Heusler Compound/III-V Semiconductor Heterostructures

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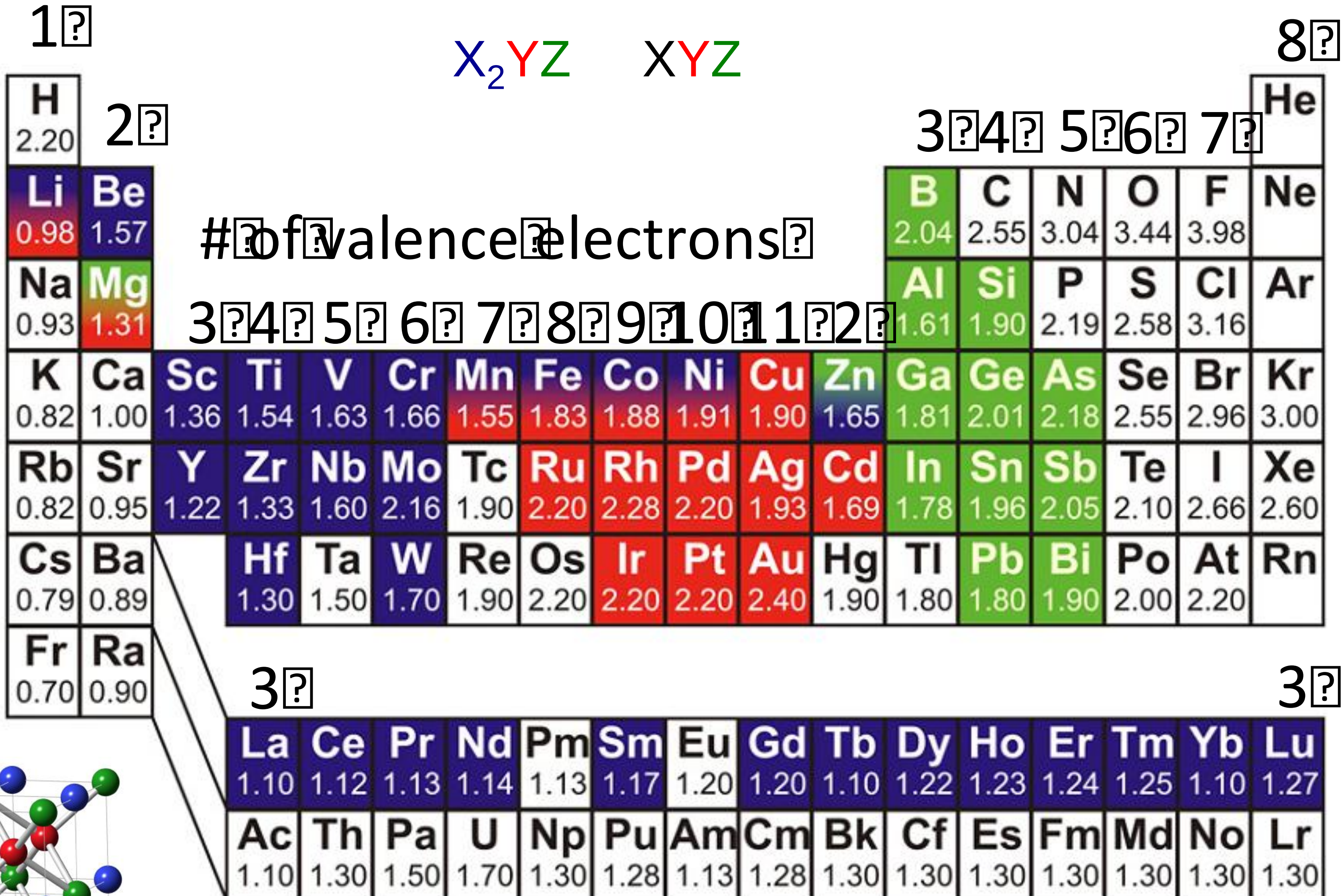
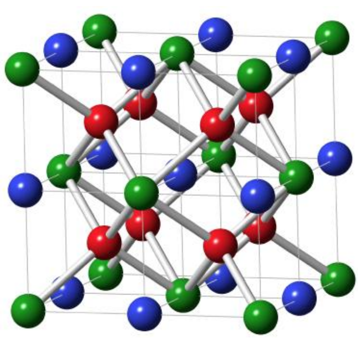
University of Alabama, AL

C-SPIN STARnet NSF

Valence Electron Counting

X_2YZ XYZ



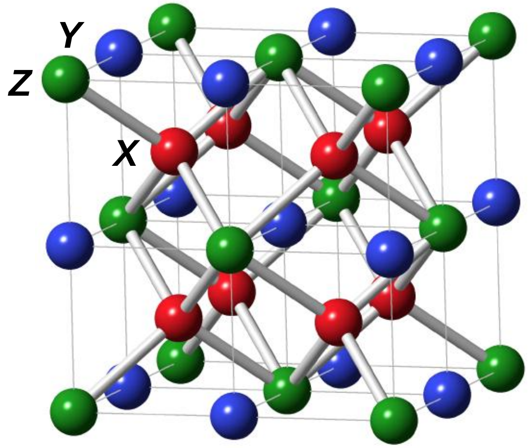


~1000s of combinations!

Graf, Felser, and Parkin, Progress in Solid State Chemistry **39,** 1 (2011)

