Electronic structure and Schottky barrier formation in Fe/GaAs magnetic junctions

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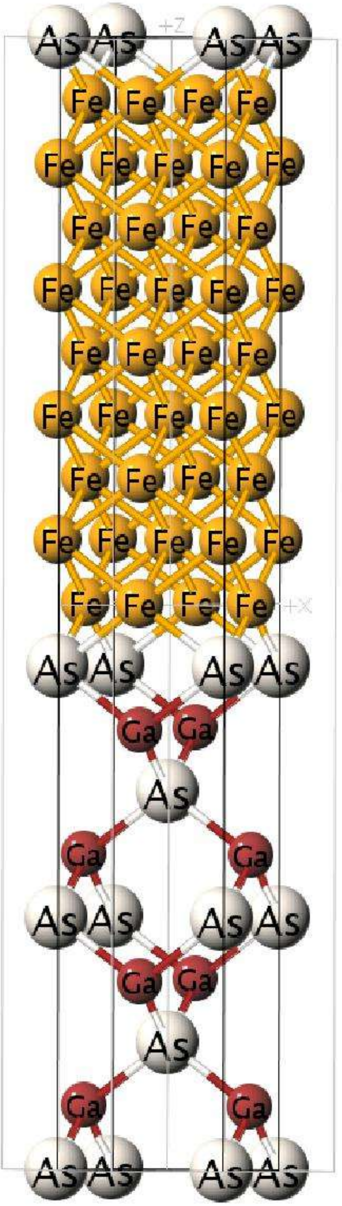
Spin Injection Prospects

- Spintronics – number of novel devices
- Until 2001 low values of spin injection <1%
- Successful experiments in electrical spin injection [1]
- 2% and 30% (at low T) using ferromagnetic Fe on GaAs
- Schottky barrier eliminates conductivity mismatch
- Also weakly dependent on temperature
- Prospects unclear, recent move towards FeCo/MgO
- Need in theoretical study of such interfaces

[1] H. J. Zhu, et al., *Phys. Rev. Lett.* **87**, 016601 (2001); A. T. Hanbicki, et al., *Appl. Phys. Lett.* **80**, 1240 (2002).

Computational Details

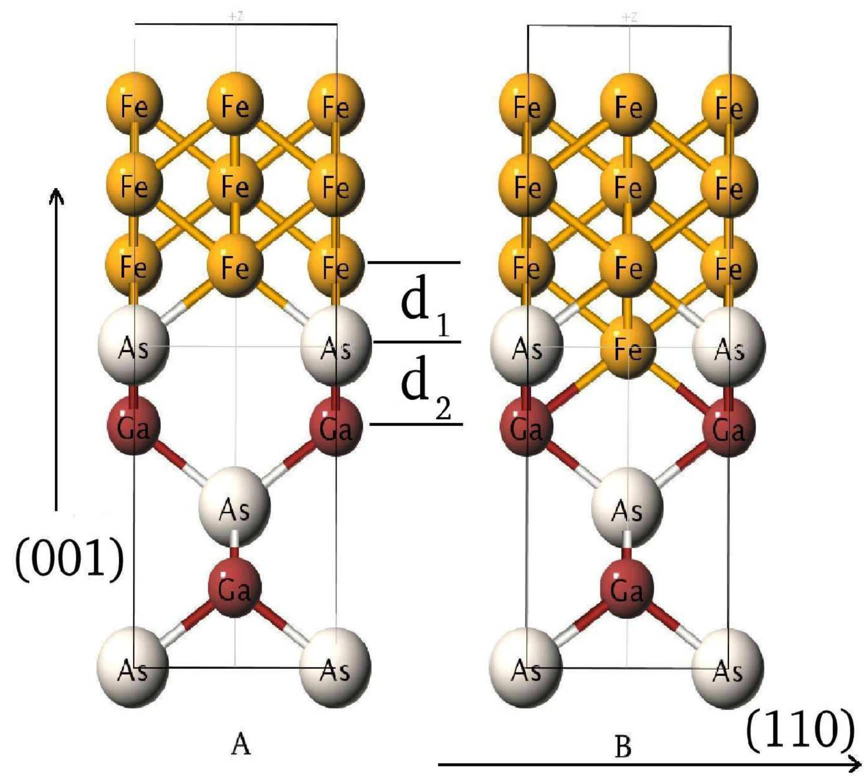
- Describe Fe/GaAs interface – large supercells
- Ignore defects, use different models instead
- Ideal (001) GaAs surface
- Contact with (001) bcc Fe, 1.36% lattice mismatch
- 9 layers of Fe and GaAs – adjacent interfaces do not interact
- GGA approximation, ultrasoft pseudopotentials
- $8 \times 8 \times 4$ **k**-points, 370 eV kinetic energy cutoff
- VASP[2]



