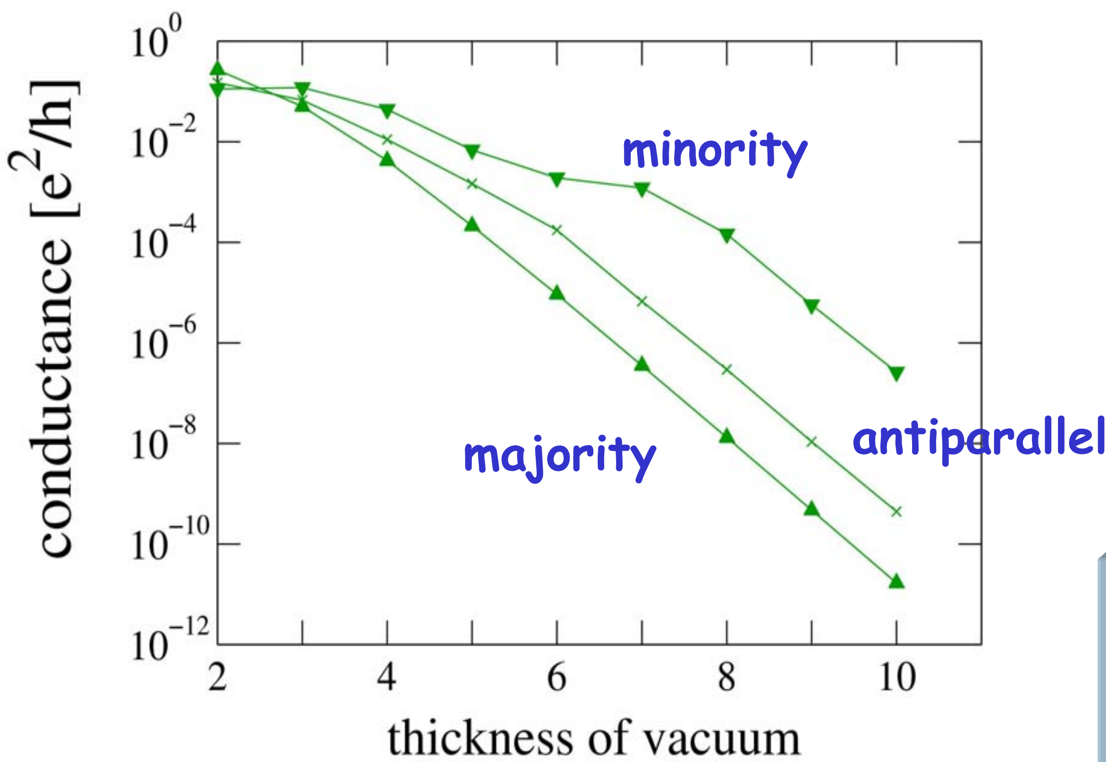
PARALLEL MOMENTS
LOW RESISTANCE

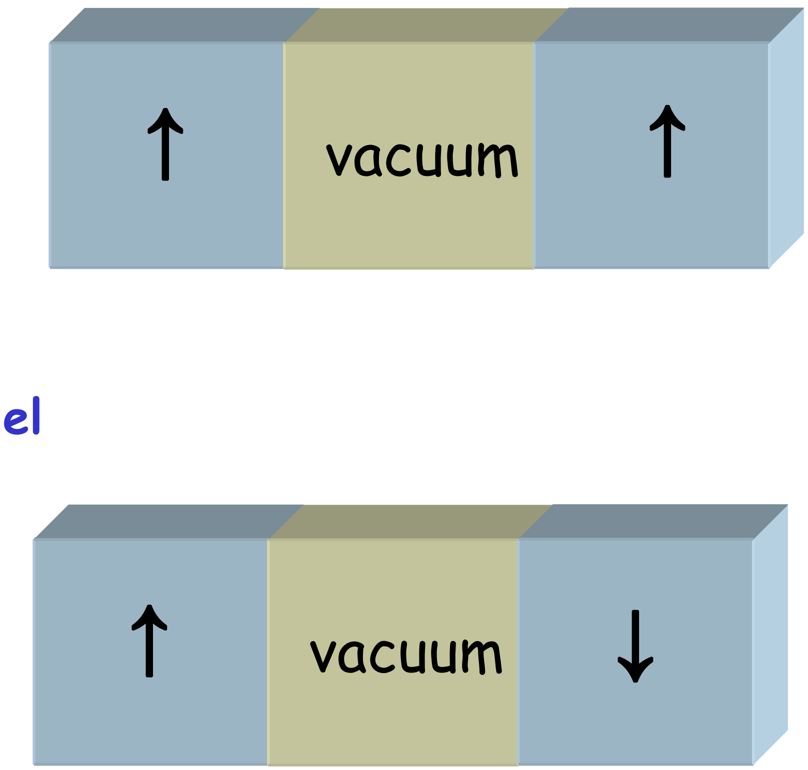
First-principles study of MTJ



- vacuum is simplest "insulator"
- vacuum is relatively easy to model
- no scattering from impurities or defects in insulator
- experiments

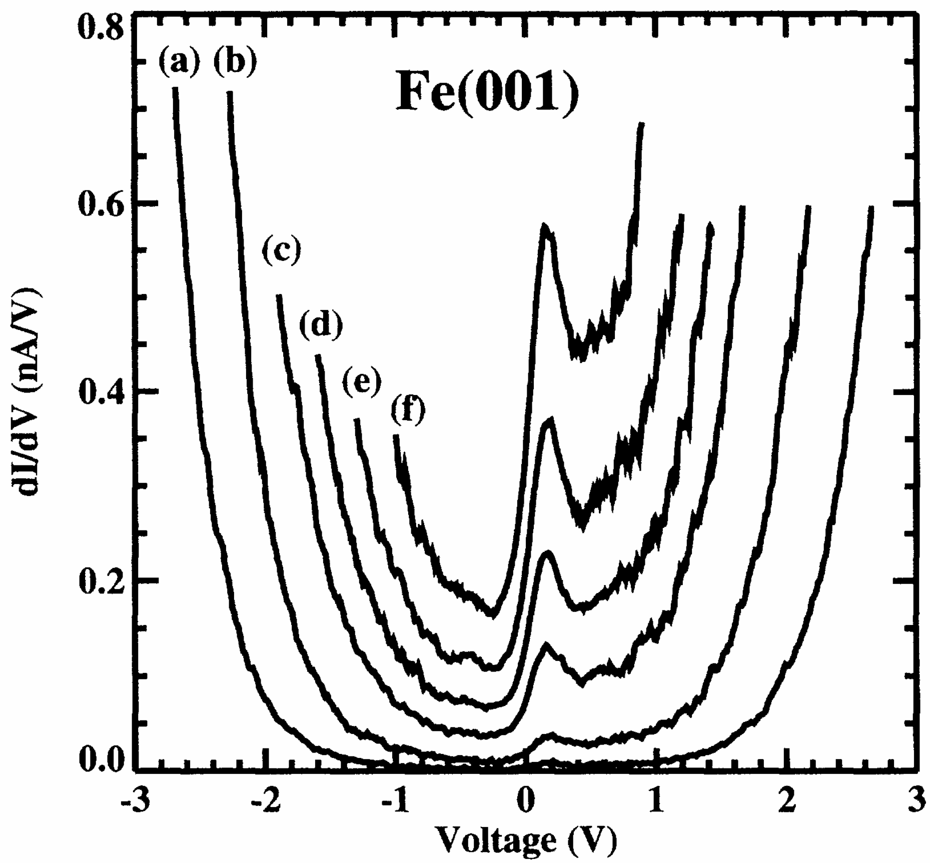
Ideal Fe/vacuum/Fe MTJ





Total antiparallel conductance is much smaller than the parallel one providing huge TMR

Observation of Fe bcc(001) surface states



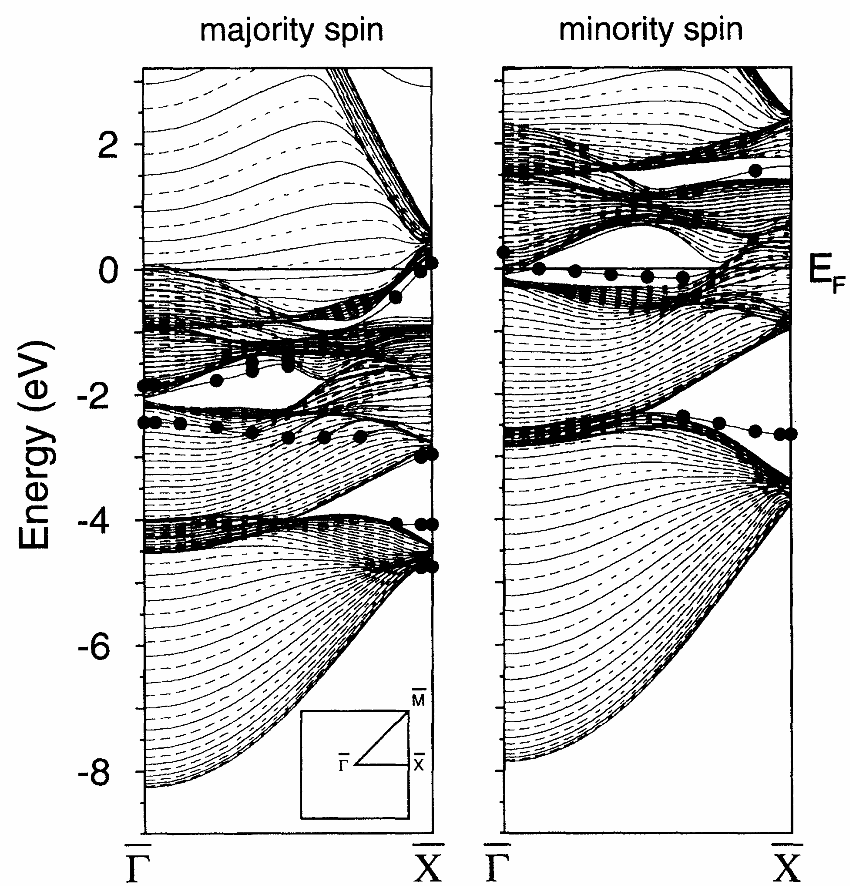
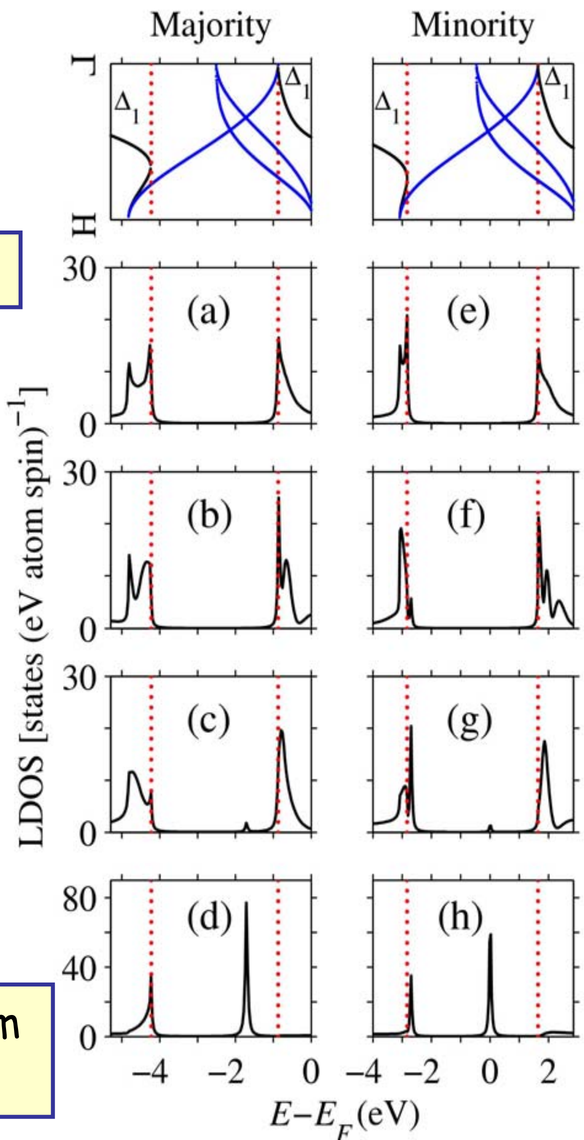


FIG. 2. Band structure of majority and minority even symmetry states along $\overline{\Gamma}$-$\overline{X}$ for a 49-layer Fe(001) film. States with high localization in the surface region are marked with circles.