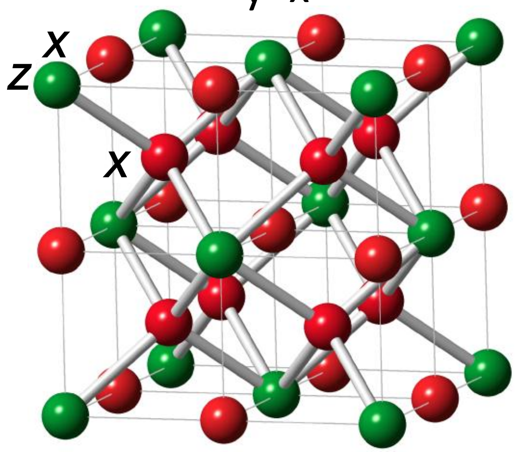
Heusler Compound Crystal Structures

Full Heusler



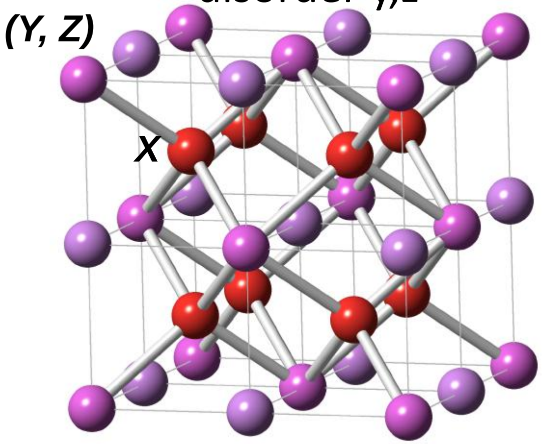
X_2YZ $L2_1$

y=x



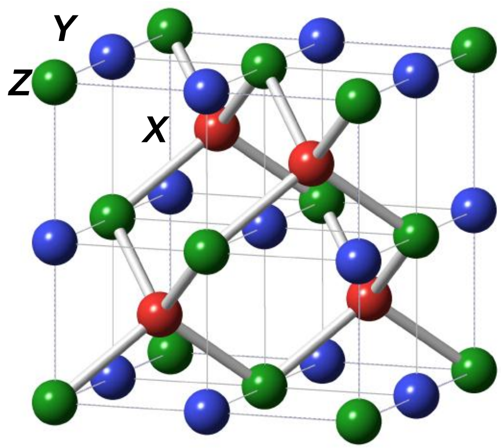
X_2XZ $D0_3$

disorder y,z

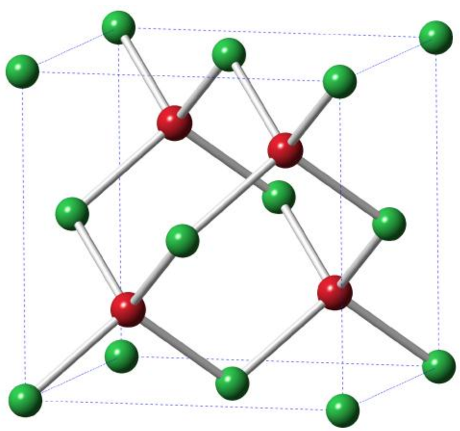


X_2YZ $B2$

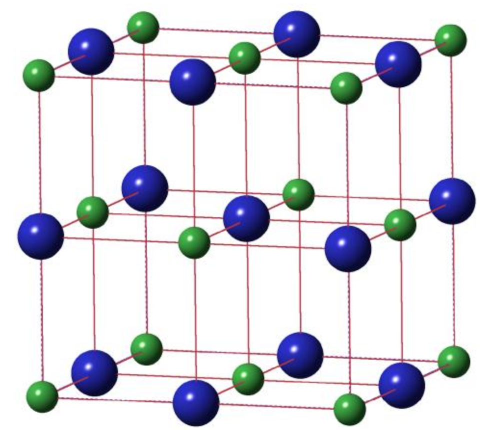
Half Heusler



XYZ $C1_b$

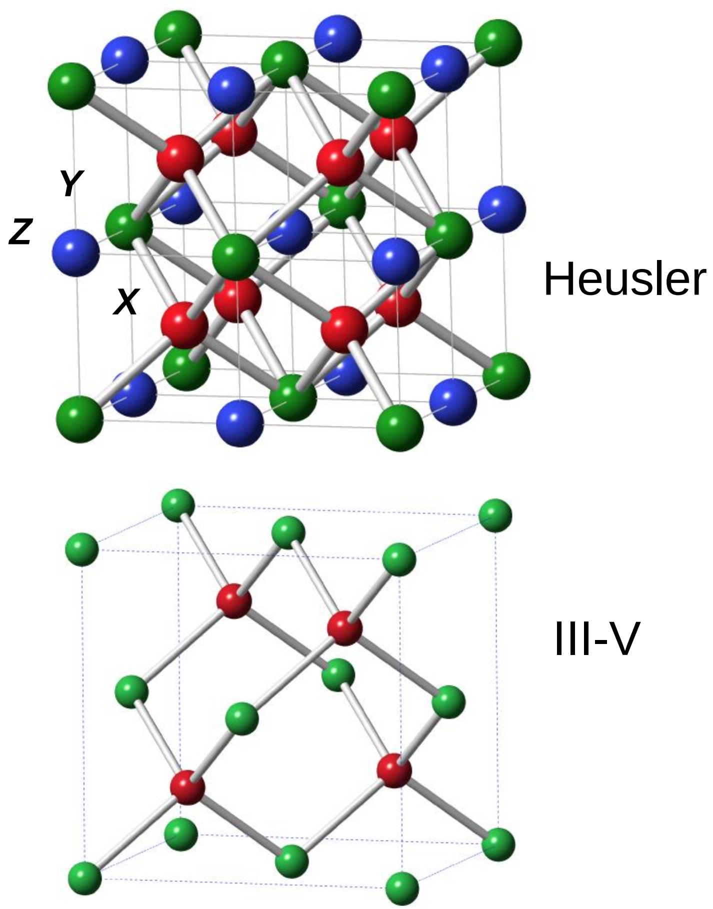


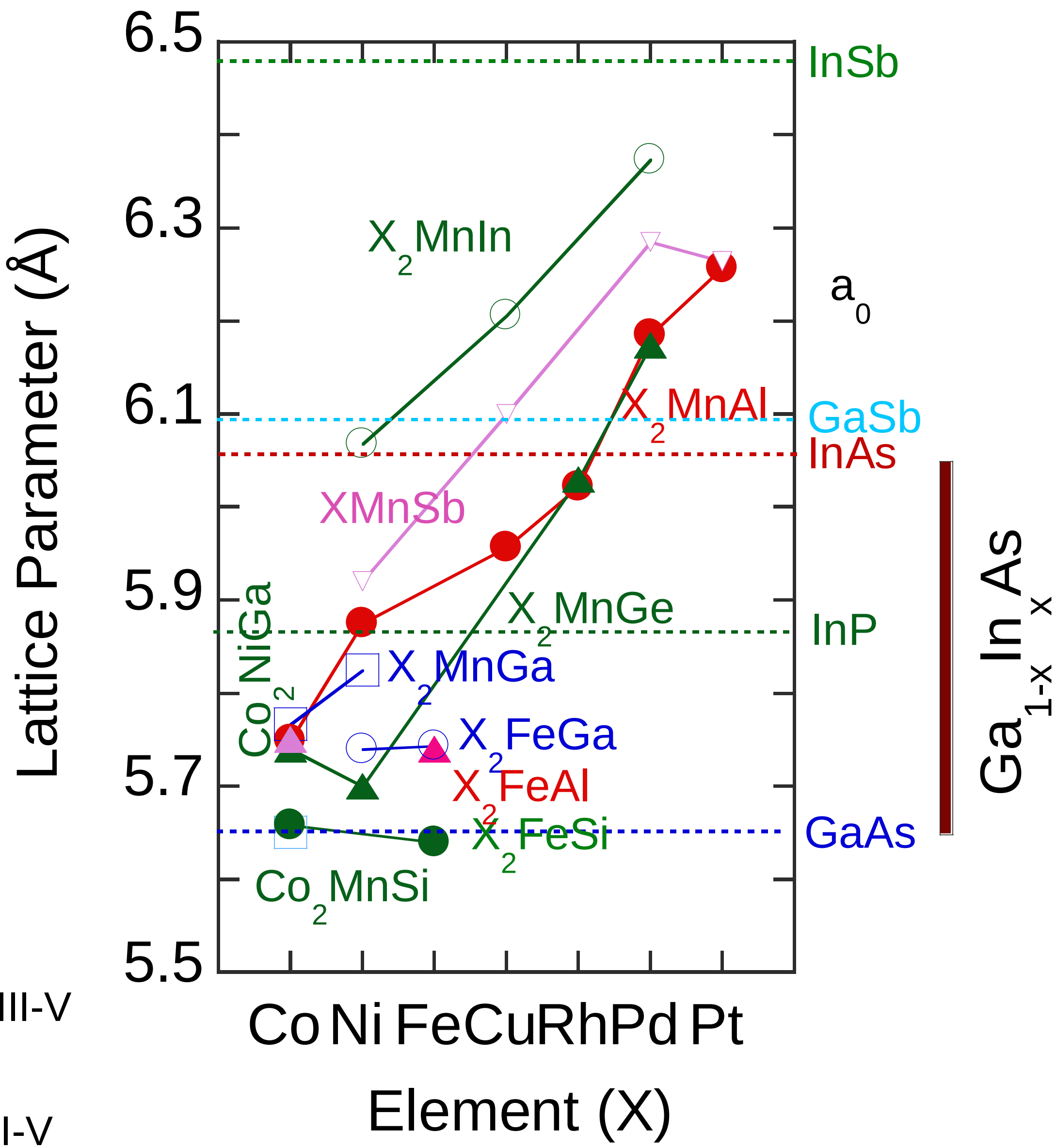
GaAs



ErAs, MgO

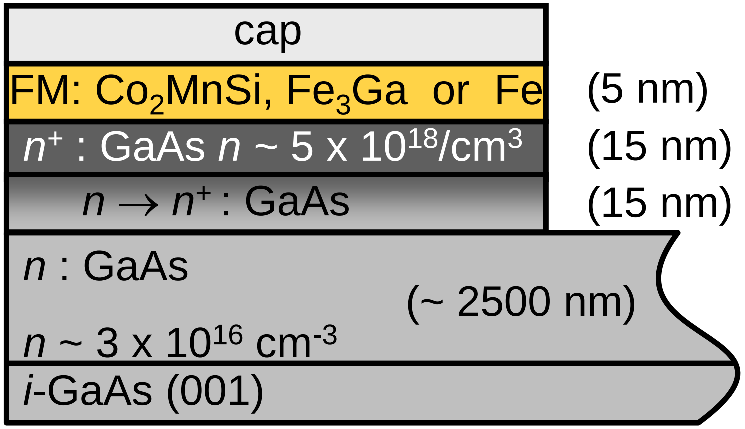
Heusler and Related Compounds: Integration with III-V Semiconductors





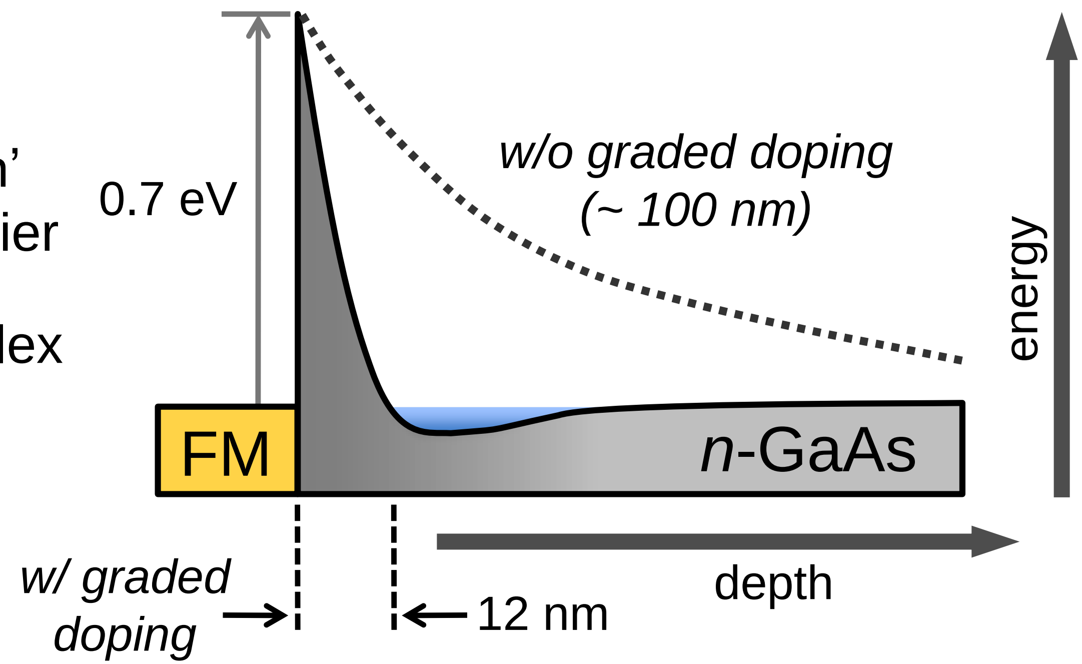
- High spin polarization
- Closely lattice matched to the III-V semiconductor
- Thermodynamic stability on III-V semiconductor

FM/*n*-GaAs Heterostructures

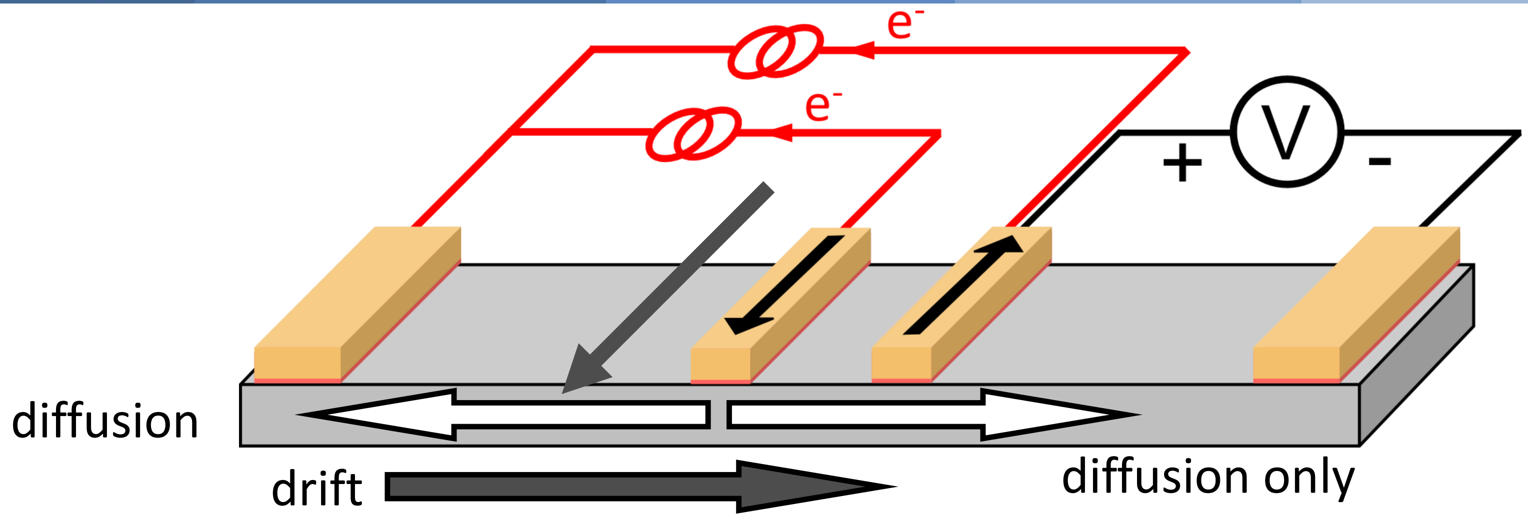


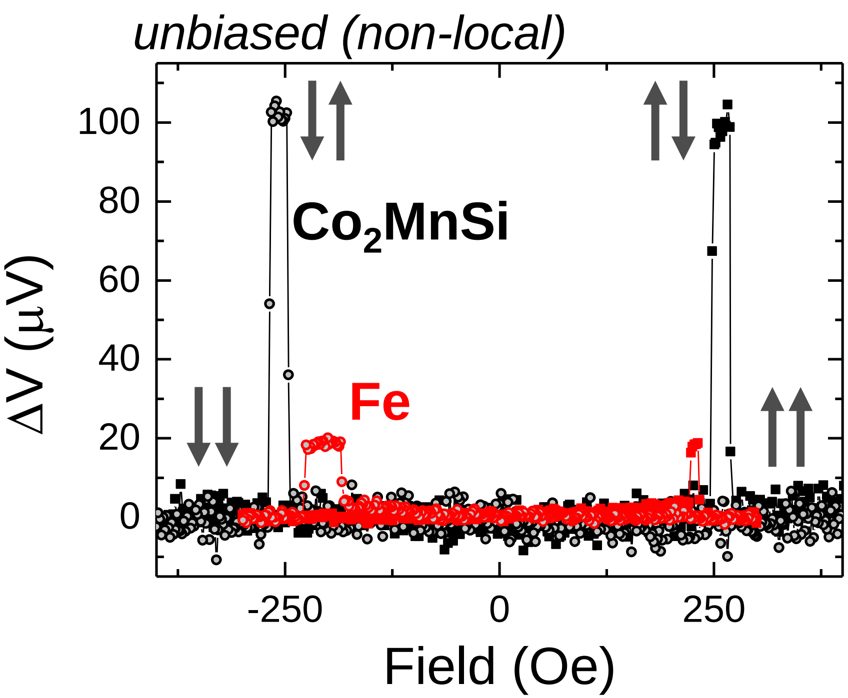
- Epitaxially grown along [001]
- Fe polarization at Fermi level
- Co_2MnSi proposed to be half-metallic
- Surface-induced FM anisotropy

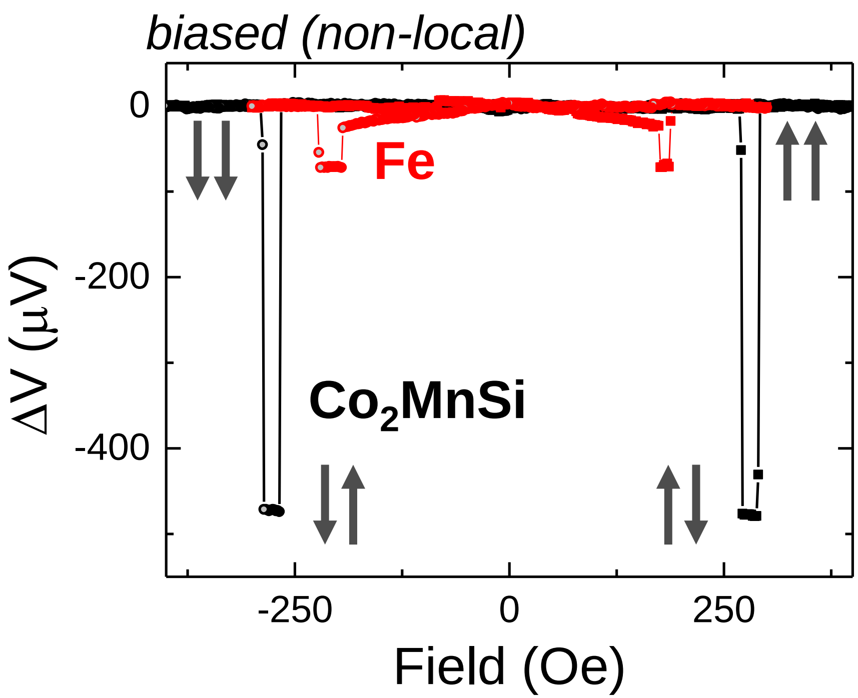
- Graded doping used to 'thin' natural forming Schottky barrier
- Interface states lead to complex bias dependence