[2] G. Kresse and J. Furthmuller, *Comput. Mater. Sci.* **6**, 15 (1996); *Phys. Rev. B* **54**, 11169 (1996).

Structure

- Several possible structures
As- or Ga-terminated
- Two sites for Fe to occupy on GaAs side of interface
- It was shown[3] that for Fe coverage exceeding 2 monolayers, model C is never energetically favorable
- Comparing formation energies
- Relax the interface with respect to d_1 and d_2
- Interfaces are isolated



$$E_{form} = E_{tot} - \sum_i N_i \mu_i$$

[3] S. C. Erwin, et al. *Phys. Rev. B* **65**, 205422 (2002).

Relaxation of the interface

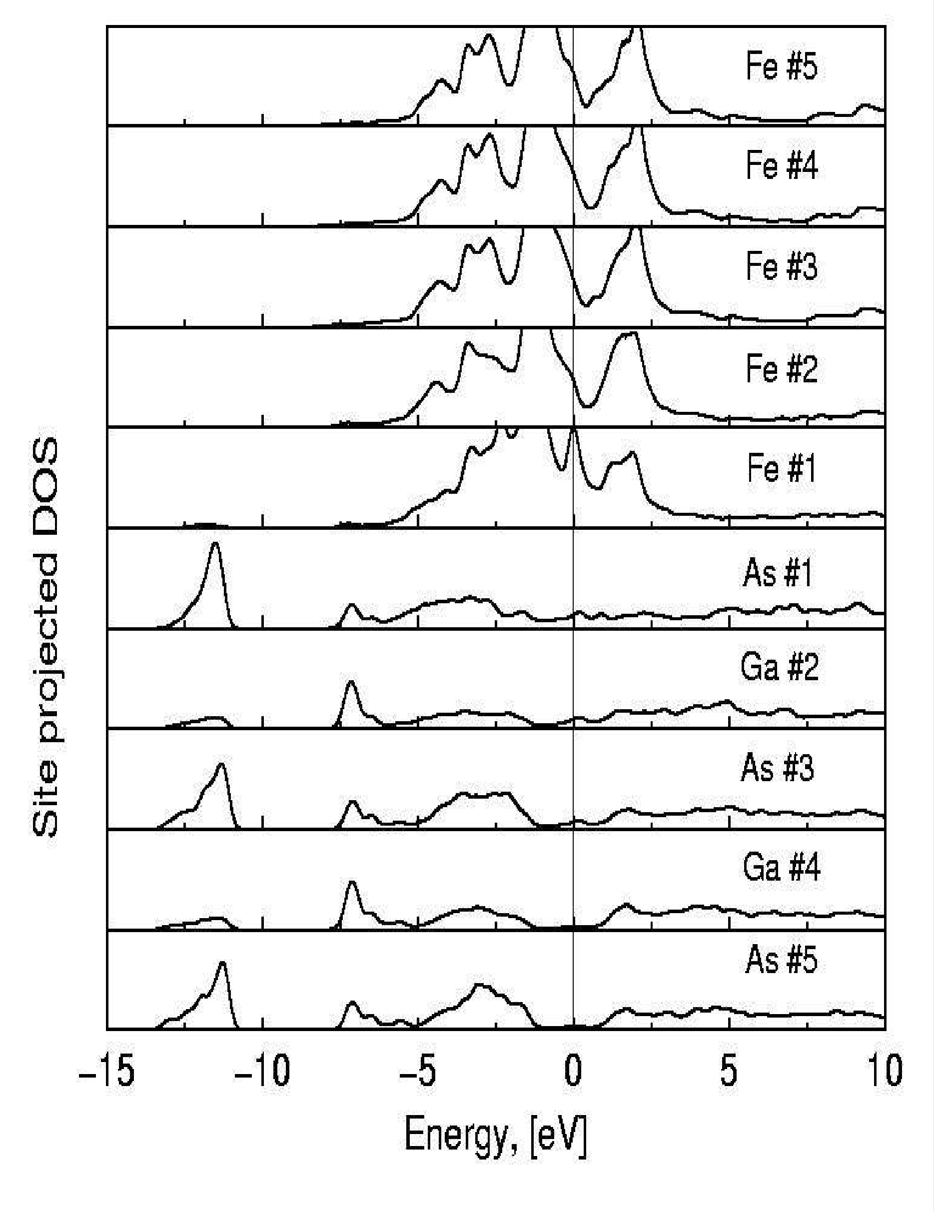
Displacements in units of a_0(GaAs) from the ideal distances between planes