Stroscio et al., PRL 1995

Polarization is negative because of the surface state

Fe bulk



Fe bulk band structure

Fe bulk LDOS* at 2d Γ point

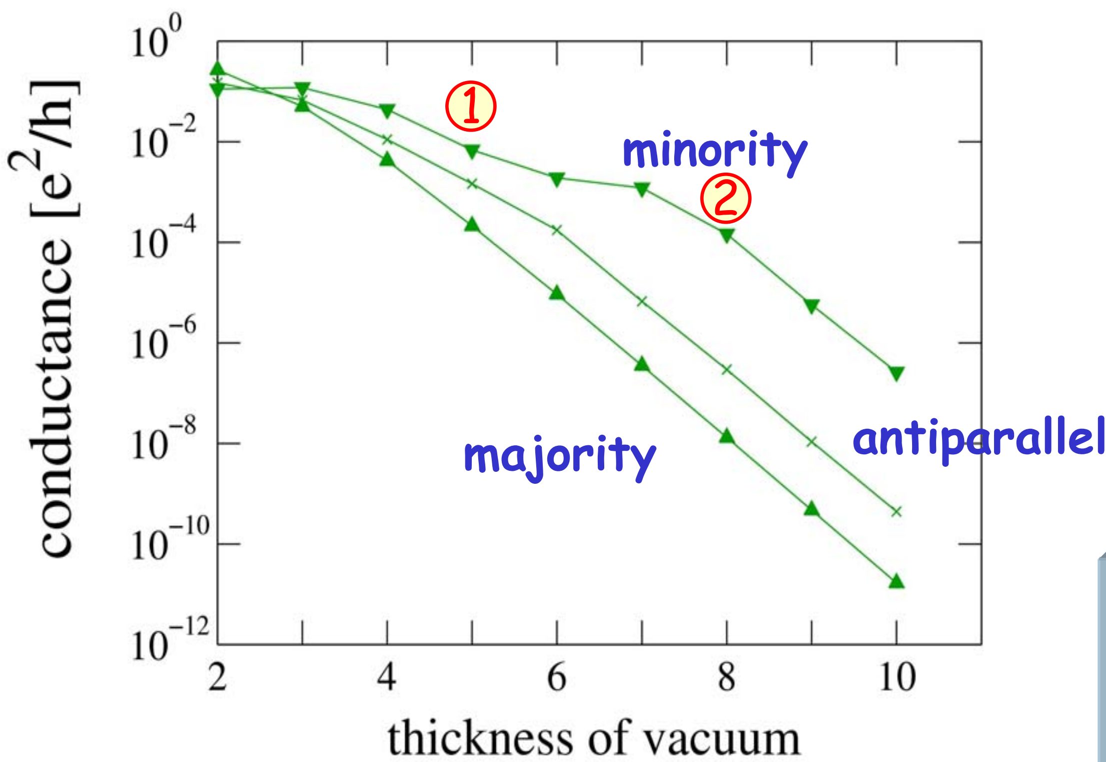
Fe interface LDOS* at 2d Γ point

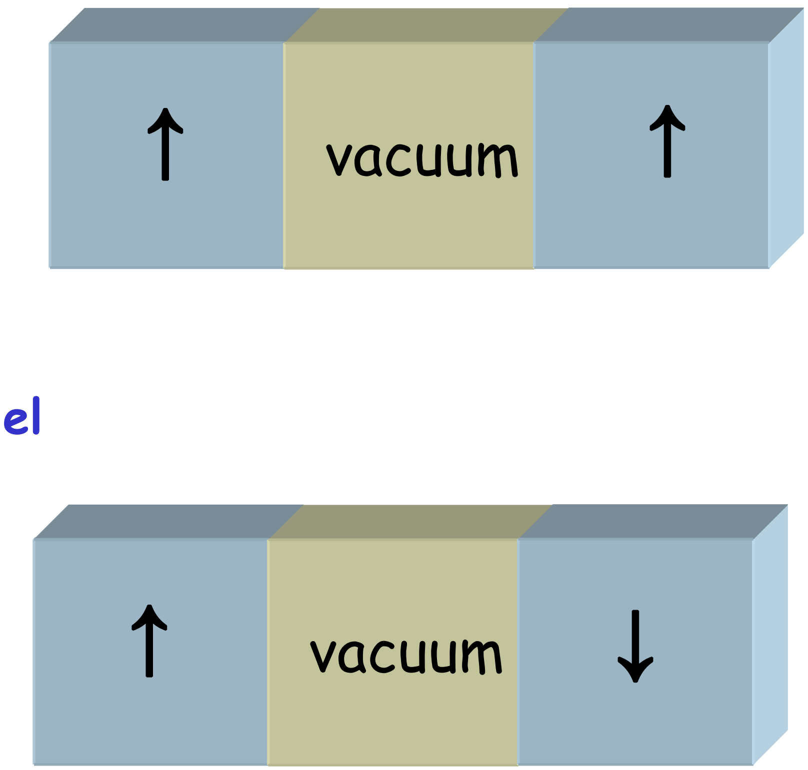
Fe/vacuum interface

Khomyakov at al, PRB 2005

* Only for states with Δ_1 symmetry

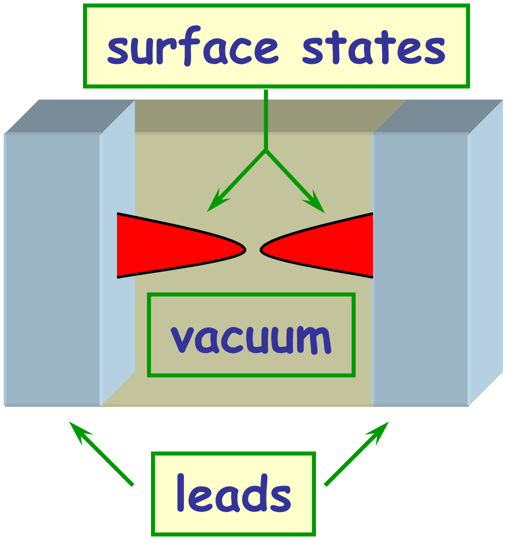
Ideal Fe/vacuum/Fe MTJ

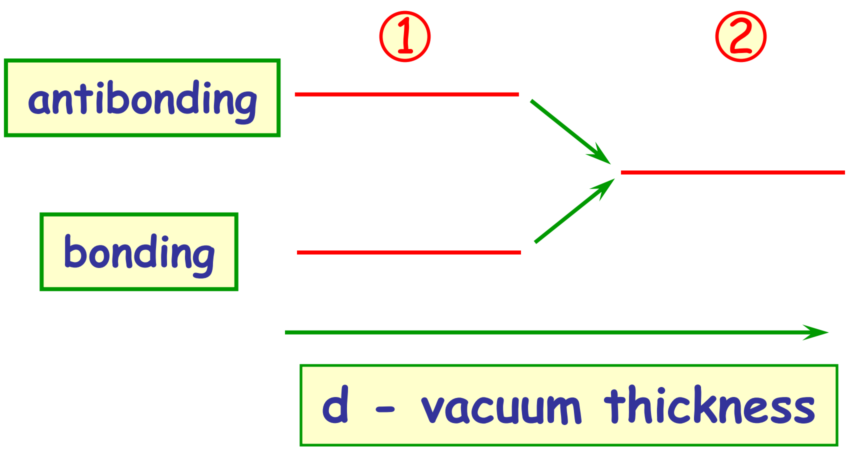


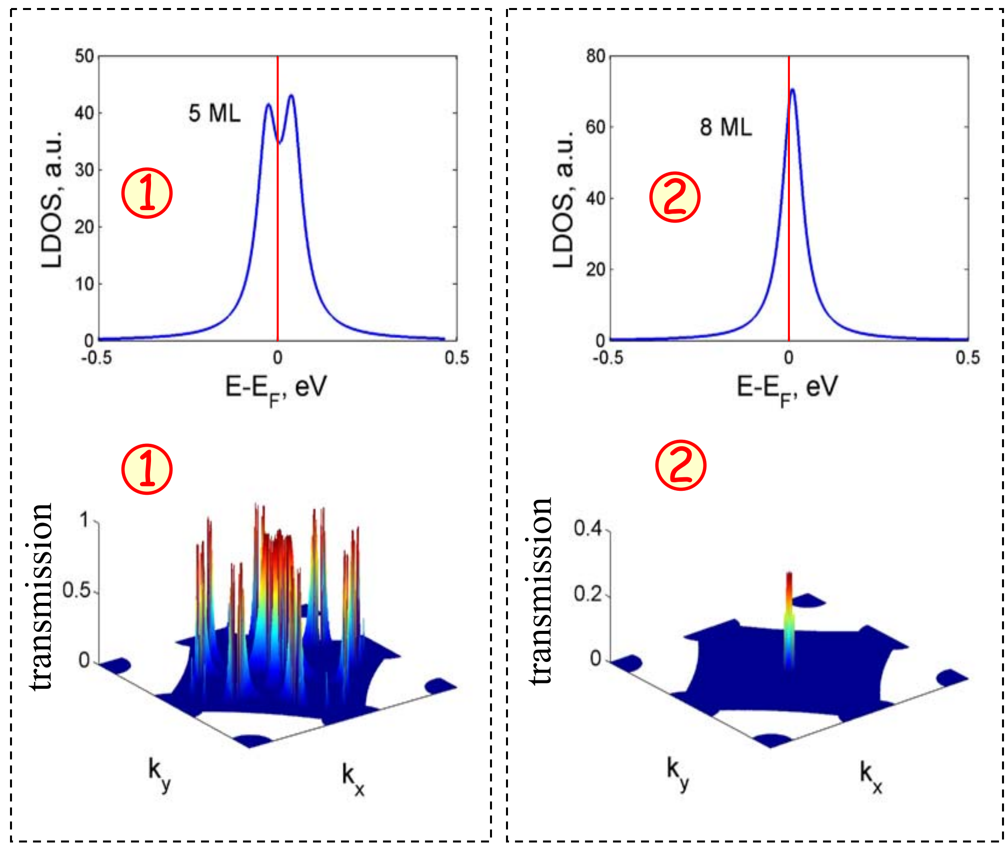


Total antiparallel conductance is much smaller than the parallel one providing huge TMR

Bonding antibonding splitting can be demonstrated by the LDOS* calculated in 2D – Γ point at the interface