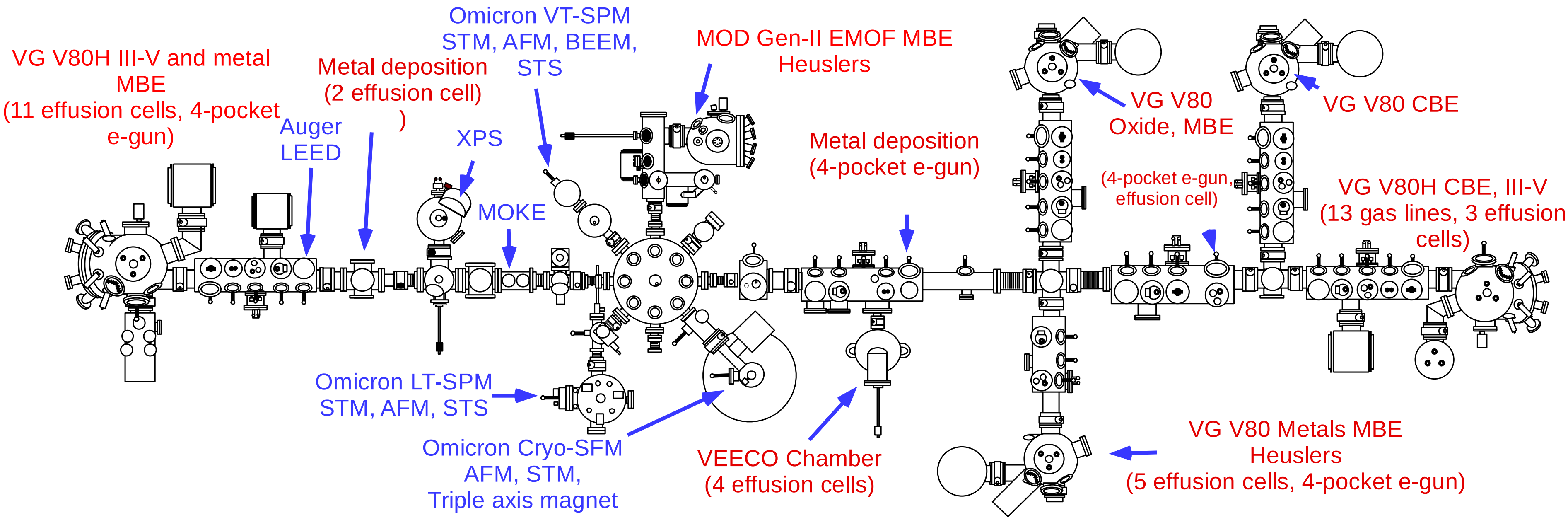
Lateral spin valve







In-situ Growth and Characterization System at UCSB



in-situ growth and atomic level characterization

Enhanced growth capabilities interconnected MBE/CBE systems for III-Vs, metals, metallic compounds and oxides

Determination of structure and chemistry at the atomic level at different stages of growth STM/AFM, Auger, XPS, LEED, RHEED, MOKE

Atomic level electronic and magnetic properties – STM/STS, BEEM (VTSTM 50-800K), LT-SPM (4-300K), Cryo-SFM (~4-300K)

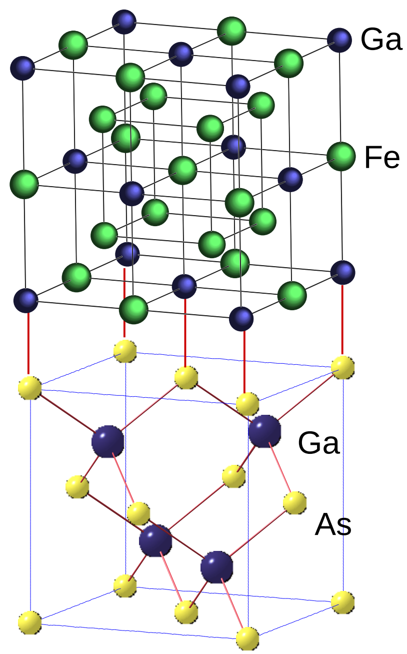
Lattice Matching and Thermodynamics

	Phase	Space Group	Structure	Type	Lattice Parameter
stable structure (Pearson) →	α-Fe_3Ga	Pm$\bar{3}$m	$L1_2$	Cu_3Au	a = 3.678 Å
	α'-Fe_3Ga	Pm$\bar{3}$m	B2	CsCl	a = 2.91 Å
	α''-Fe_3Ga	Fm$\bar{3}$m	$D0_3$	BiF_3	a = 5.808 Å
	β-Fe_3Ga	$P6_3$/mmc	$D0_{19}$	Ni_3Sn	a = ?, c = ?

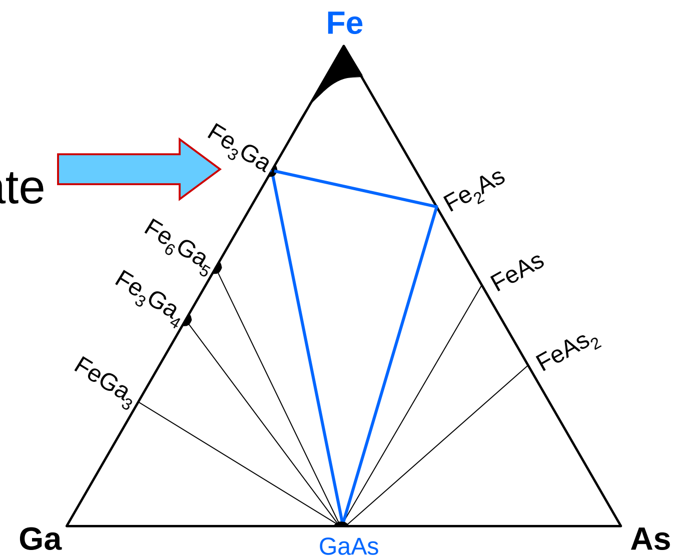
Fe_3Ga
DO_3 structure
a_0 = 5.812 Å

2.8% mismatch to GaAs

GaAs
Zincblende structure
a_0 = 5.653 Å



Fe_3Ga is a good candidate



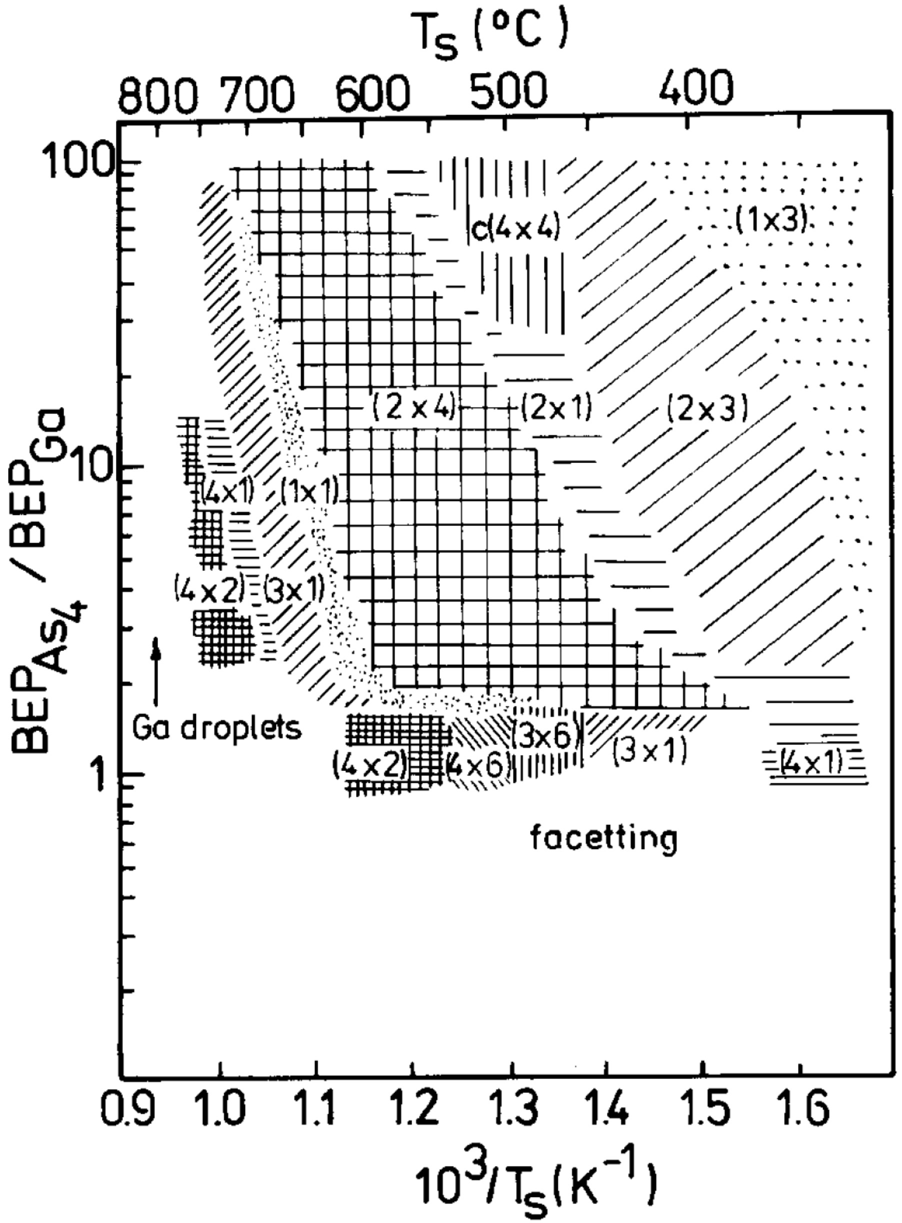
Fe_3Ga T_c ~900K

Kawamiya et al., J. Phys. Soc. Jap., **33**, 1318 (1972)
Okamoto, in Binary Alloy Phase Diagrams (ASM (1993))

Schultz, et al., APL, **92,** 091914 (2008)
Kawamiya et al., J. Phys. Soc. Jap. **33**, 1318 (1972)
Ikeda et al., J. Alloys Comp. **347**, 198 (2002)

Surface Phase Diagram of GaAs(001) (misoriented 2° towards (-111)As)

GaAs(001) has multiple surface reconstructions depending on As/Ga surface composition

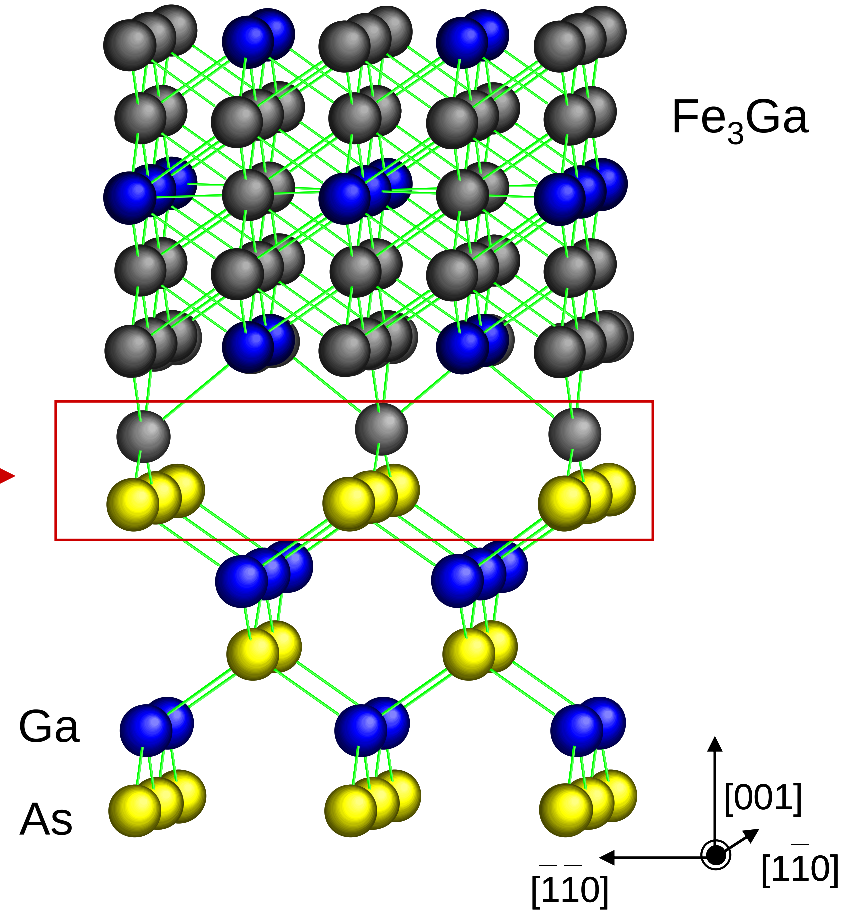


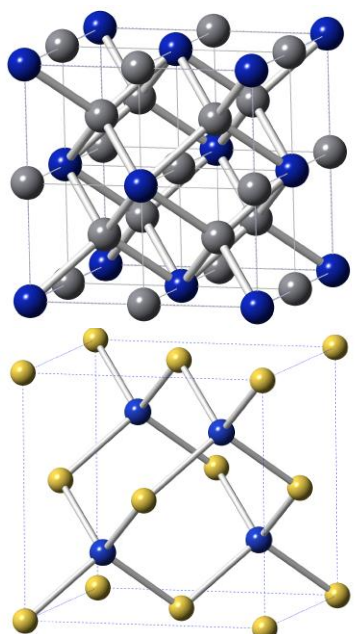
Däweritz, L. and R. Hey, Surface Science **236**, 15 (1990)