	As-termianted		**Ga-terminated**	
	Δd_1	Δd_2	Δd_1	Δd_2
Model A	0.0	0.025	0.022	0.017
Model B	0.017	0.068	0.018	0.058

- Comparable distortions in both models and terminations In model B the As(or Ga)-Fe bonding is stretched by similar amounts (Δd_1)
- Ga-As distance changes considerably more (Δd_2) in model B – extra Fe atom (extra electrons occupy antibonding orbitals)
- Relaxed energies: A favored for As-termination; B favored for Ga-termination

Layer-resolved DOS

- DOS in most bulk-like layers resemble bulk DOS
- Tails of Fe states penetrate into GaAs
- MIGs (?) in the GaAs bandgap pinning the Fermi level
- Gap is practically recovered in the GaAs layer furthest from interface



Schottky barriers

Schottky barrier height $\phi_p = \Delta E_v + \Delta V$ - band structure $\Delta E_v = E_F - E_v$ (taken from two bulk calculations) + potential line-up ΔV (extracted from the SC electrostatic potential):

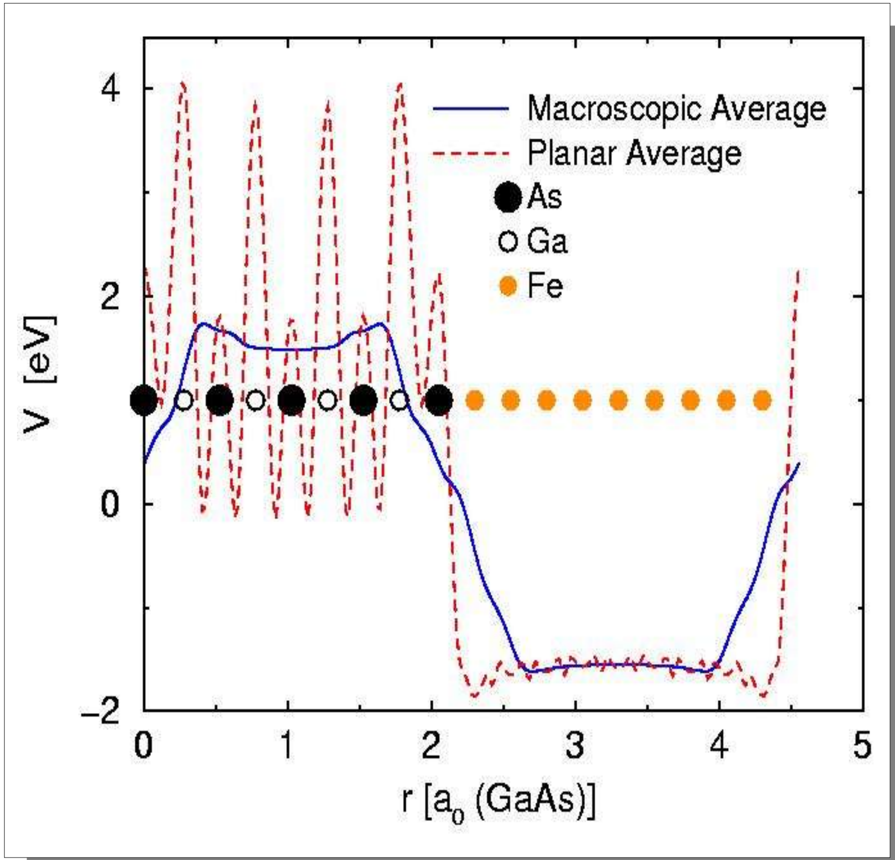
i) 3D data averaged over (001) plane

$$\bar{f}(z) = \frac{1}{S}\int_S f(x,y,z)\,dxdy$$

ii) macroscopic average eliminates bulk-like oscillations

$$\langle \bar{f}(z) \rangle = \frac{1}{a_0}\int_{z-a_0/2}^{z+a_0/2} f(z')\,dz'$$

and approaches bulk constants inside each slab, their difference ΔV



Schottky barriers

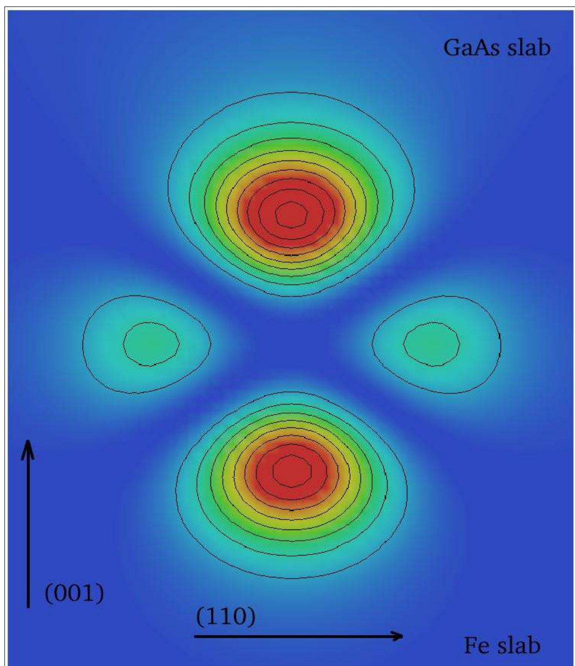
Schottky barrier heights (*eV*) for ideal and relaxed models