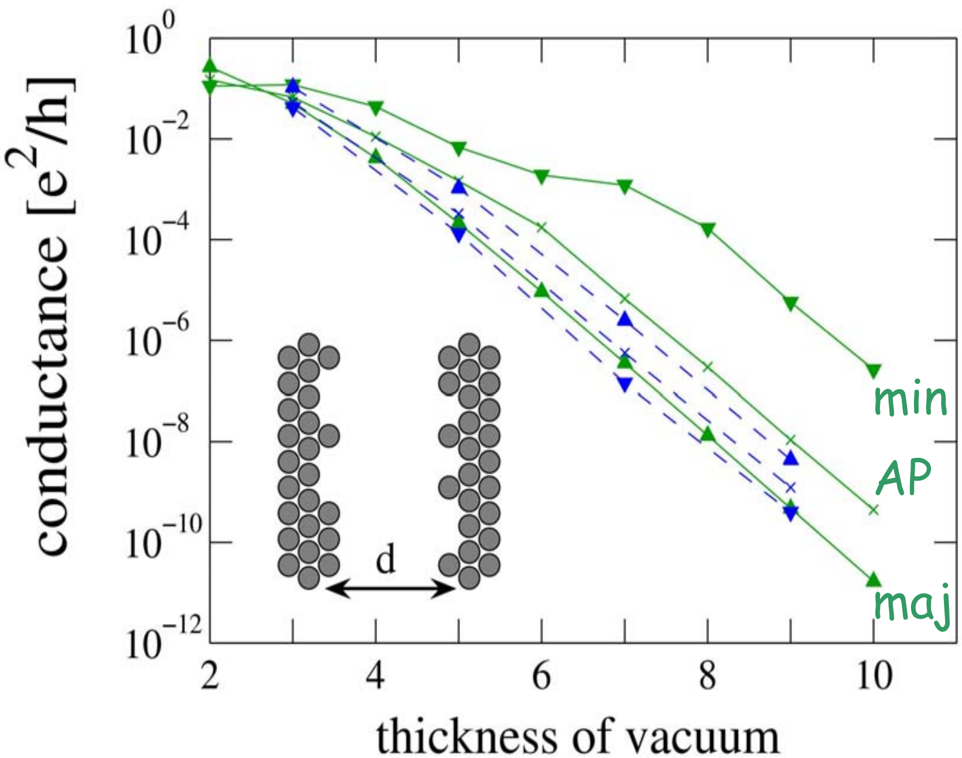
* Only for states with Δ_1 symmetry

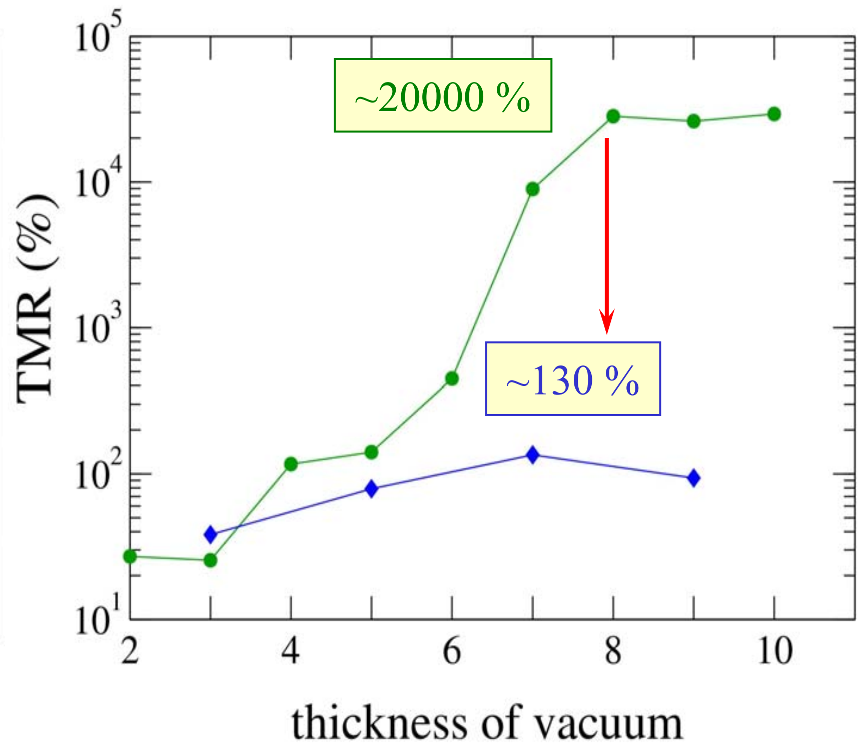
Wunnicke et al. PRB**65** (2002)

What about disorder, roughness ?

Model flexibly in lateral supercells

Fe/vacuum/Fe interface roughness



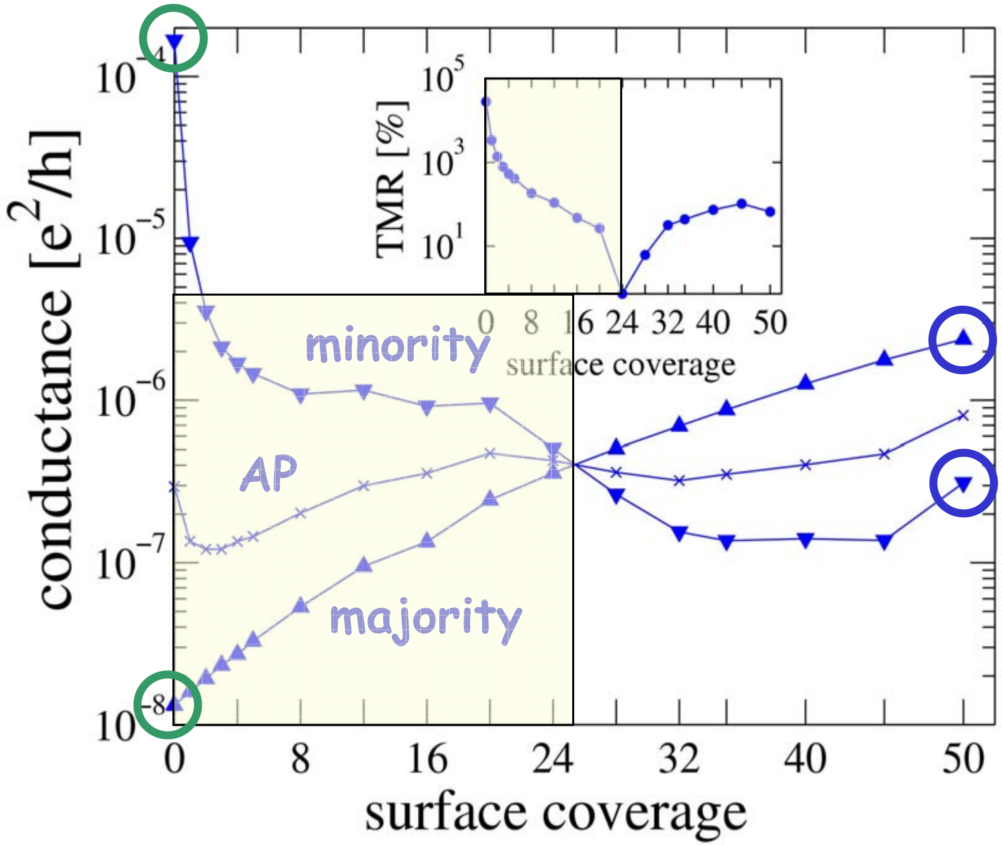


In case of roughness (with 50% of interface coverage) the majority conductance is higher than minority for the parallel configuration

For an ideal junction TMR is about 20000%. Interface roughness reduces the TMR to values comparable to those observed experimentally

Xu et al. PRB**73** (2006)

Transport for a fixed vacuum barrier thickness as a function of roughness



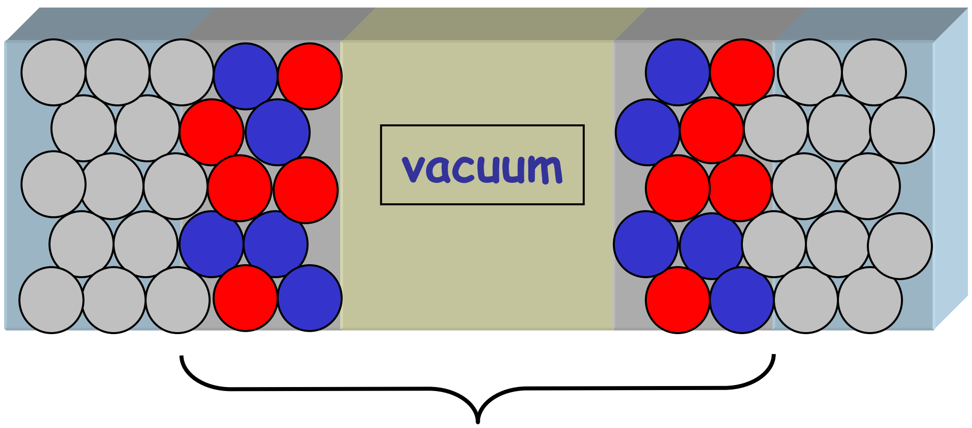
Till ~25% of surface coverage the minority conductance decreases as the roughness increases leading to a rapid decline of TMR

Majority conductance increases all the time resulting in an increasing TMR in a range of surface coverage greater than 25%

Xu et al. PRB**73** (2006)