Initiation of Fe_3Ga Growth on GaAs

- **GaAs surface reconstruction**
- As-rich
- Ga-rich
- how As- or Ga- rich, multiple reconstructions are possible

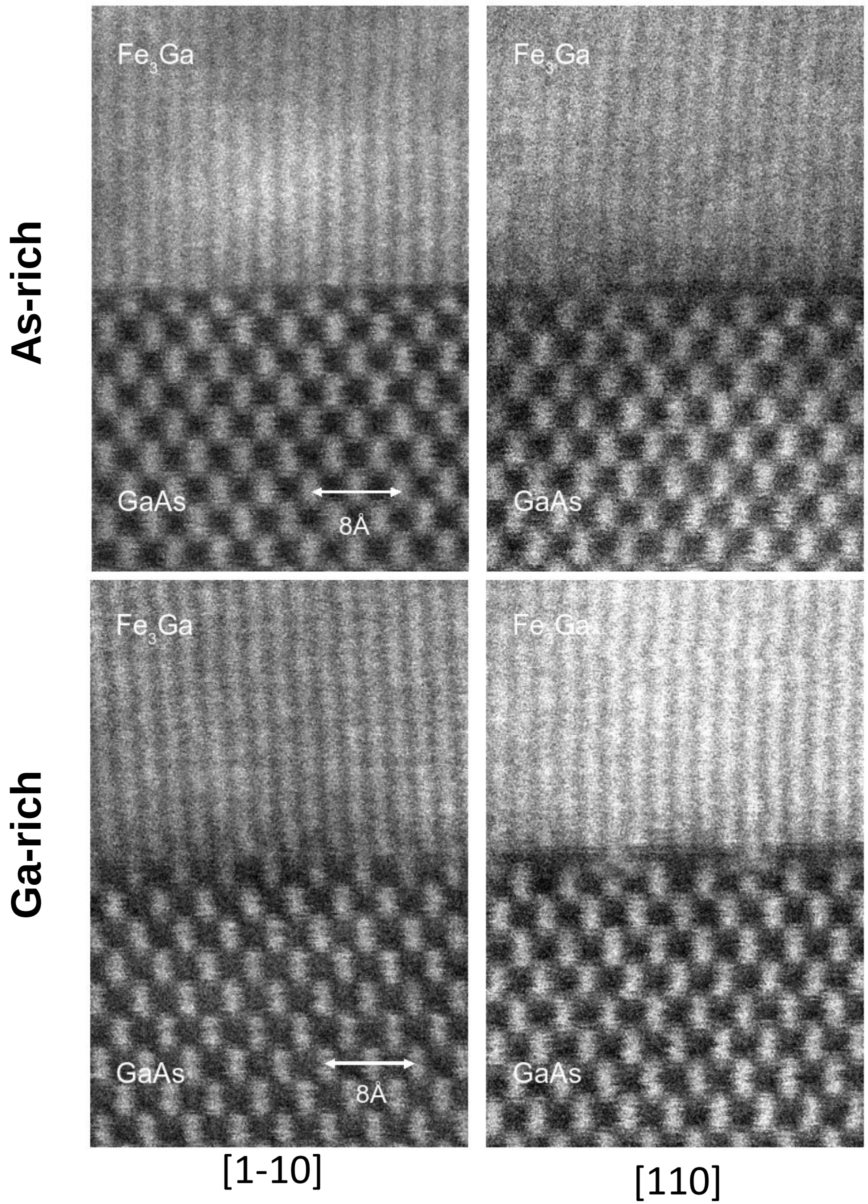
- **Initiation of Fe_3Ga growth**
- Fe first
- Ga first
- Co-deposition of Fe+Ga



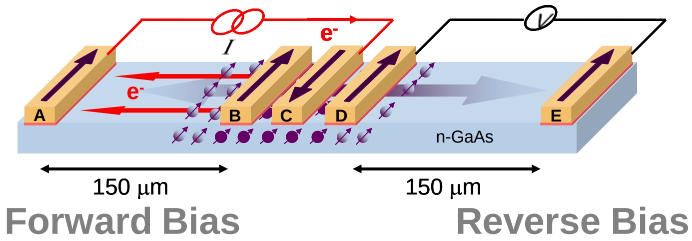


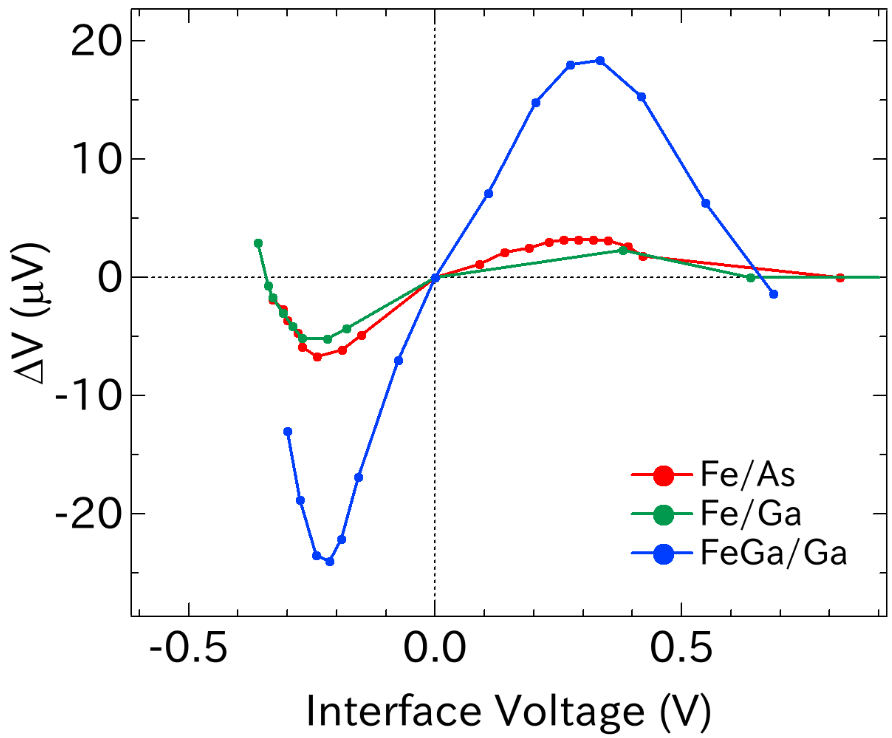
Fe_3Ga/GaAs Interfaces Dependence on Growth Sequence

HAADF-STEM images



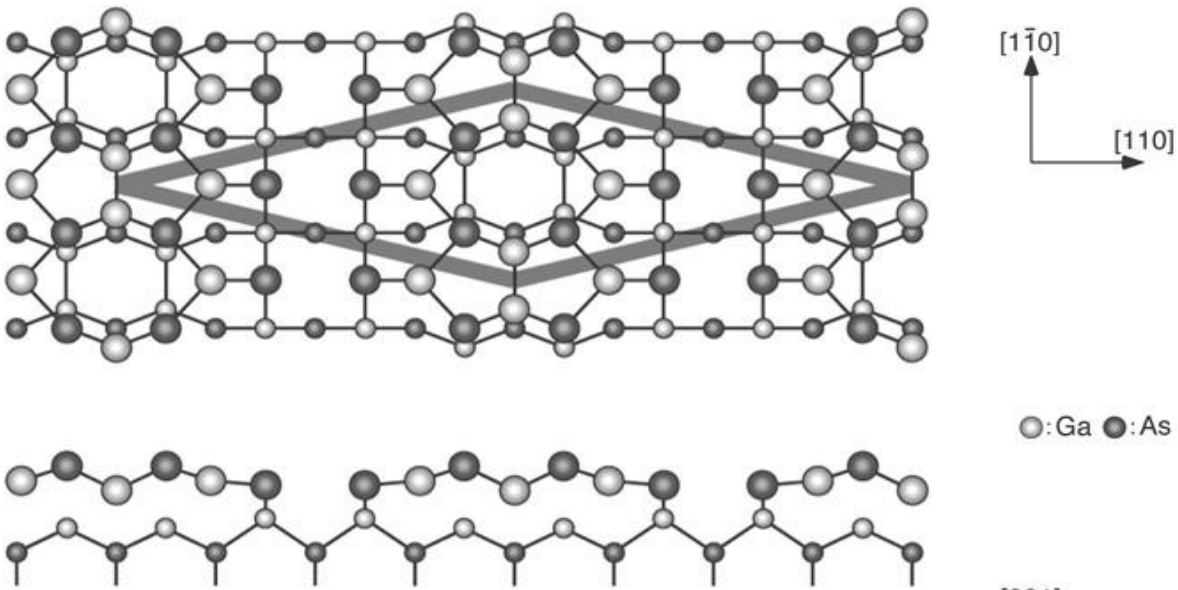
Bias dependence of the non-local signal



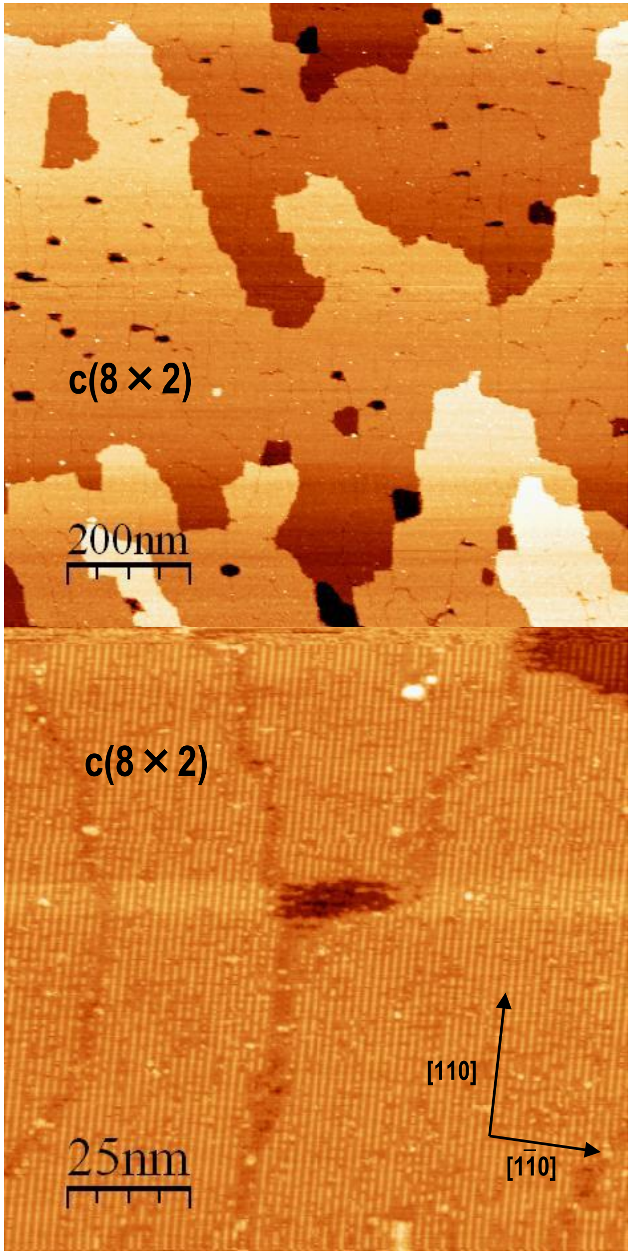


- Different atomic structures for As- and Ga-rich interface
- Distinct magnitude and bias dependence of Spin-Valve signal