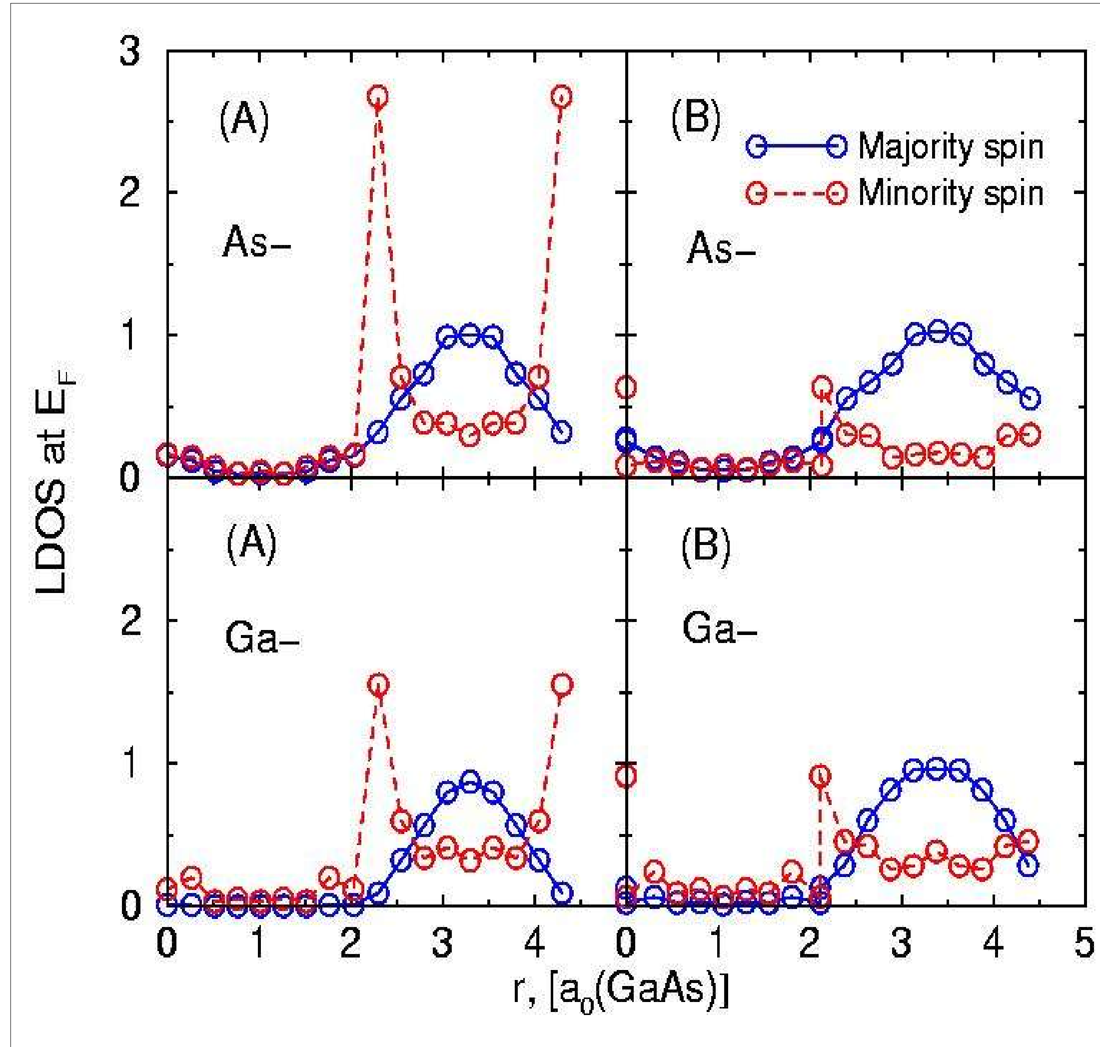
	As-termianted		Ga-terminated	
	Ideal	Relaxed	Ideal	Relaxed
Model A	0.65	0.70	0.51	0.44
Model B	0.94	0.88	0.83	0.63

- Schottky barriers depend on structure
- Relaxed interfaces show good agreement with experiment ~0.72 – 0.75 eV
- What is the mechanism of the Fermi level pinning?
  - GaAs surface states
  - MIGs
  - Interface defects

Spin-polarized DOS at E_F

- Layer-resolved DOS
- Minority spin states dominate at the interface
- Peak caused by localized $d_{3z^2-r^2}$ orbital