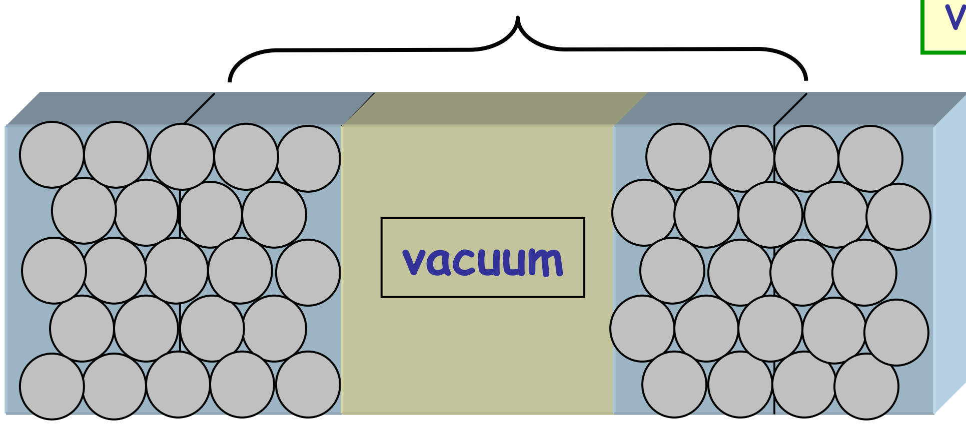
FeCo/vacuum/FeCo alloy leads

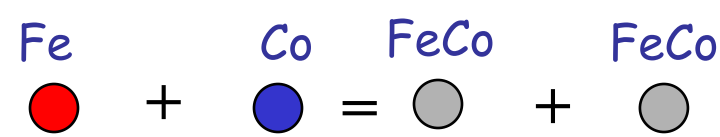
disordered (alloy) leads

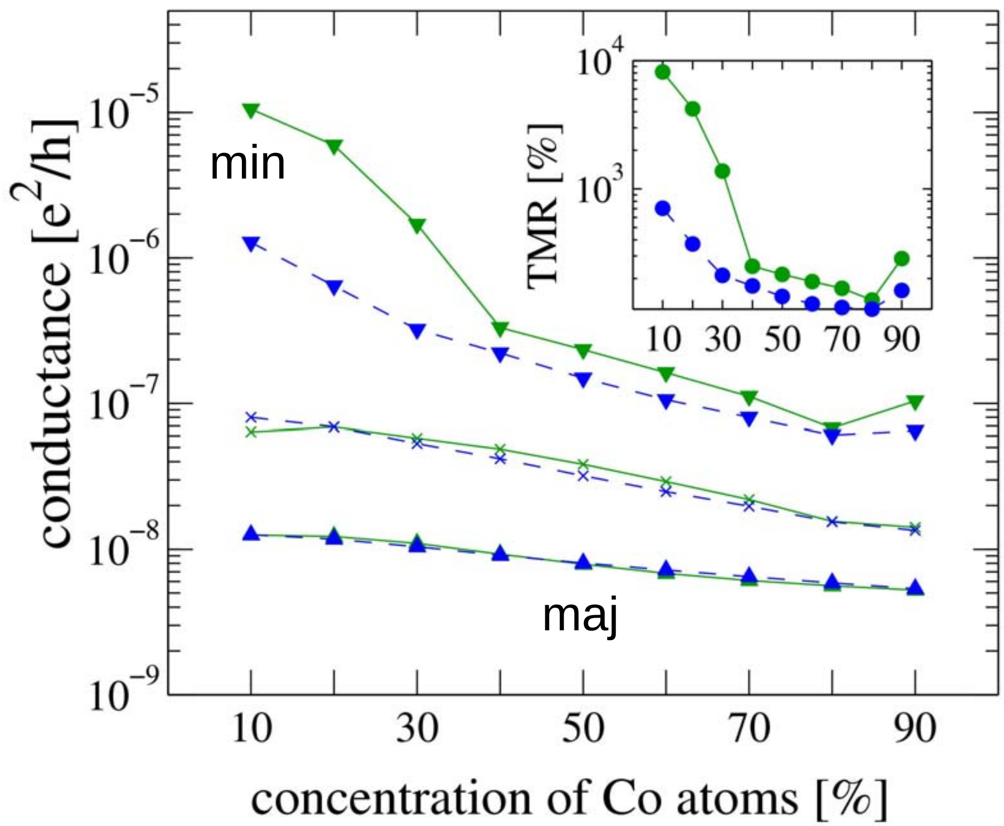


scattering region

ideal leads -
virtual crystal approximation







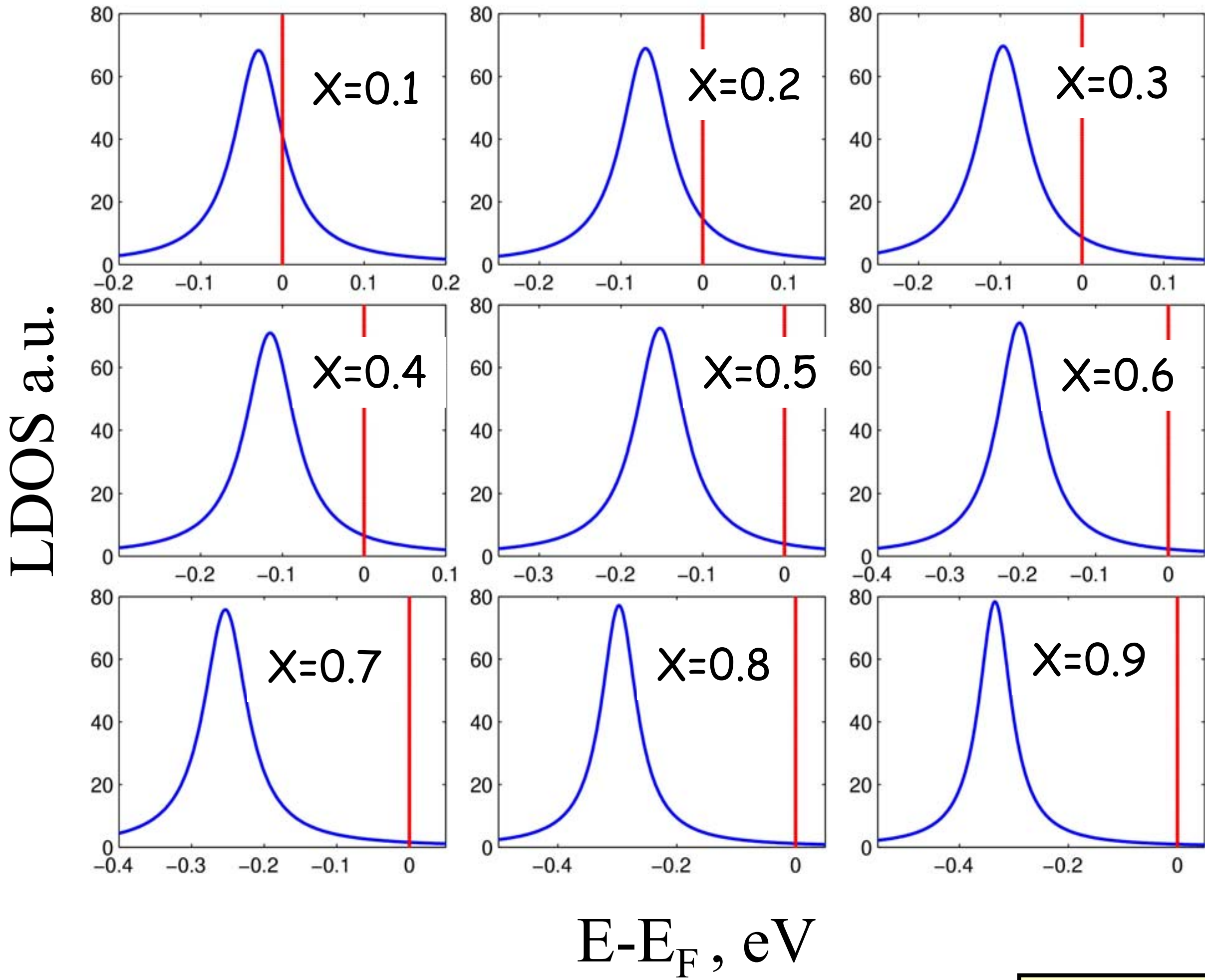
Blue lines represent conductances in case of disordered leads

Green lines represent conductances in case of ideal leads

Effect of the alloy leads is not as strong as the effect of roughness especially for higher concentration of Co

Xu et al. PRB**73** (2006)

interfacial LDOS* at 2d Γ point for $Fe_{1-x}Co_x$ alloy



Fermi level moves away from the surface state maximum as the Co concentration increases

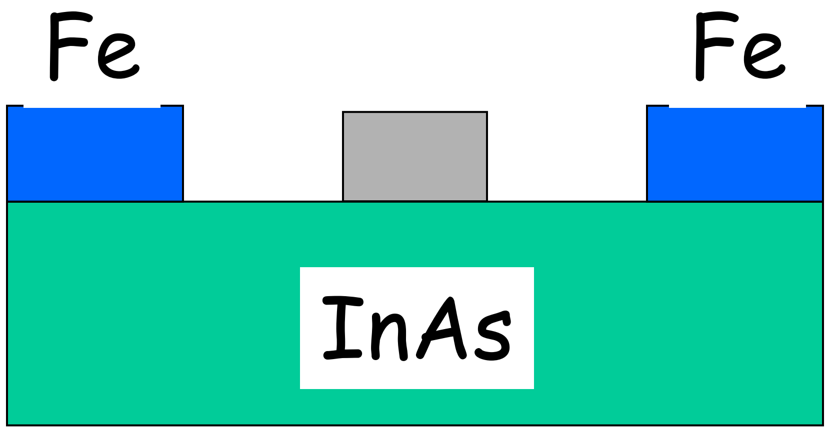
*** Only for states with Δ_1 symmetry**

Spin injection from Fe into InAs

V.Karpan[1], M.Zwierzycki[1,3], P.J.Kelly[1],
K.Xia[1,2], G.E.W.Bauer[4]

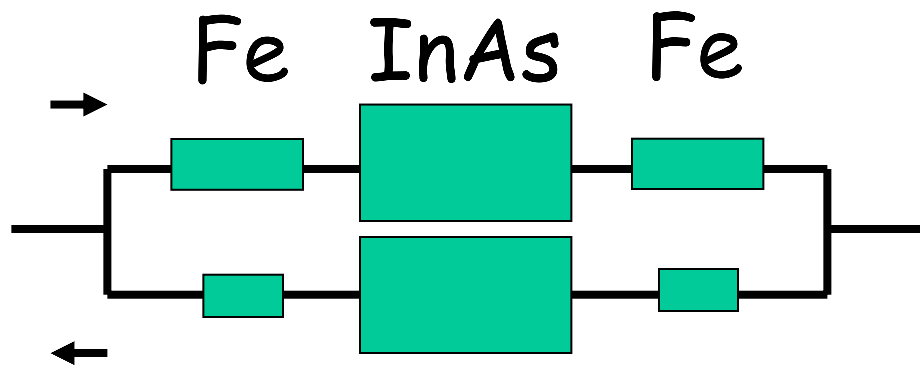
[1] *University of Twente, Enschede, The Netherlands*
[2] *Institute of Physics, Beijing, China*
[3] *Max-Planck Institute for Solid State Research, Stuttgart, Germany*
[4] *Kavli Institute of NanoScience, Delft University of Technology, The Netherlands*

Spin injection



"Spin-transistor"
Datta & Das, APL **56** (1990)

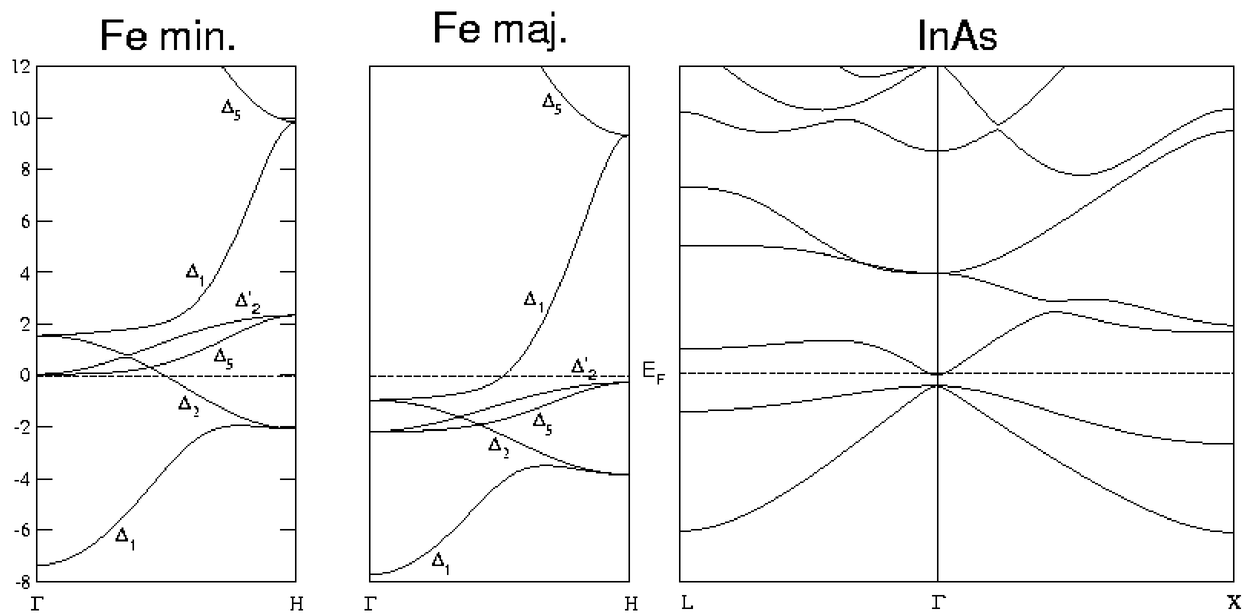
"Conductance mismatch"



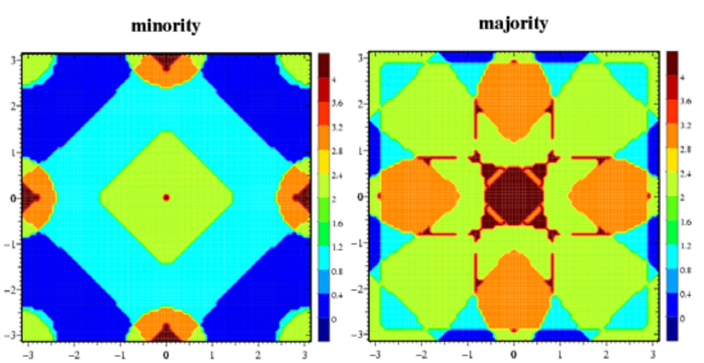
Schmidt et al. PRB **62** (2000)

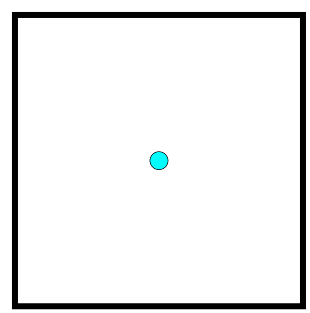
The "Conductance mismatch" argument ignores the possibility of spin-dependent interface resistances - how large are they ?