GaAs(001) c(8x2) Ga-rich surface

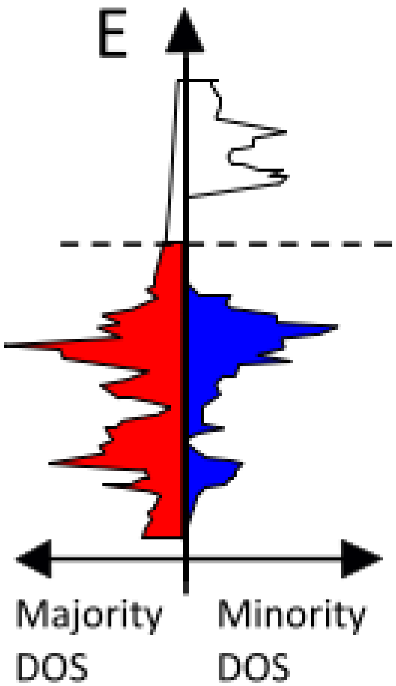


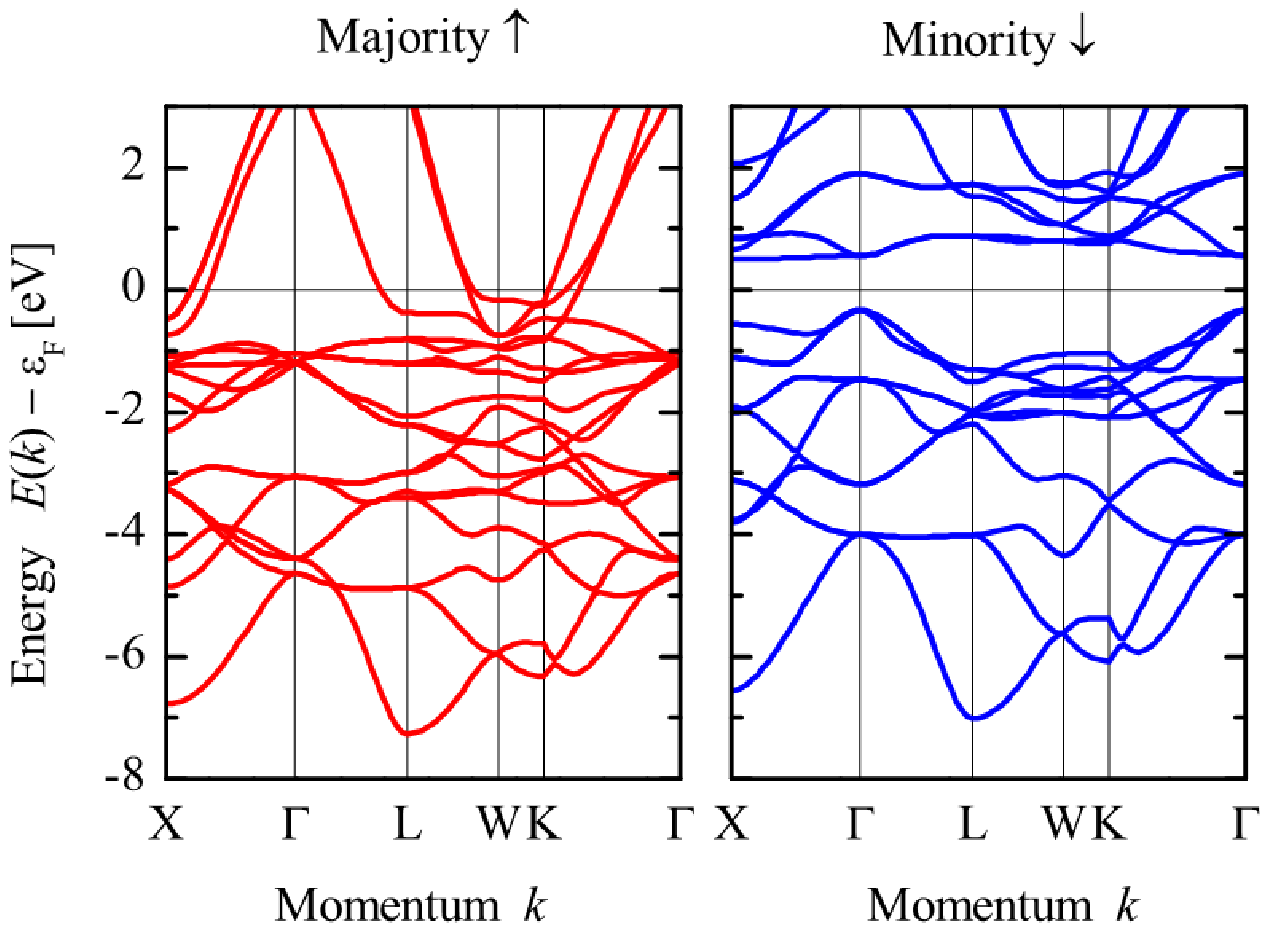
ζ model for c(8x2)



A. Ohtake, Surface Science Reports **63,** 295 (2008)

Co_2MnSi Band Structure – half-metal





- Large minority spin gap of approximately 1eV is centred around the Fermi level

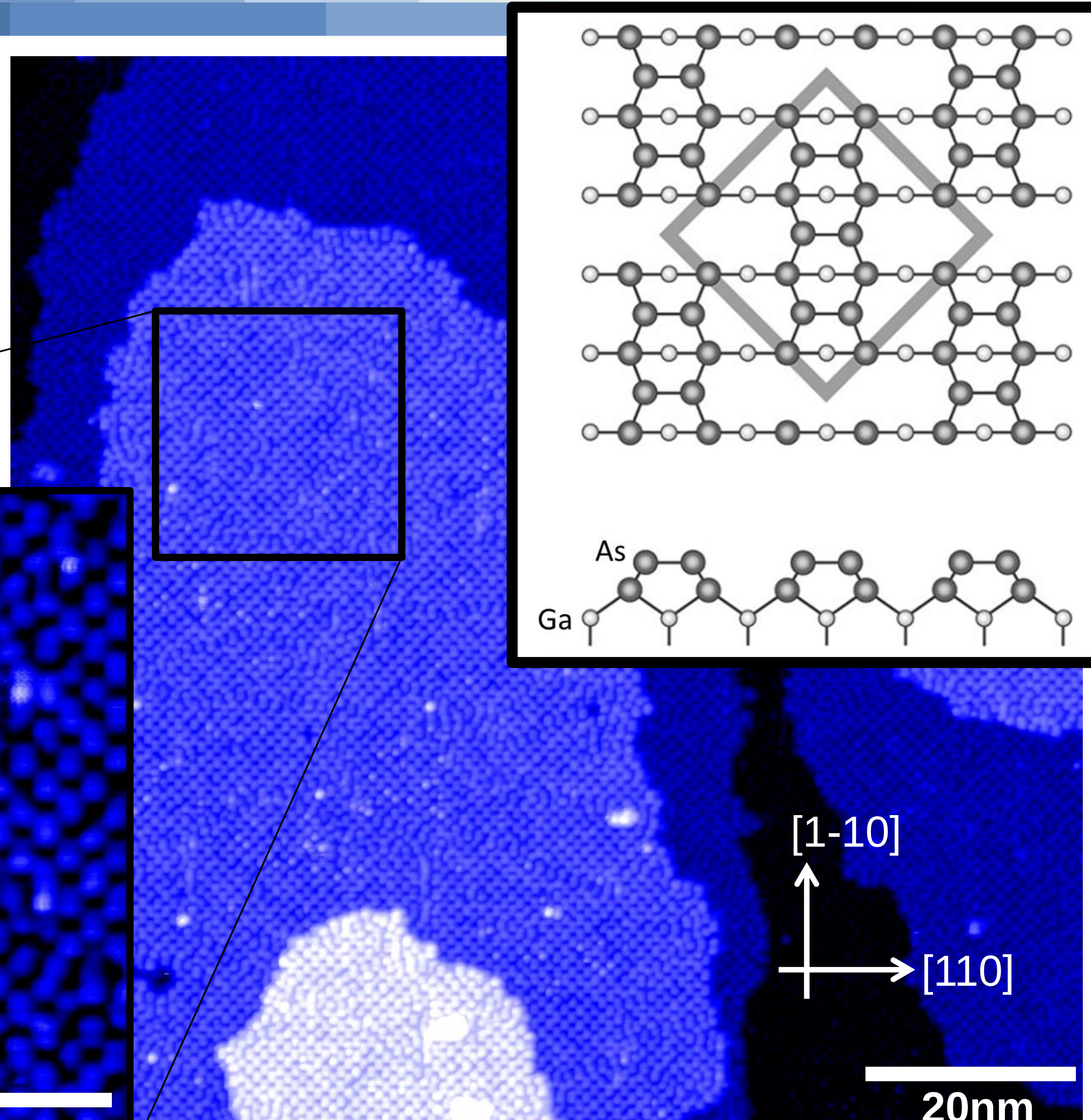
Co_2MnSi – 0.06% mismatch to GaAs – not thermodynamically stable on GaAs

Balke, B., S. Ouardi, et al. (2010). Solid State Communications **150**(11–12): 529-532.

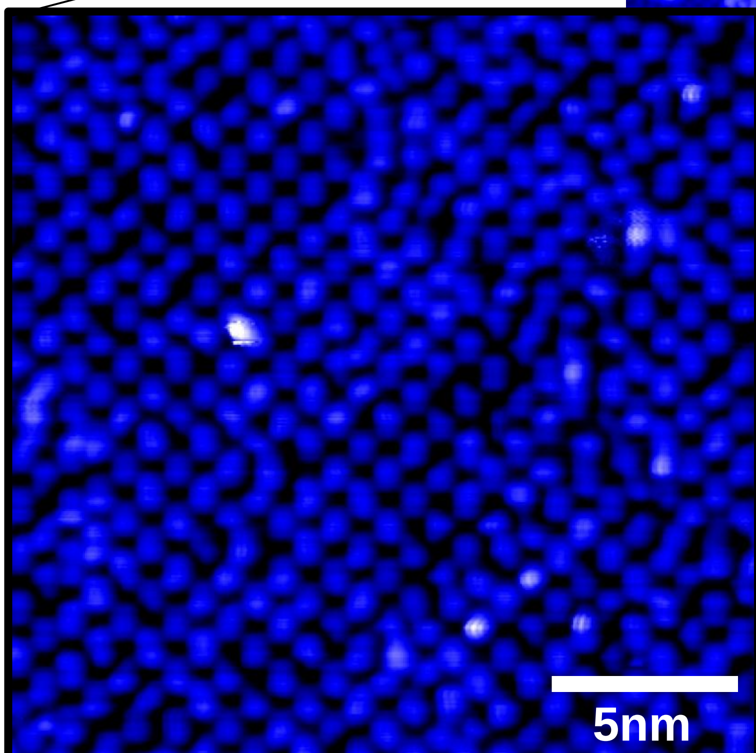
M. Jourdan et al., Nature Communications, **5** 3974 (2014)

GaAs(001) c(4x4) As-rich surface

Extra ¾ ML of As

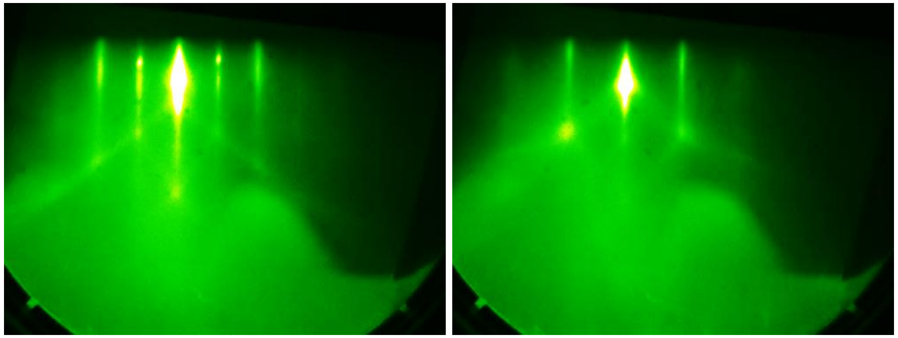


Filled States image

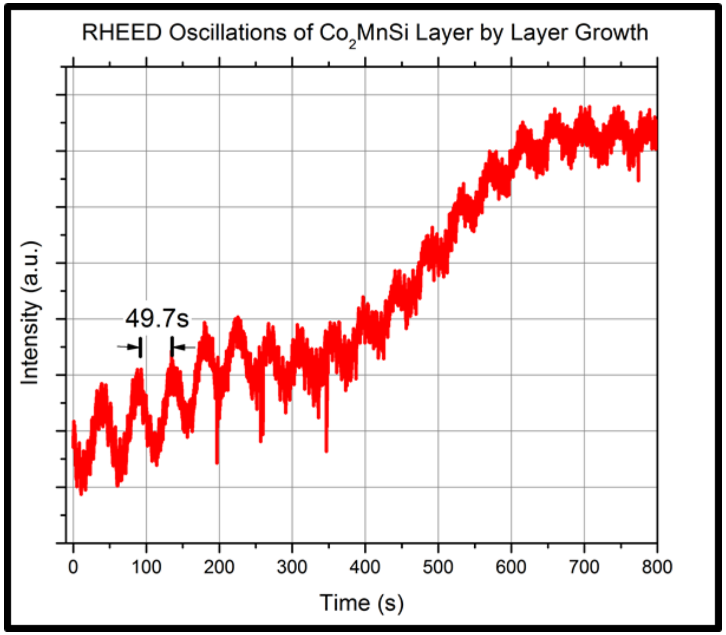


Growth of Co_2MnSi on GaAs(001)-c(4x4)