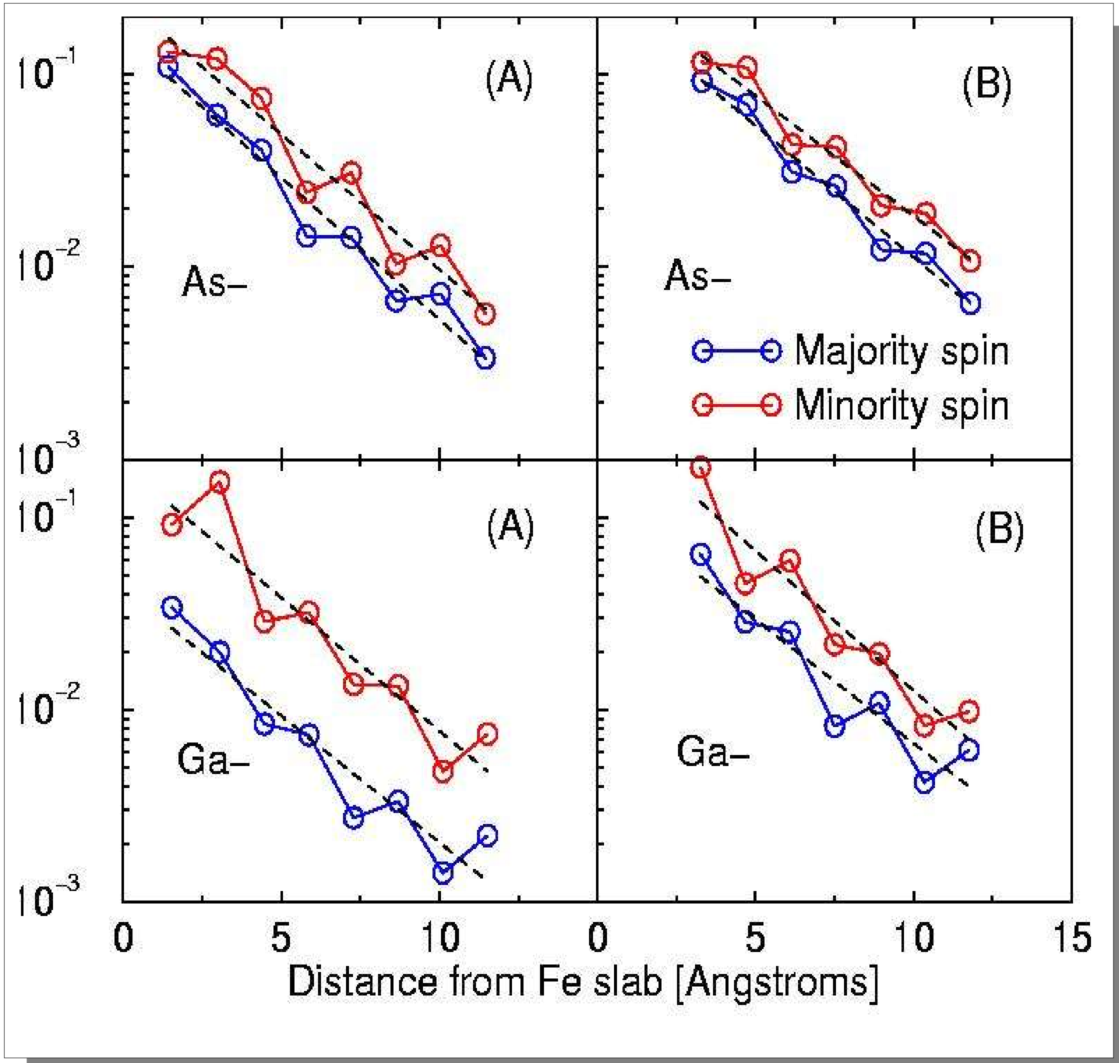




- Similar to free Fe surface
- Fermi level pinned by this MIG state

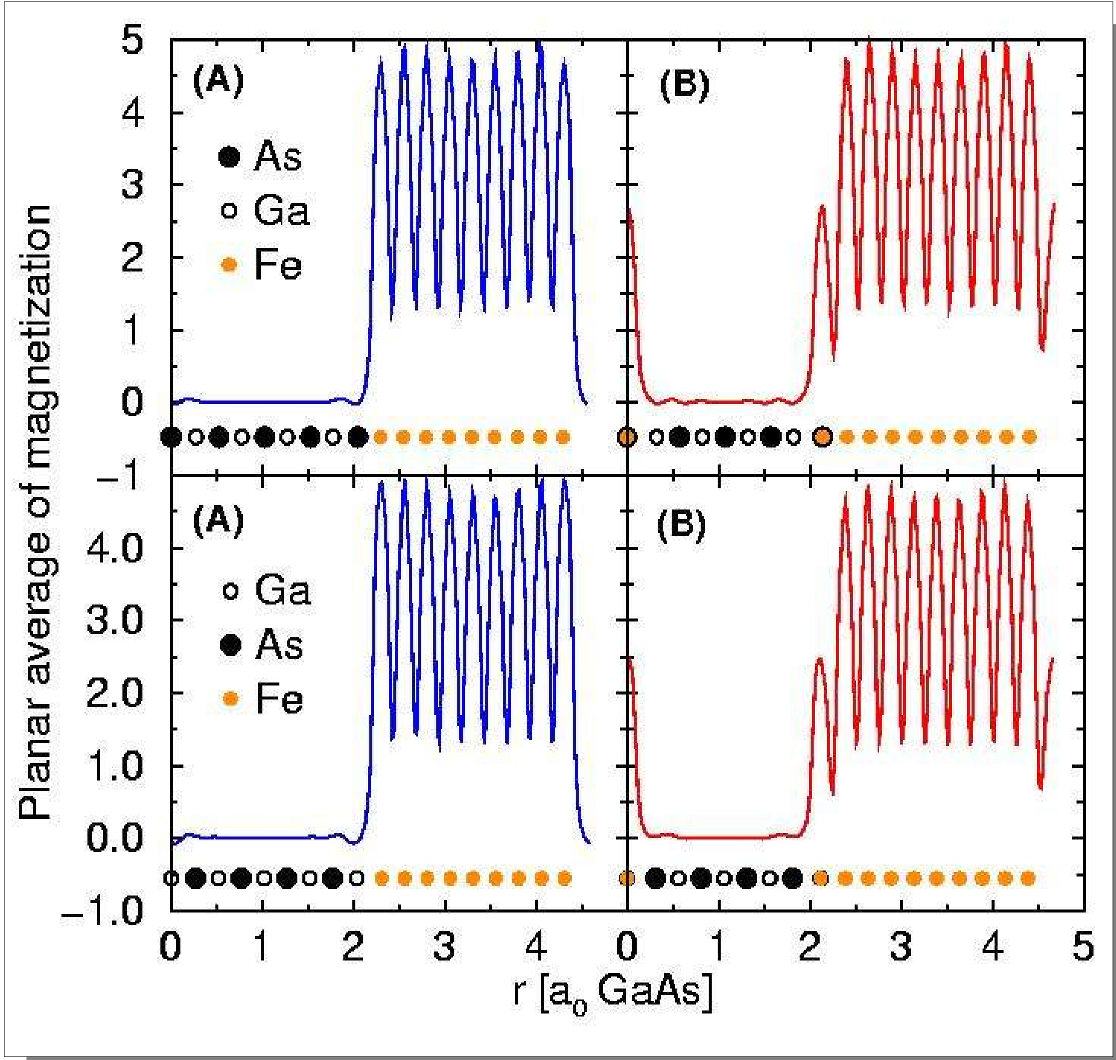
Spin-polarized DOS at E_F in GaAs

- 17 ML GaAs slab
- Exponentially decaying MIGs
- Minority states continue to dominate
- Significant proximity effect
- Decay lengths range from 2.95Å to 3.5 Å



Magnetization profiles

- No induced magnetic moment in GaAs
- Model A: average magnetzation drops from ~2.4-2.7μ_B in Fe to zero in GaAs
- Model B: from ~2.6-2.7μ_B in Fe to zero in GaAs
- Bulk-like magnetic moments at the interface
- recent experiments[4] on Fe/GaAs(100)-4×6 interface



[4] J. S. Claydon, et al. *Phys. Rev. Lett* **93**, 037206 (2004).

Conclusions

- Calculated relaxed geometries of Fe/GaAs interfaces
- Calculated Schottky barriers for relaxed structures are in better agreement with experiment
- Fermi level is pinned by MIGS, i.e. Fe $d_{3z^2-r^2}$ state
- Bulk-like magnetic moments at the interface
- Significant proximity effect inside GaAs slab
- Minority spin polarization at the interface