Origin of conductance mismatch



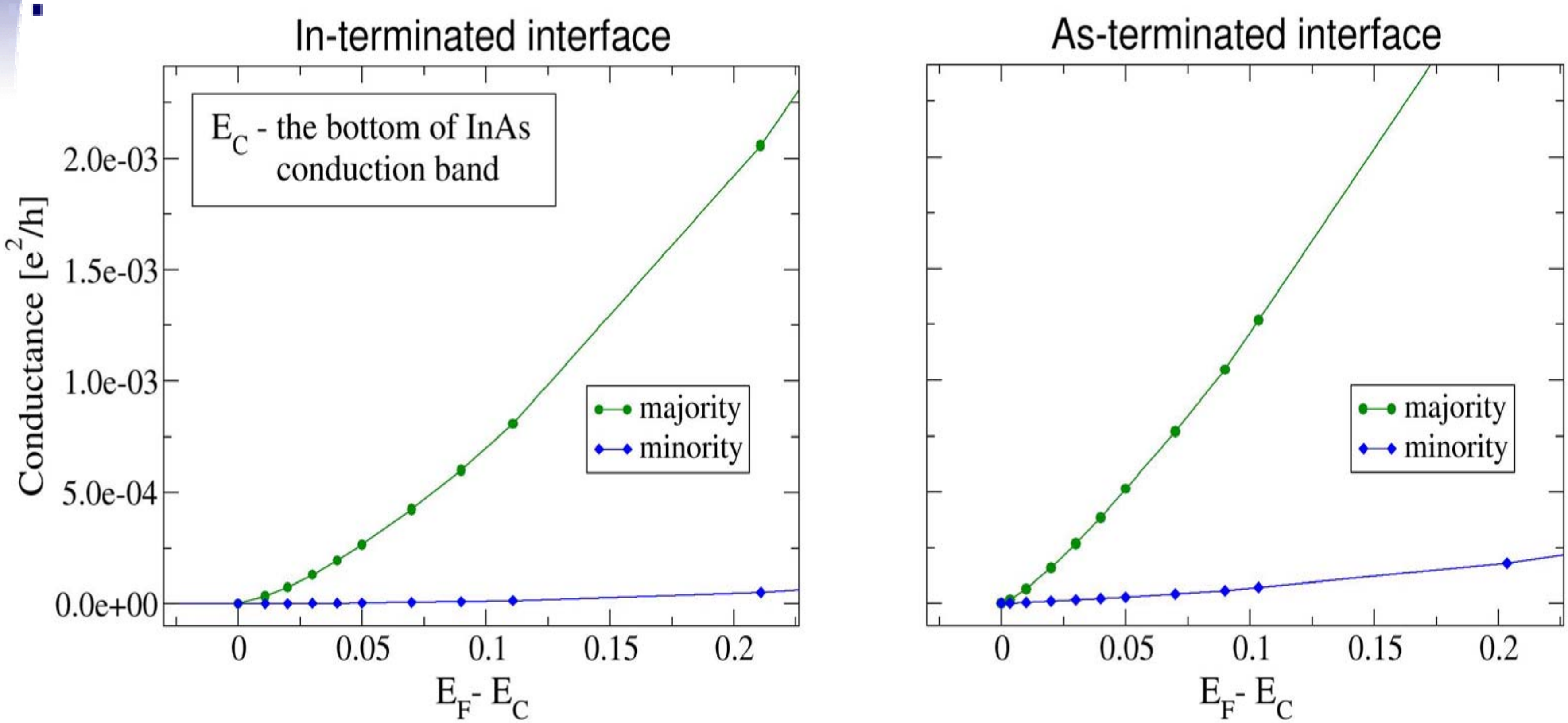
Fermi surface projections





What about the spin dependence of the interface resistance ?

Ideal Fe/InAs interface conductances

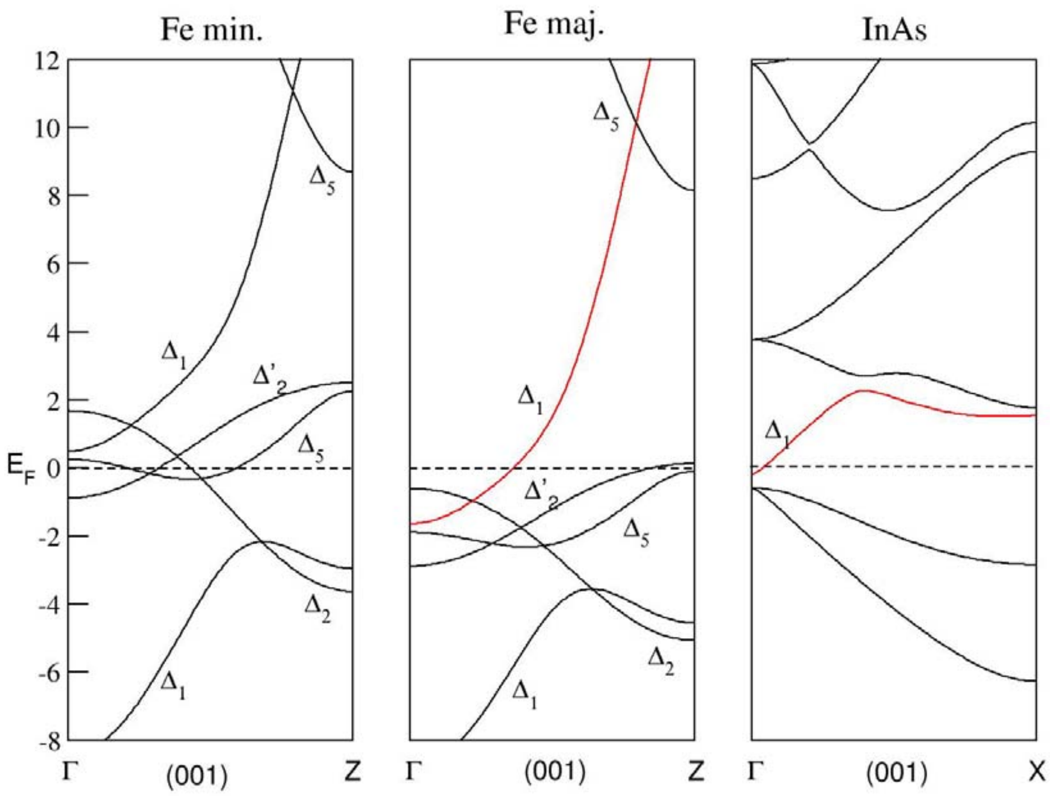


$$\frac{G_{\uparrow} - G_{\downarrow}}{G_{\uparrow} + G_{\downarrow}}$$

~ 98% $E_F - E_C \sim 0.02$ eV   ~ 89%

Zwierzycki et al. PRB **67** (2003)
Wunnicke et al. PRB **65** (2002)

Origin of large spin-dependent conductance mismatch: symmetry of states at Fermi energy



Interface Resistances

- Estimate the spin-dependent interface resistances – valid in the diffusive regime – using

$$SR_{A/B} = \frac{Sh}{e^2}\left[\frac{1}{tr\{t\,t^{+}\}} - \frac{1}{2}\left(\frac{1}{N_A} + \frac{1}{N_B}\right)\right]$$

and compare these resistances to the resistance of a thickness L of bulk doped InAs.

$$L_{InAs}\,\rho_{InAs} \sim SR_{Fe/InAs}$$

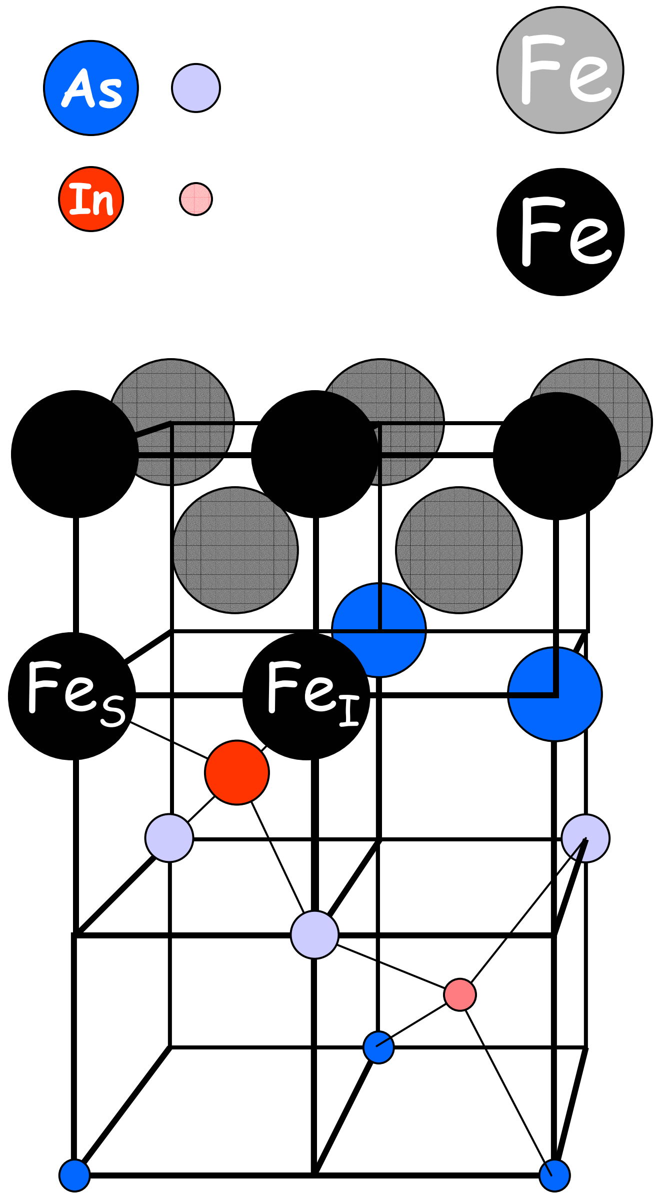
Use LT ρ: $\rho_{InAs}(10^{17}\ cm^{-3}) \sim 0.3\times10^{-4}\Omega m$