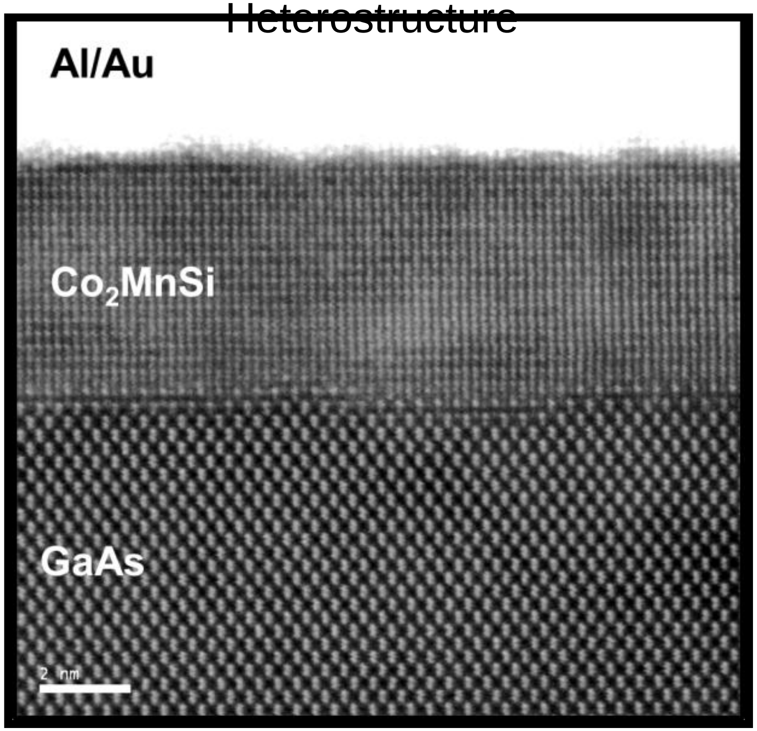
[110] [010]

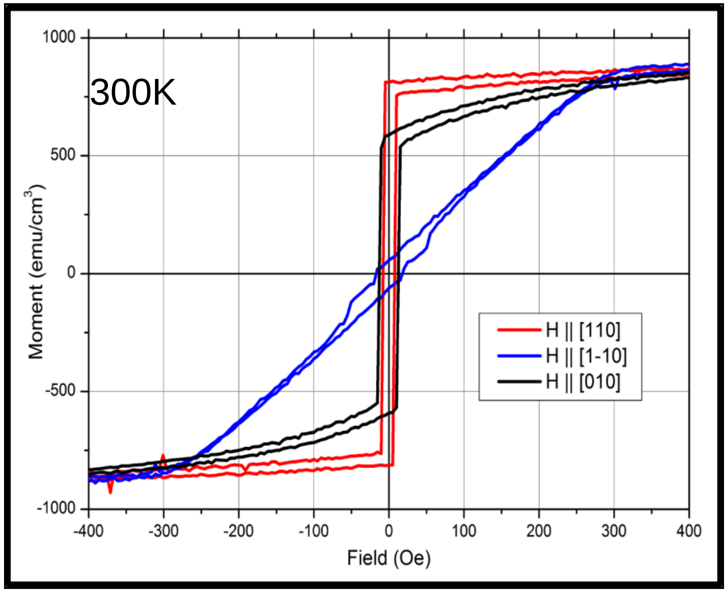


Growth Temperature ~270° C

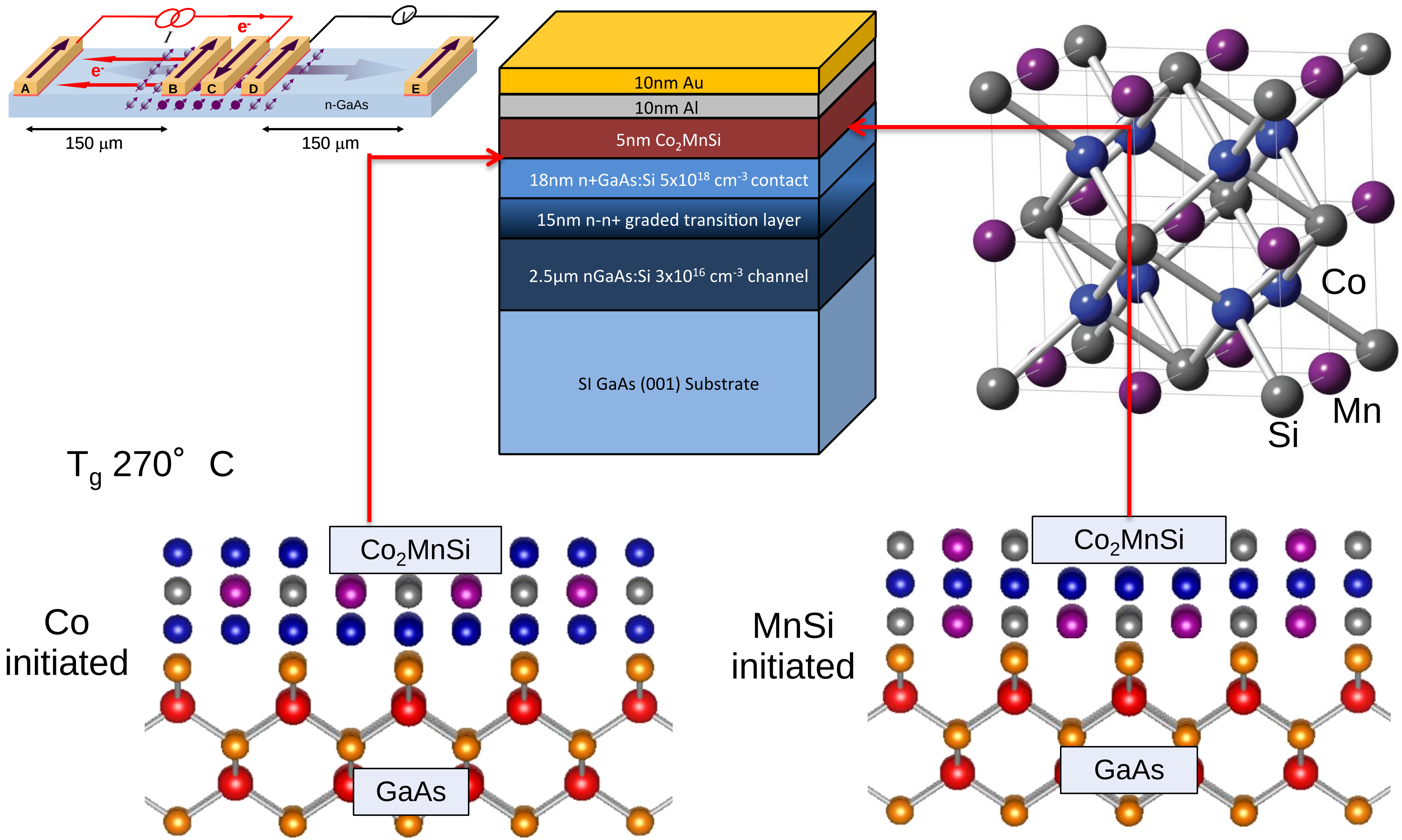


HAADF-STEM of CMS/GaAs Heterostructure





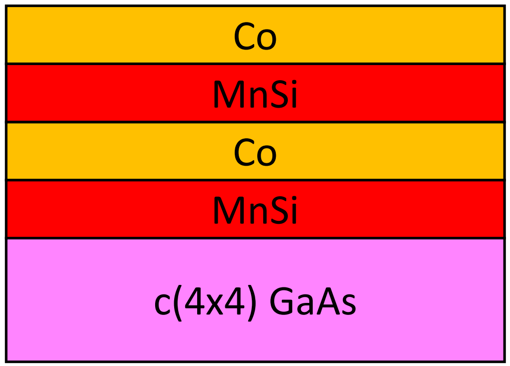
Co_2MnSi/GaAs Spin Contacts



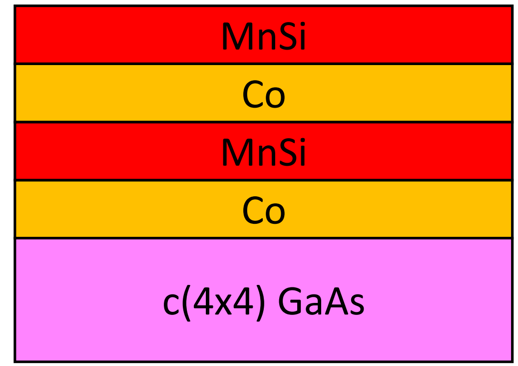
How does the initiation layer affect nucleation and structure?

Grow Co_2MnSi seed layer using two different nucleation sequences

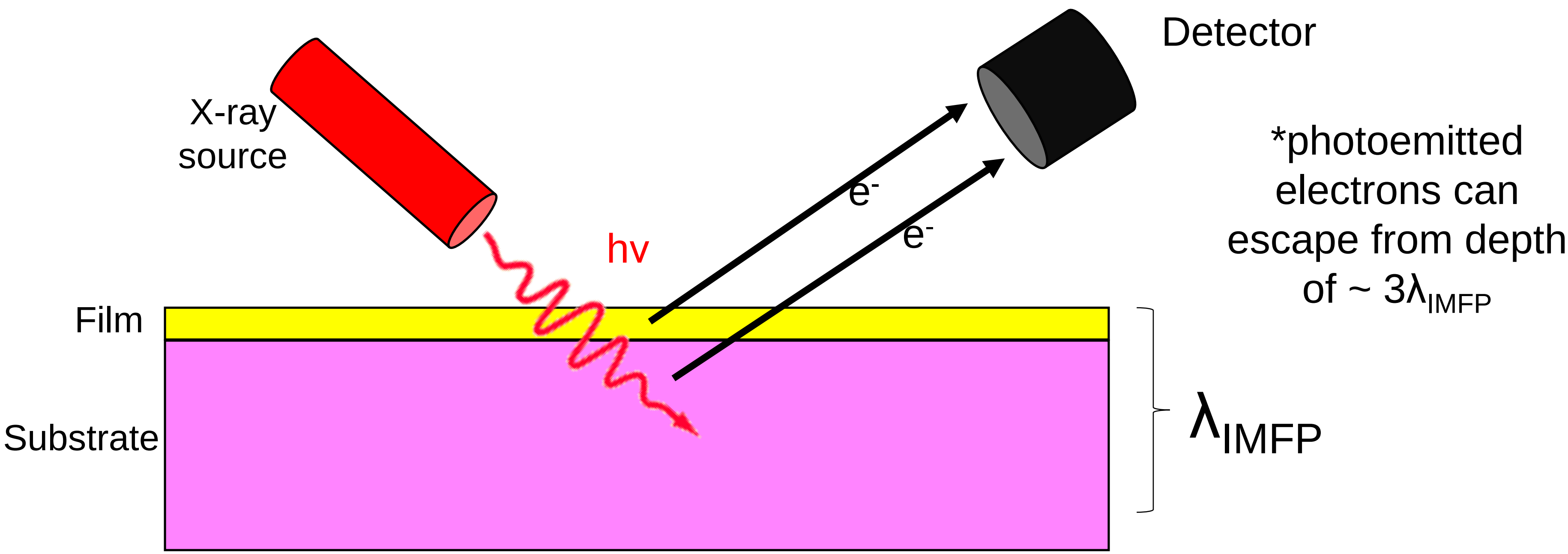
MnSi initiated growth



Co initiated growth

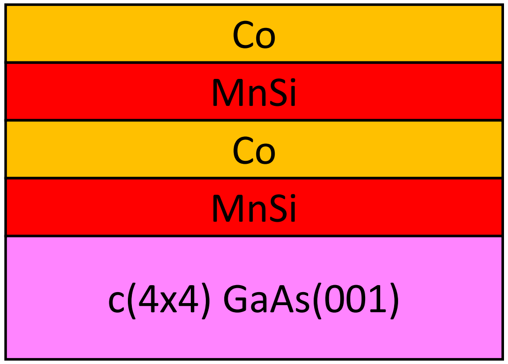


X-ray photoemission spectroscopy (XPS) allows study of core level intensity as a function of film thickness



1ML MnSi Initiated Growth

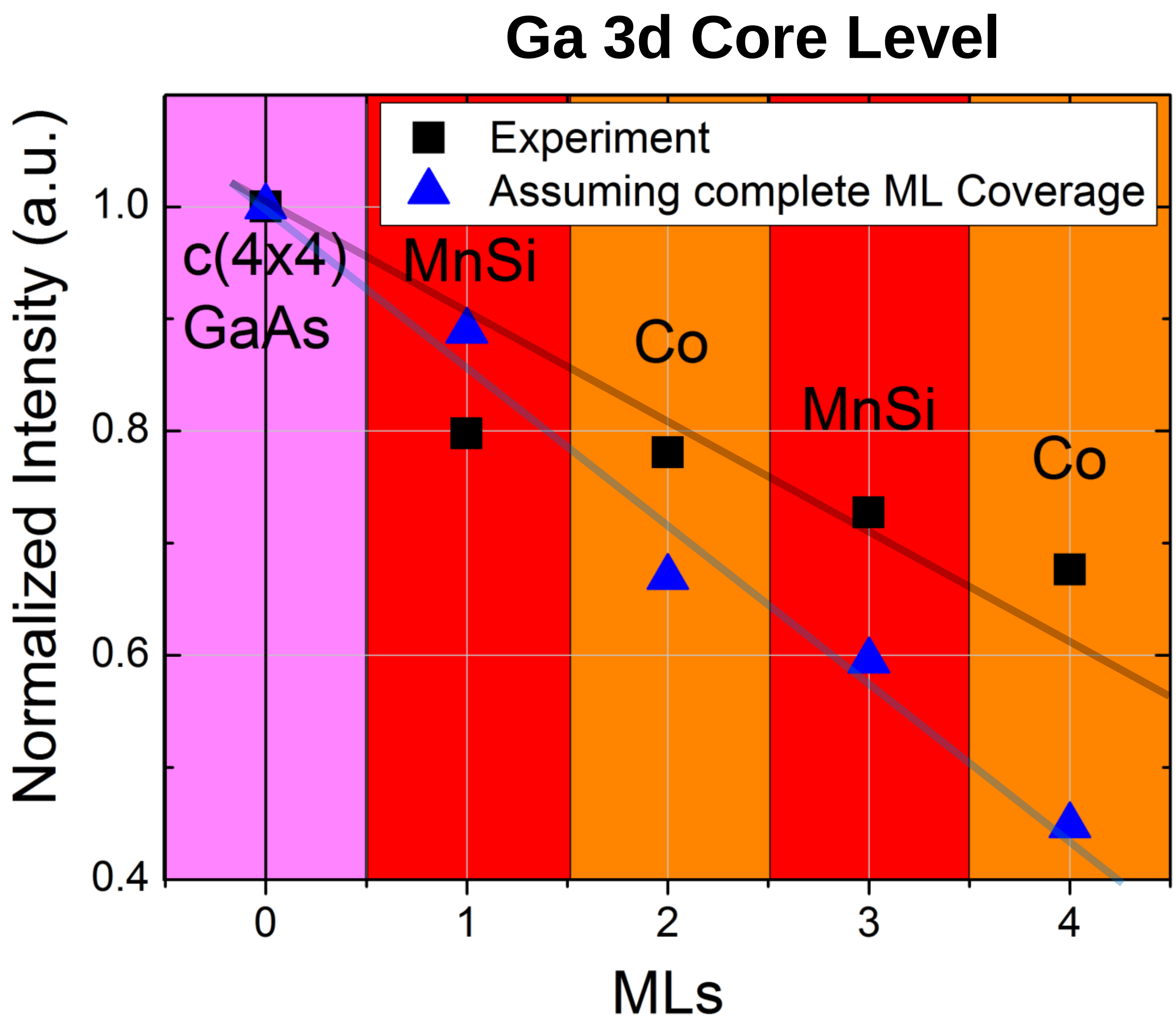
MnSi initiated growth



As and Ga 3d core levels show similar decreases in intensity for each layer deposited

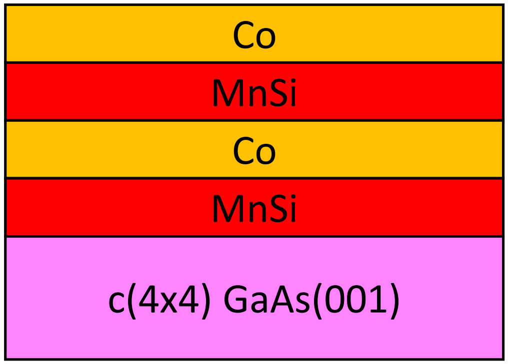
As and Ga intensity does not attenuate as fast as expected for simple ML by ML coverage on GaAs

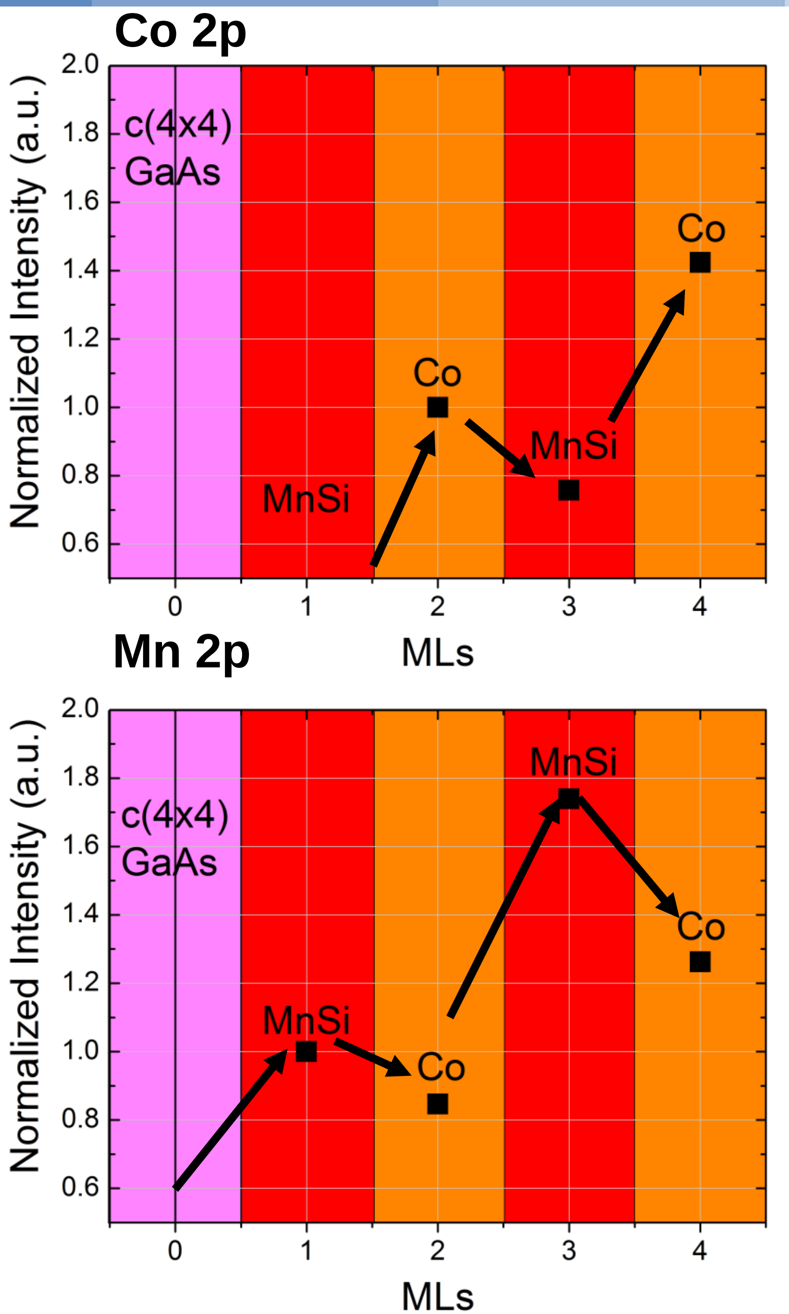
Suggests that Ga and As must be riding on the surface or island growth



1ML MnSi Initiated Growth

MnSi initiated growth





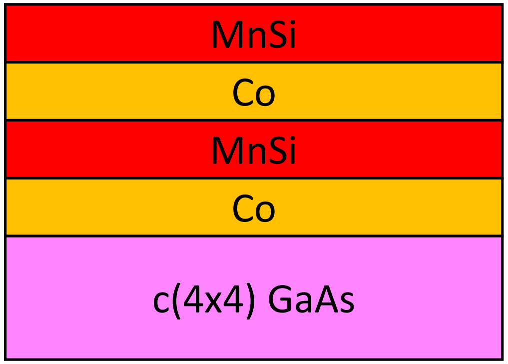
MnSi deposition attenuates Co 2p peak

Co deposition attenuates Mn 2p peak

MnSi layers cover Co layers and Co layers cover MnSi layers (simple layer-by-layer growth)

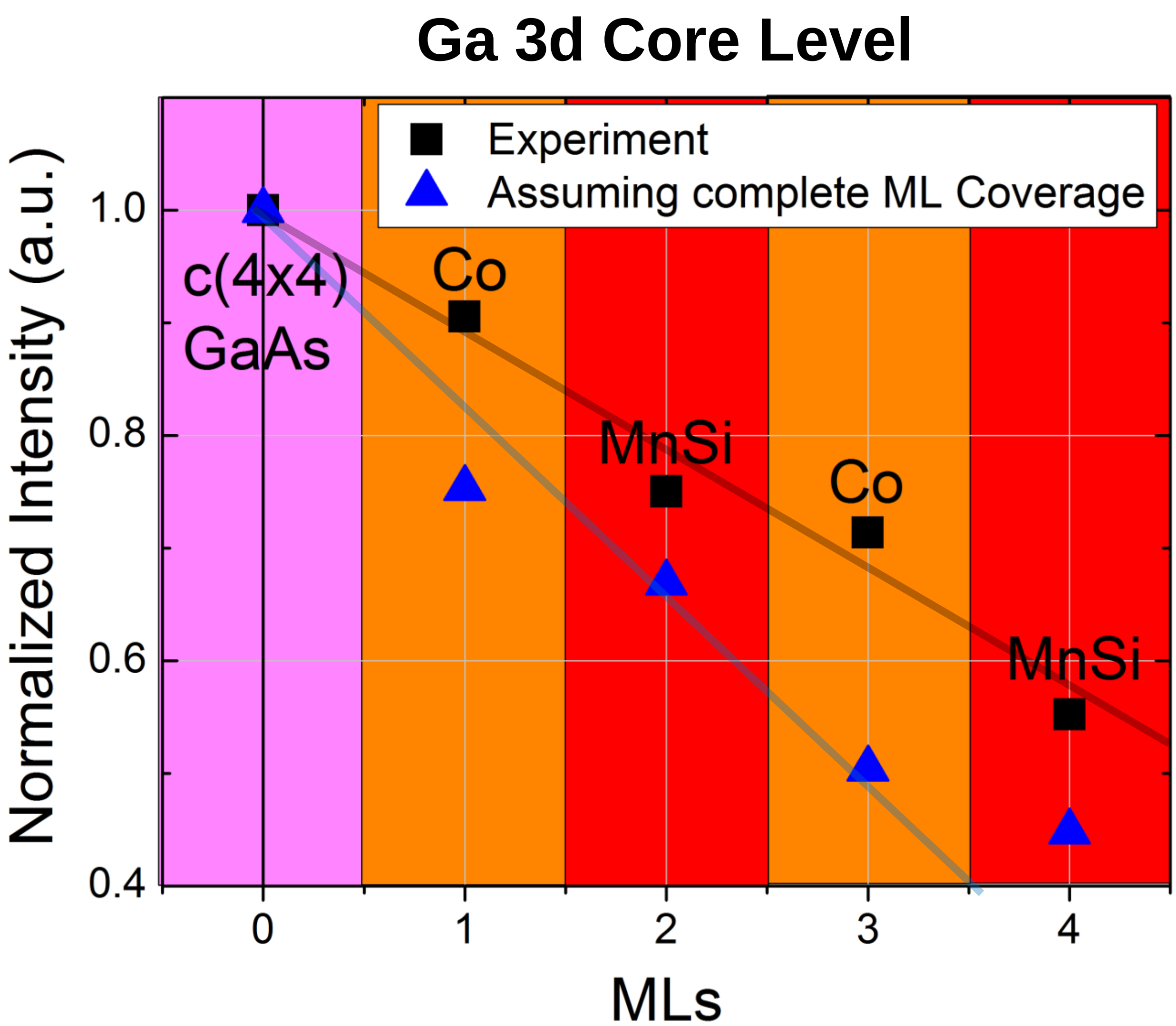
1ML Co Initiated Growth

Co initiated growth



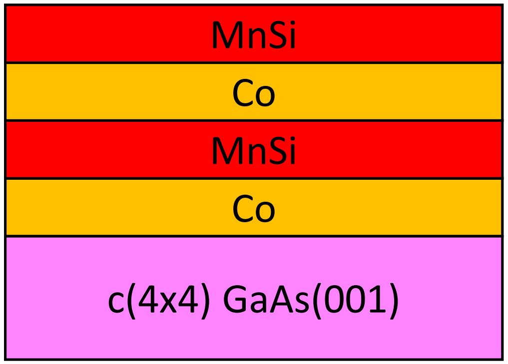
As and Ga 3d core levels show similar decreases in intensity for each layer deposited

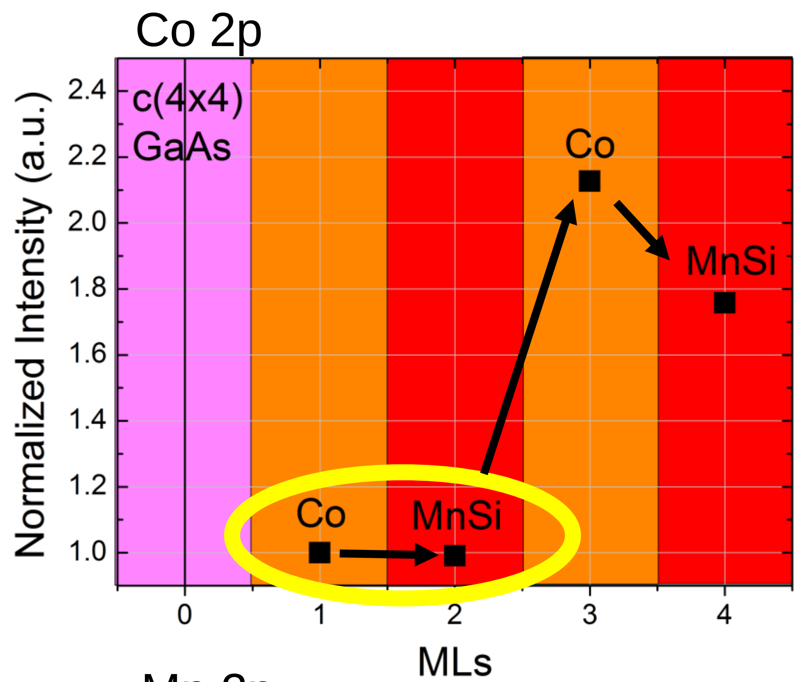
Similar to MnSi initiated growth, Ga and As core levels do not attenuate as fast as expected for simple layer-by-layer coverage, implying **Ga and As ride on surface during growth**