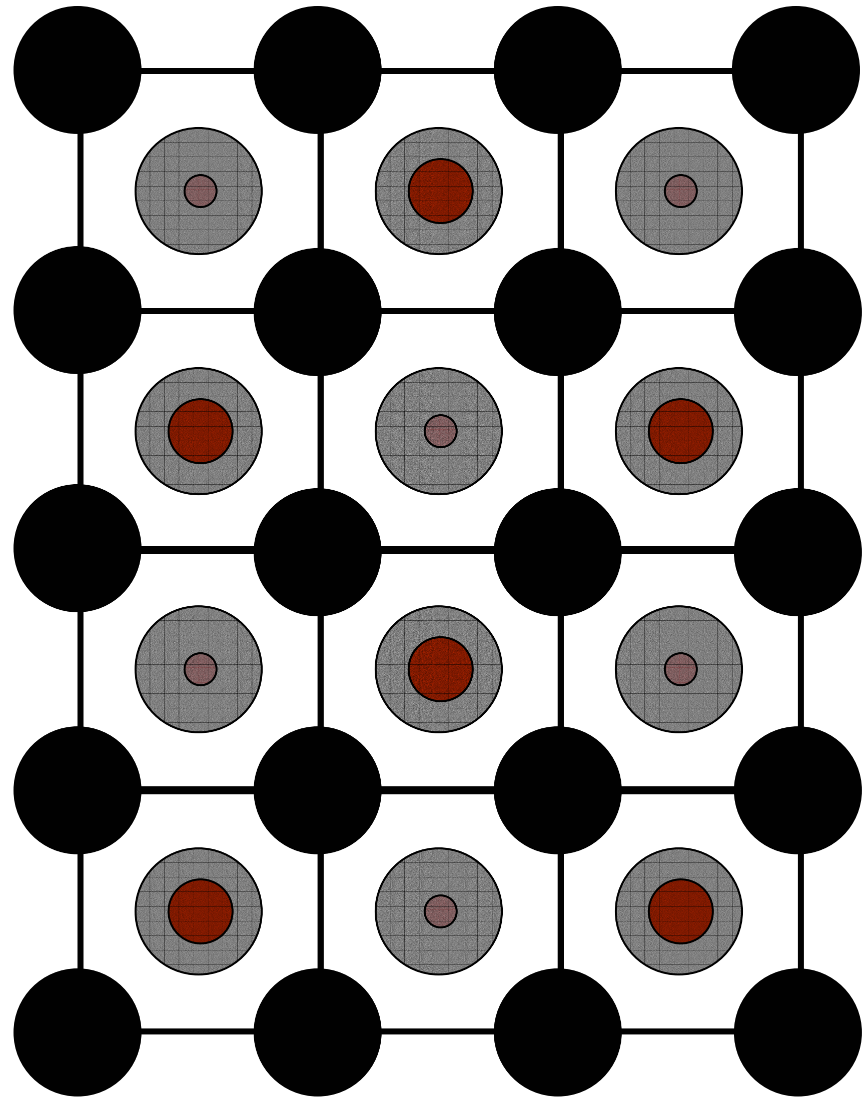
$f\Omega m^2$	In-term	As-term
R_{maj}	5.5×10^4	2.1×10^4
R_{min}	7.1×10^6	5.2×10^5

↓

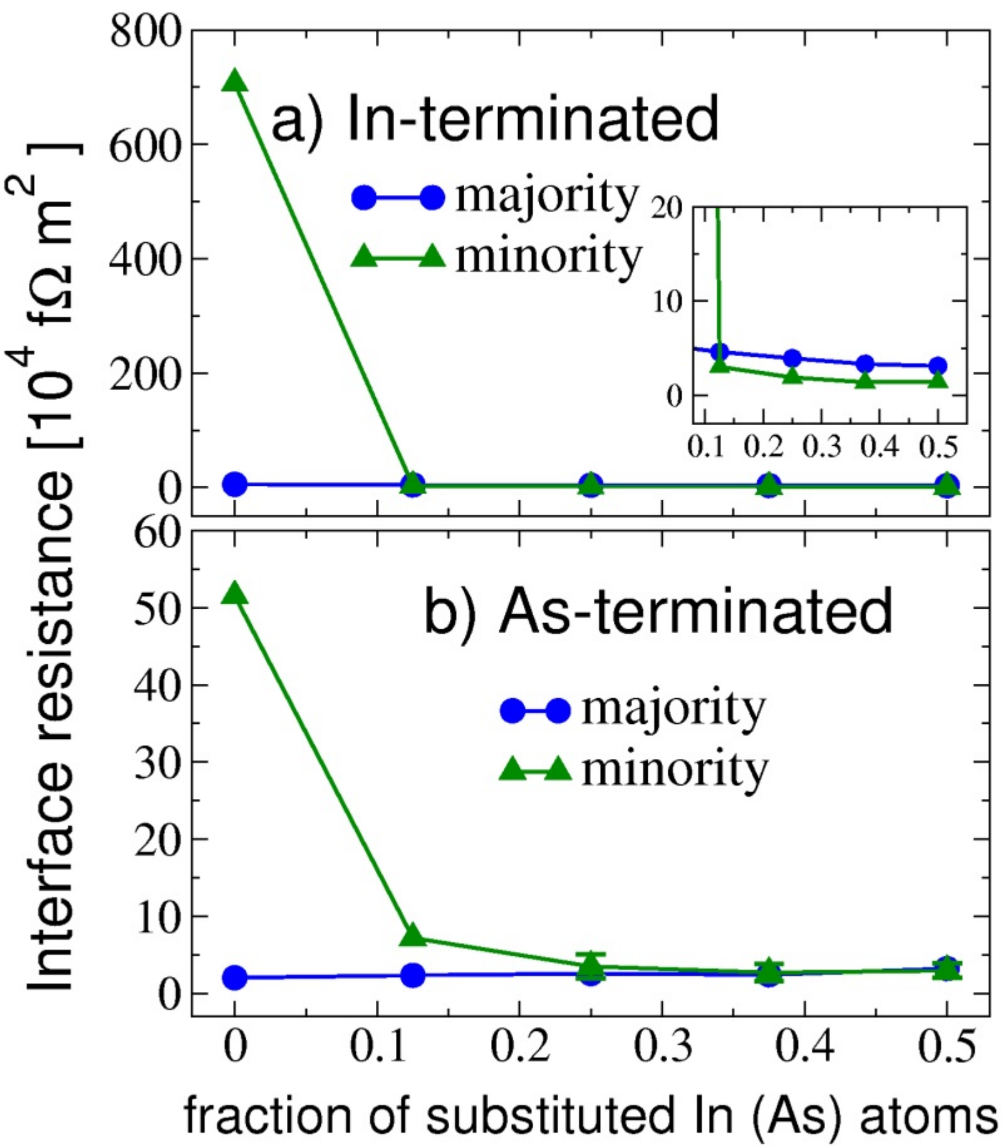
L_{InAs} = 0.7 μm – 240 μm

Effect of Interface Disorder ?





... or in terms of interface resistances

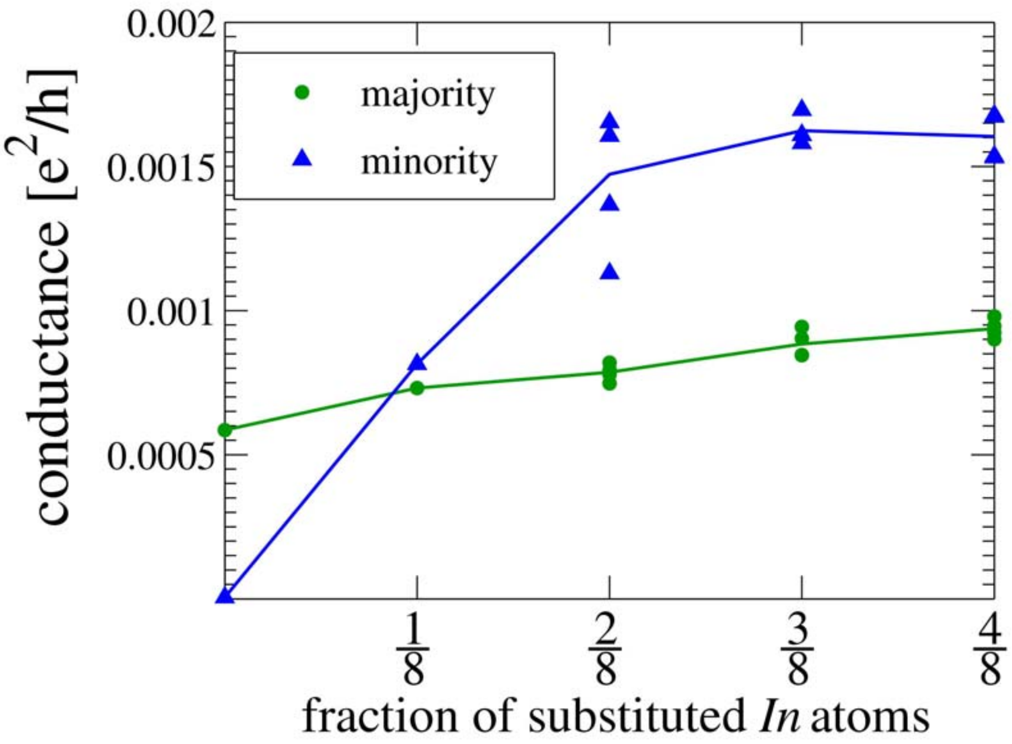


8 In (As) interface atoms in a 2x2 lateral supercell. Replace In (As) with Fe:

A small amount of disorder is sufficient to destroy the spin asymmetry of the interface resistance

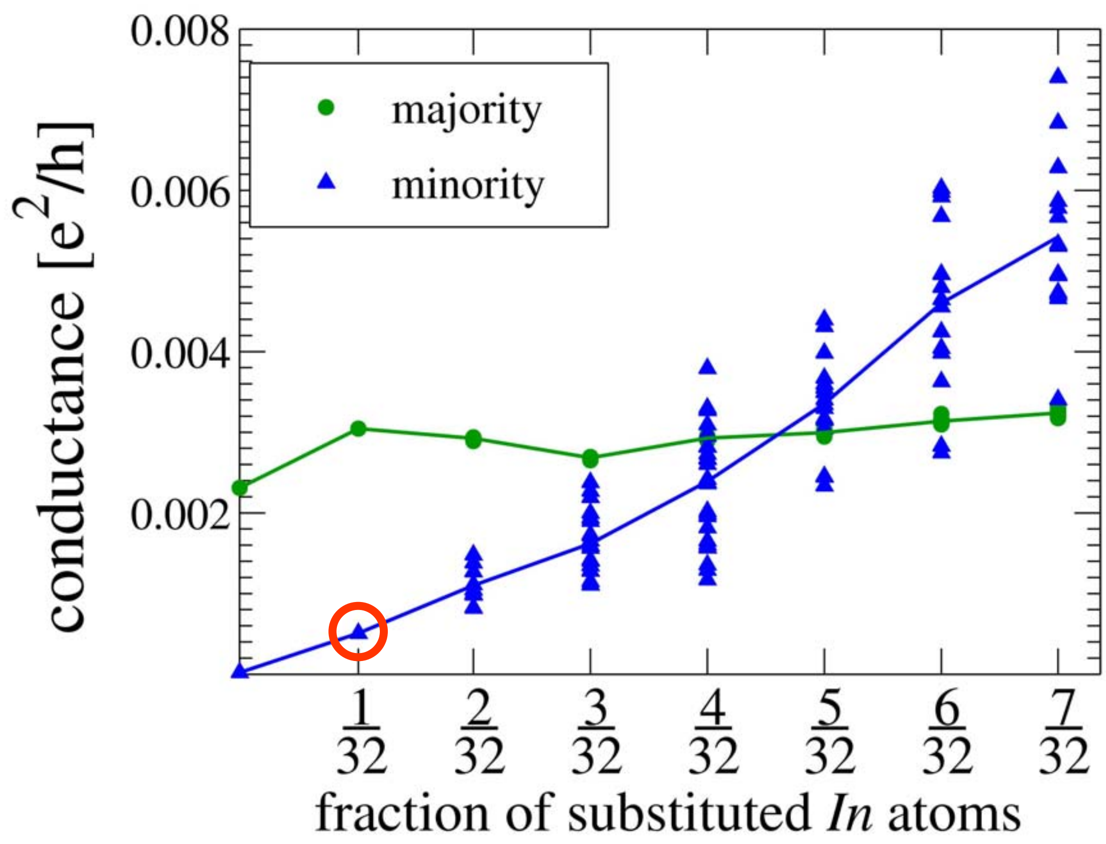
Zwierzycki et al. PRB**67** (2003)

Spin-dependent transmission

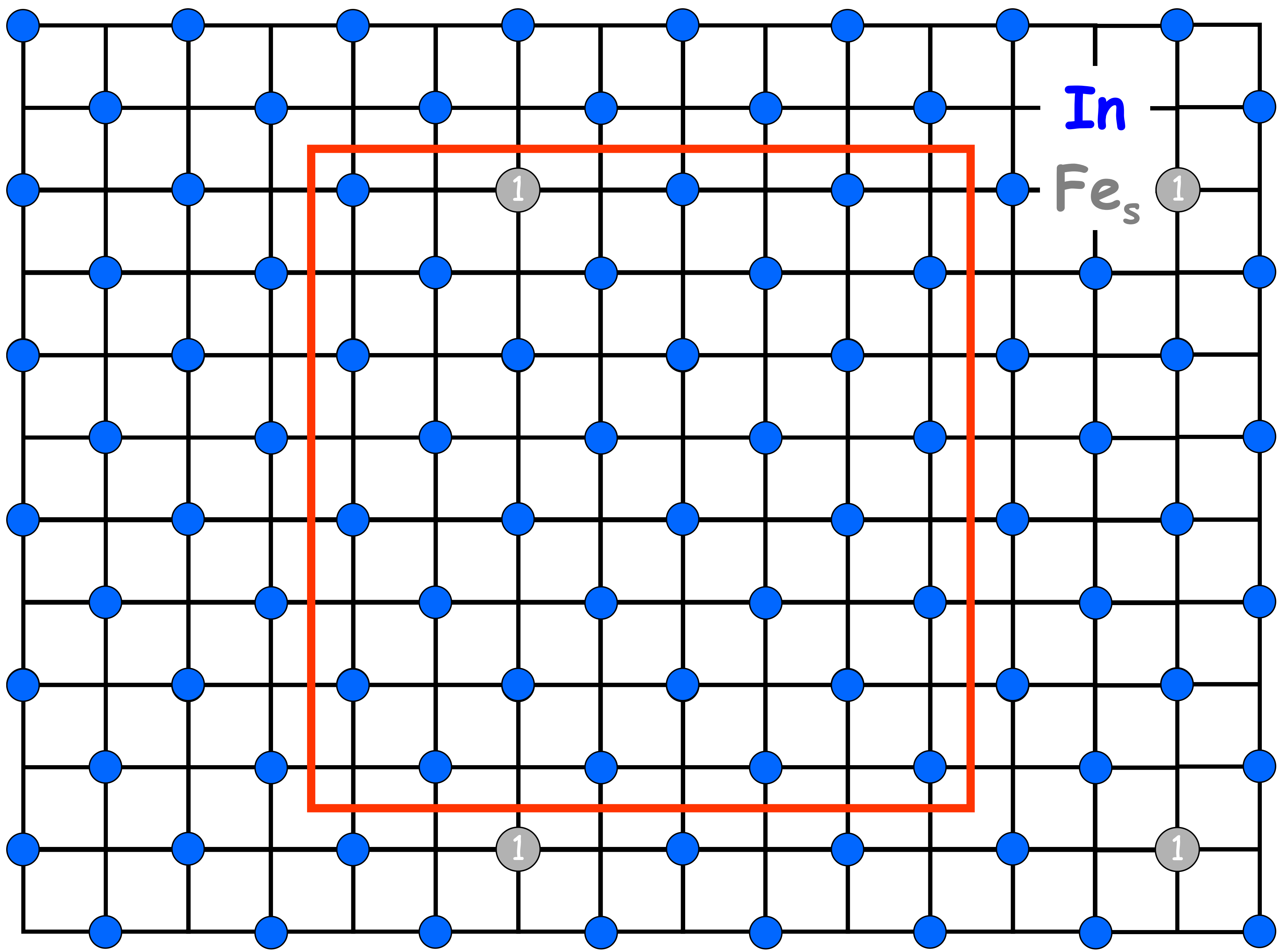


High concentration of impurities -
where is the proportionality regime ?

Spin-dependent transmission

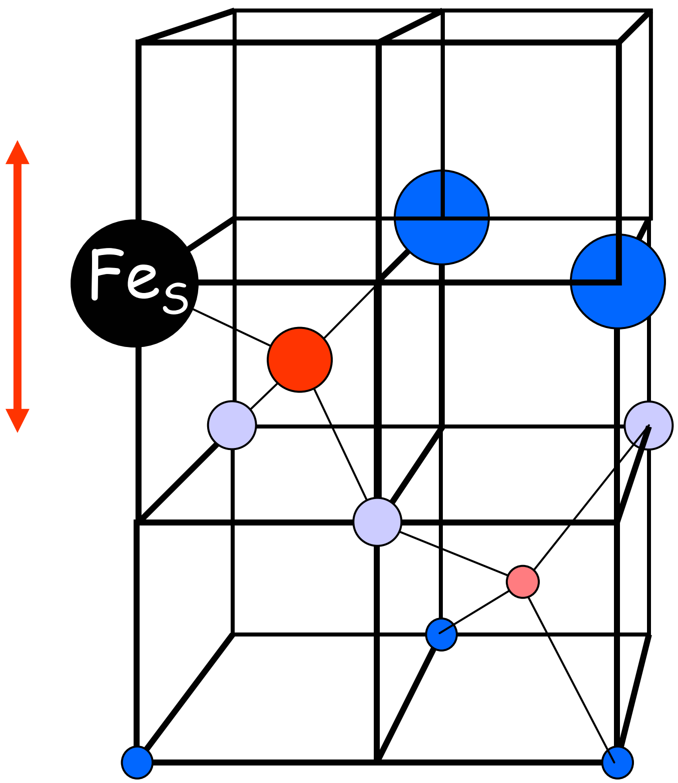


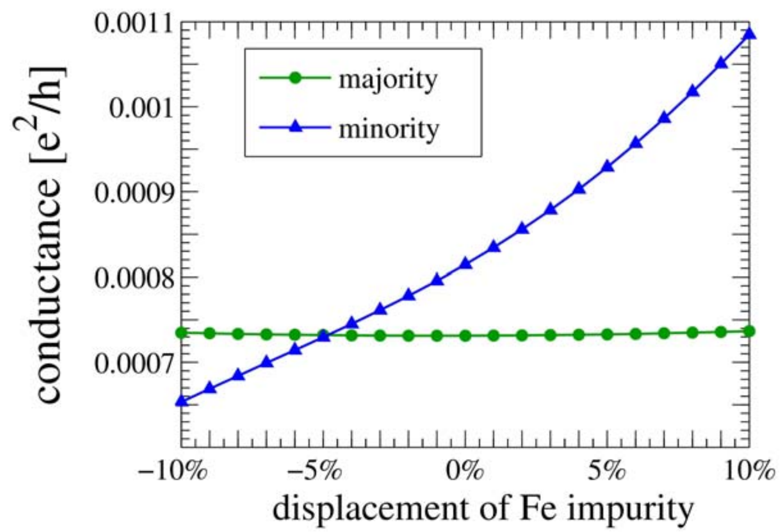
Focus on a single substitutional Fe impurity on In site



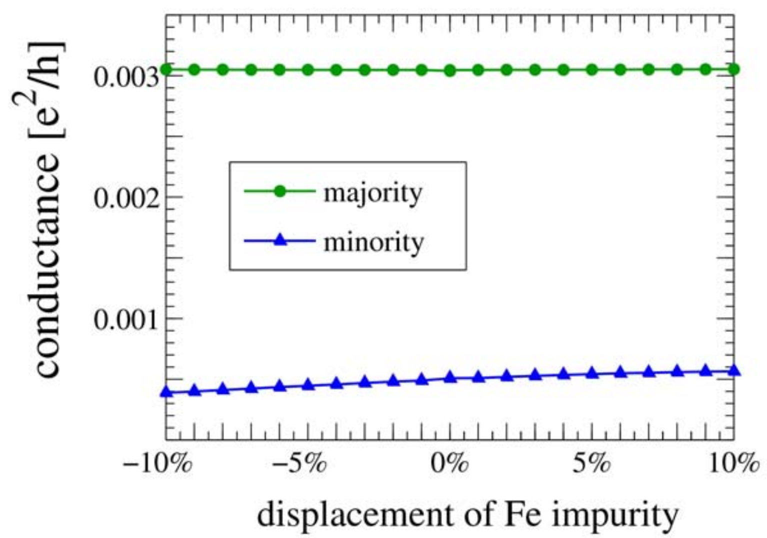
In
Fe_s
1
1
1
1

Effect of displacing a single Fe_s





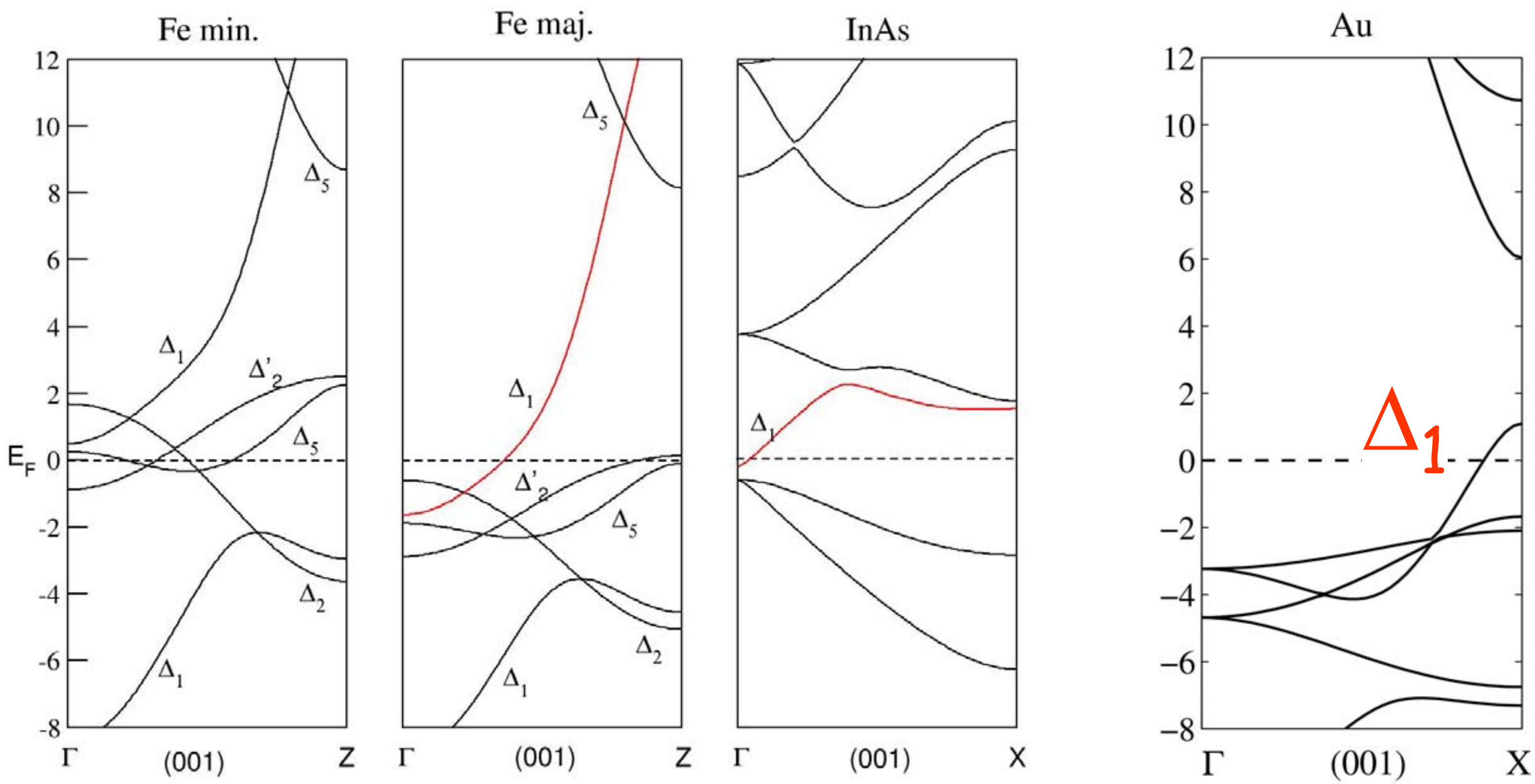
1/8



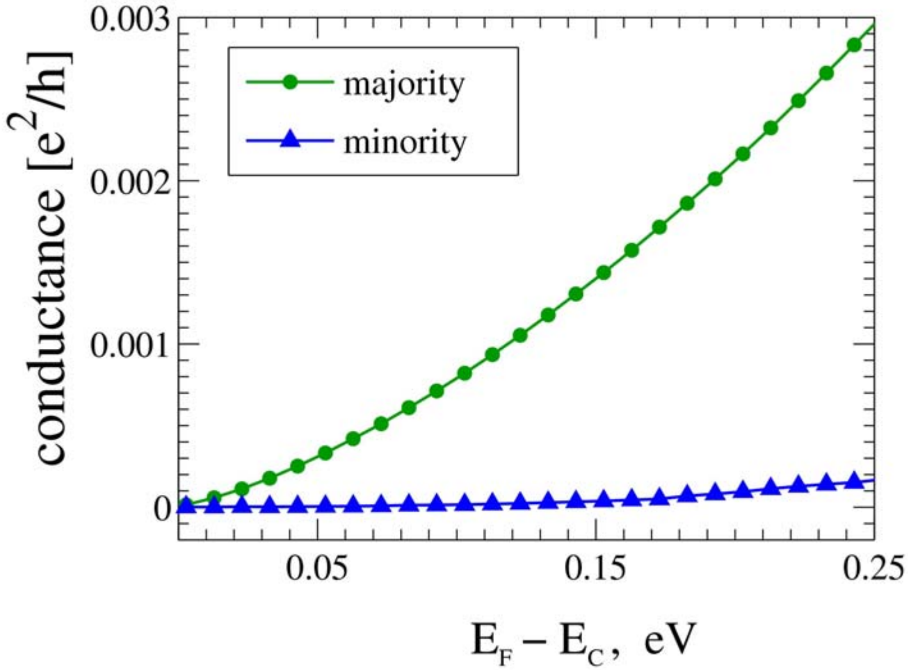
1/32

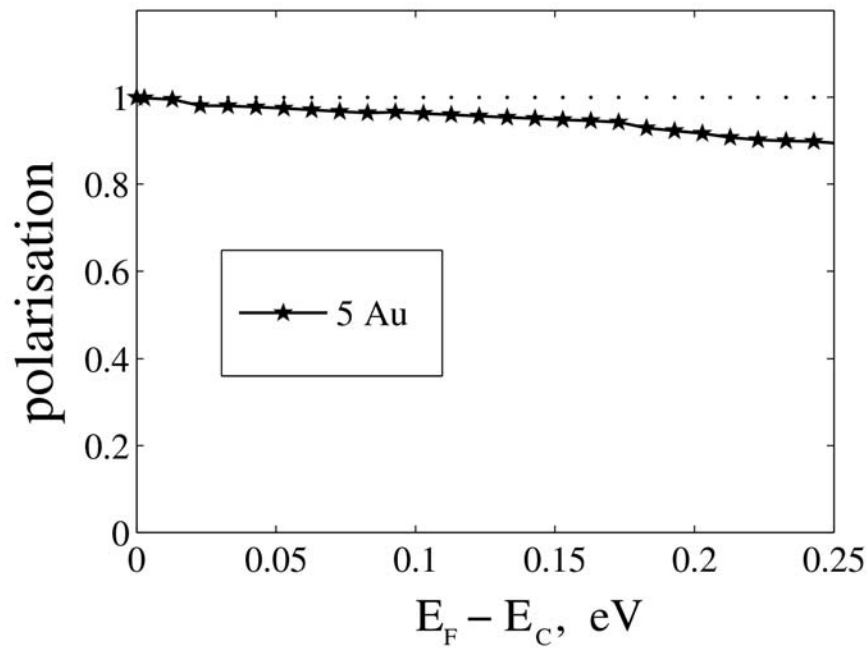
The transmission polarization is seen to depend very sensitively on the concentration and configuration of impurities

Alternatively: prevent Fe from contacting the InAs by inserting a barrier between Fe and InAs which preserves the transmission polarization

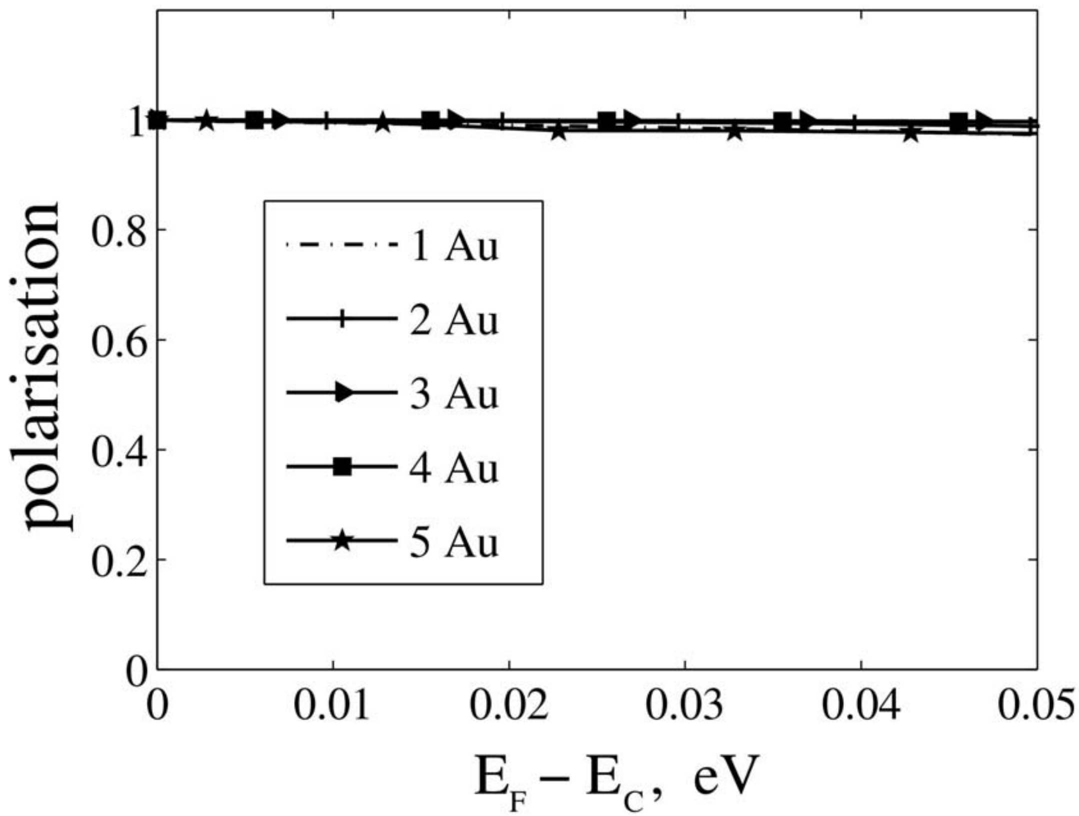


$Fe|Au_5|InAs$


0.003
0.002
0.001
0
conductance [e^2/h]
majority
minority
0.05
0.15
0.25
E_F – E_C, eV

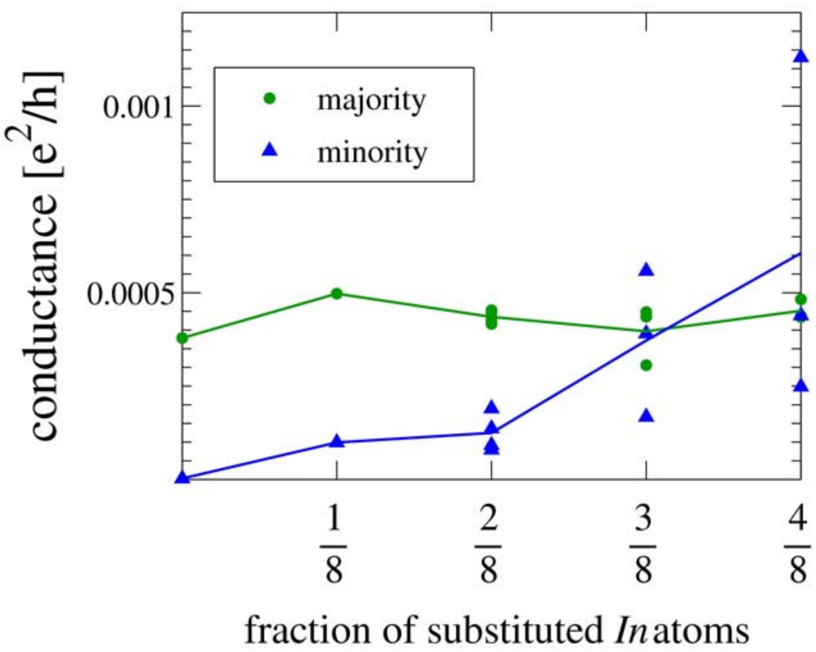

1
0.8
0.6
0.4
0.2
0
polarisation
5 Au
0
0.05
0.1
0.15
0.2
0.25
E_F – E_C, eV

Au thickness-dependence Fe|Au$_n$|InAs

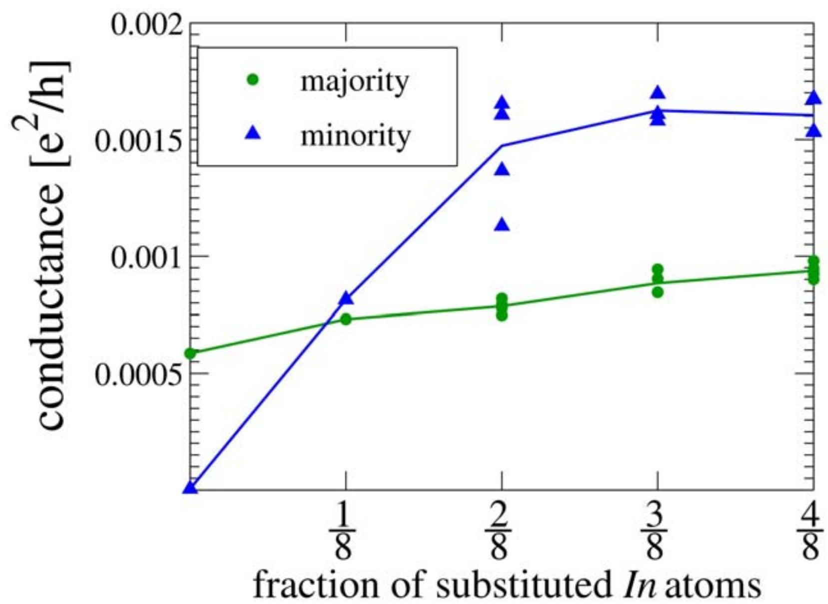


Effect of disorder at Fe|Au interface on the transmission polarization for Fe|Au_5|InAs

with Au



without Au



Interface sharpening ?
Co/Au (250-300°C): den Broeder et al PRL**60** (1988)

- Electrons can be strongly reflected at a perfect interface (no disorder) between two different metals because of bandstructure mismatch

- The transmission through an interface with a ferromagnetic material is strongly spin-dependent

- The spin-dependence of the interface resistance should be enough to make spin-injection observable for sufficiently clean Fe/SC interfaces

- Important to have detailed characterization of interface structure !