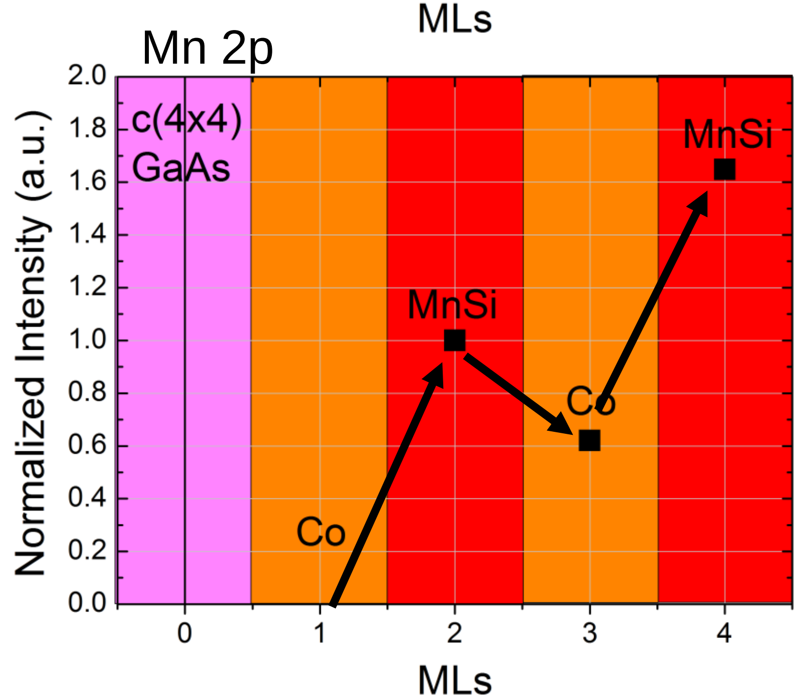


1ML Co Initiated Growth

Co initiated growth





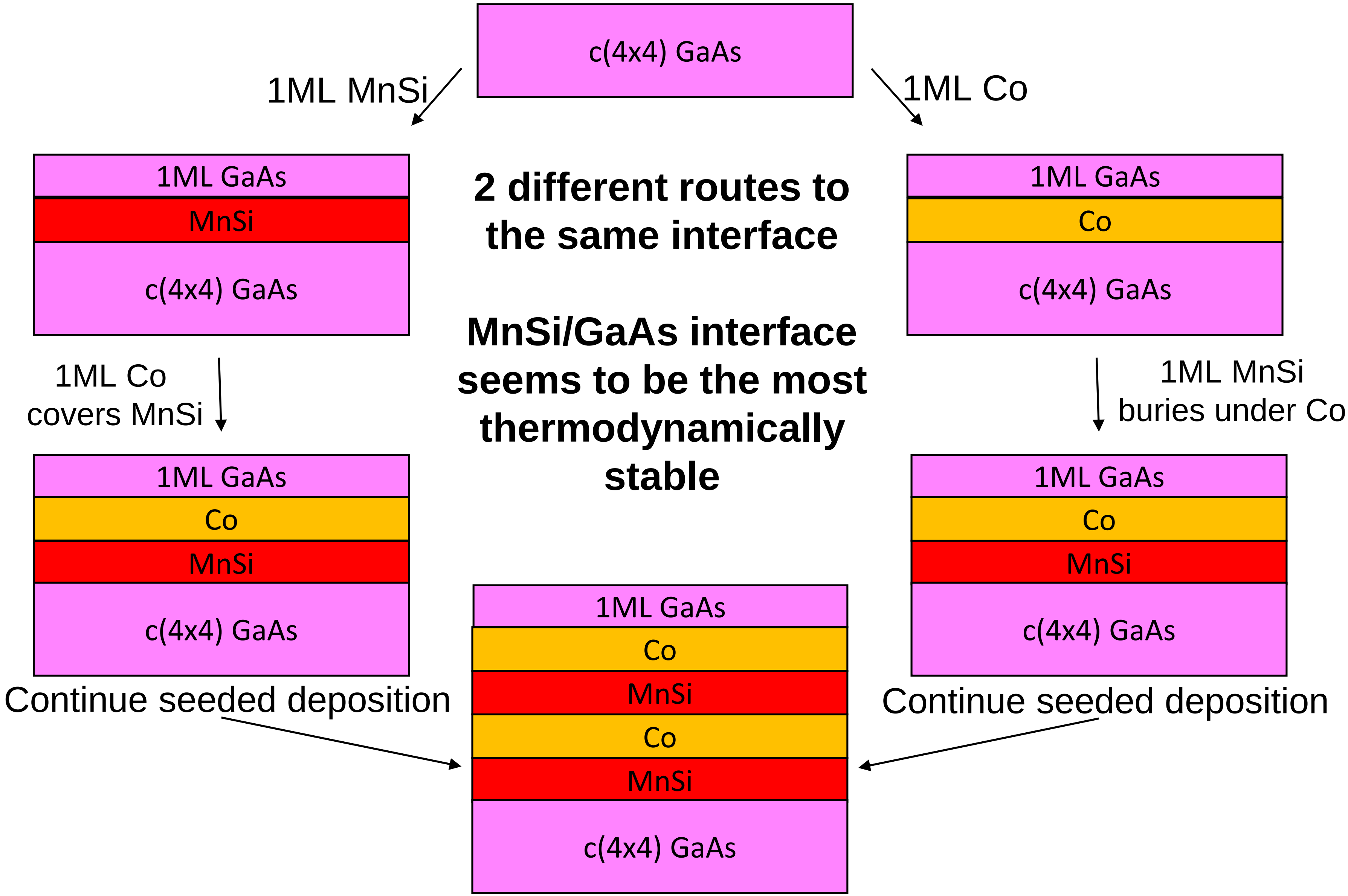


Co deposition attenuates Mn 2p peak

For first MnSi monolayer, the Co 2p peak is not attenuated at all, indicating that MnSi goes “under” the first Co layer

MnSi/GaAs interface is the most stable and forms regardless of deposition sequence

Growth Model of Co_2MnSi on c(4x4) GaAs(001)

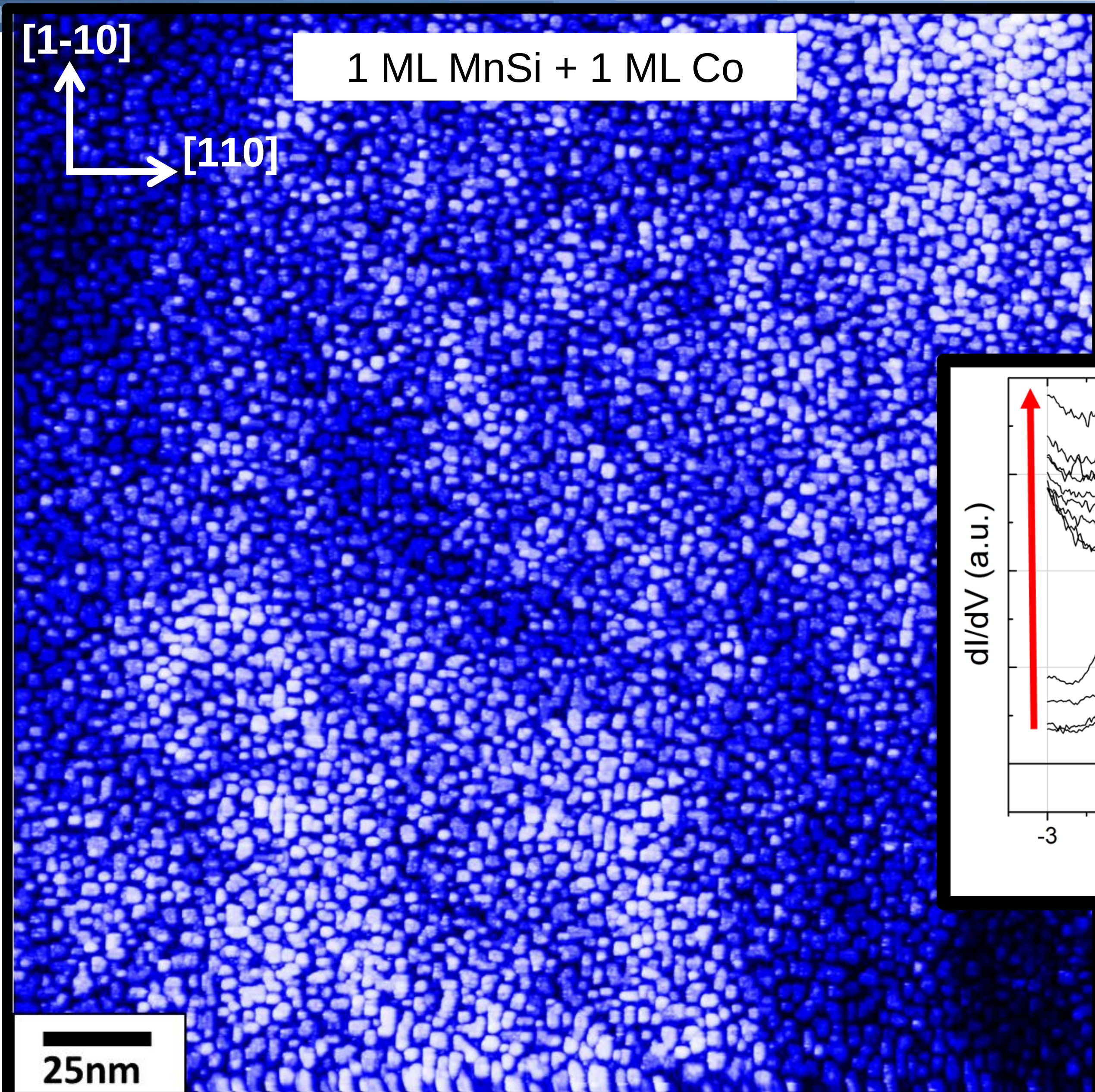


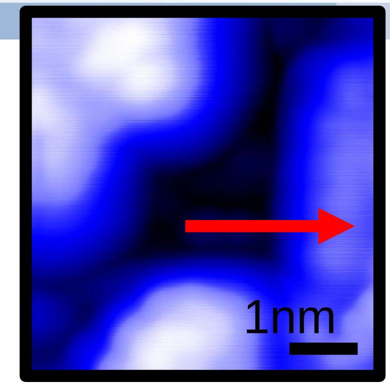
2 different routes to the same interface

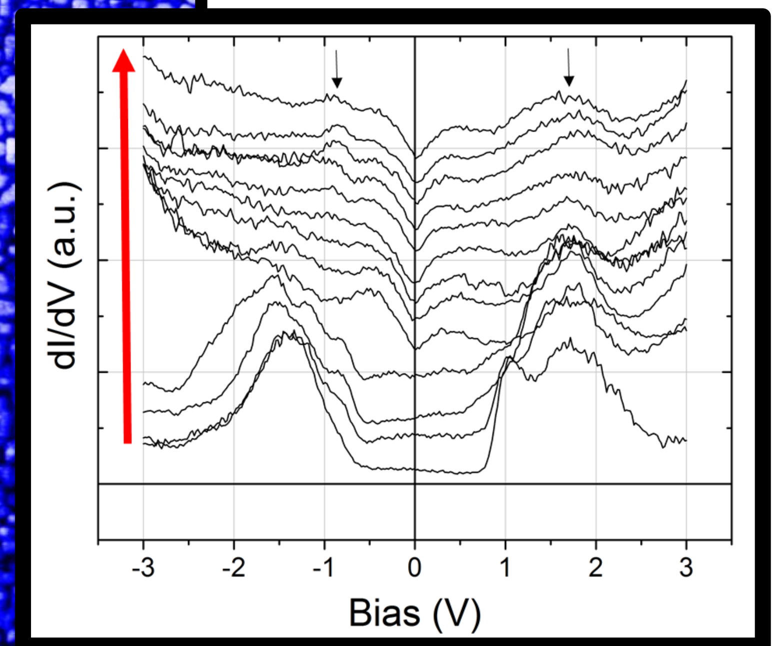
MnSi/GaAs interface seems to be the most thermodynamically stable

Final interface is similar regardless of nucleation sequence

Evidence of GaAs on surface of 5.6Å tall Co_2MnSi island on GaAs

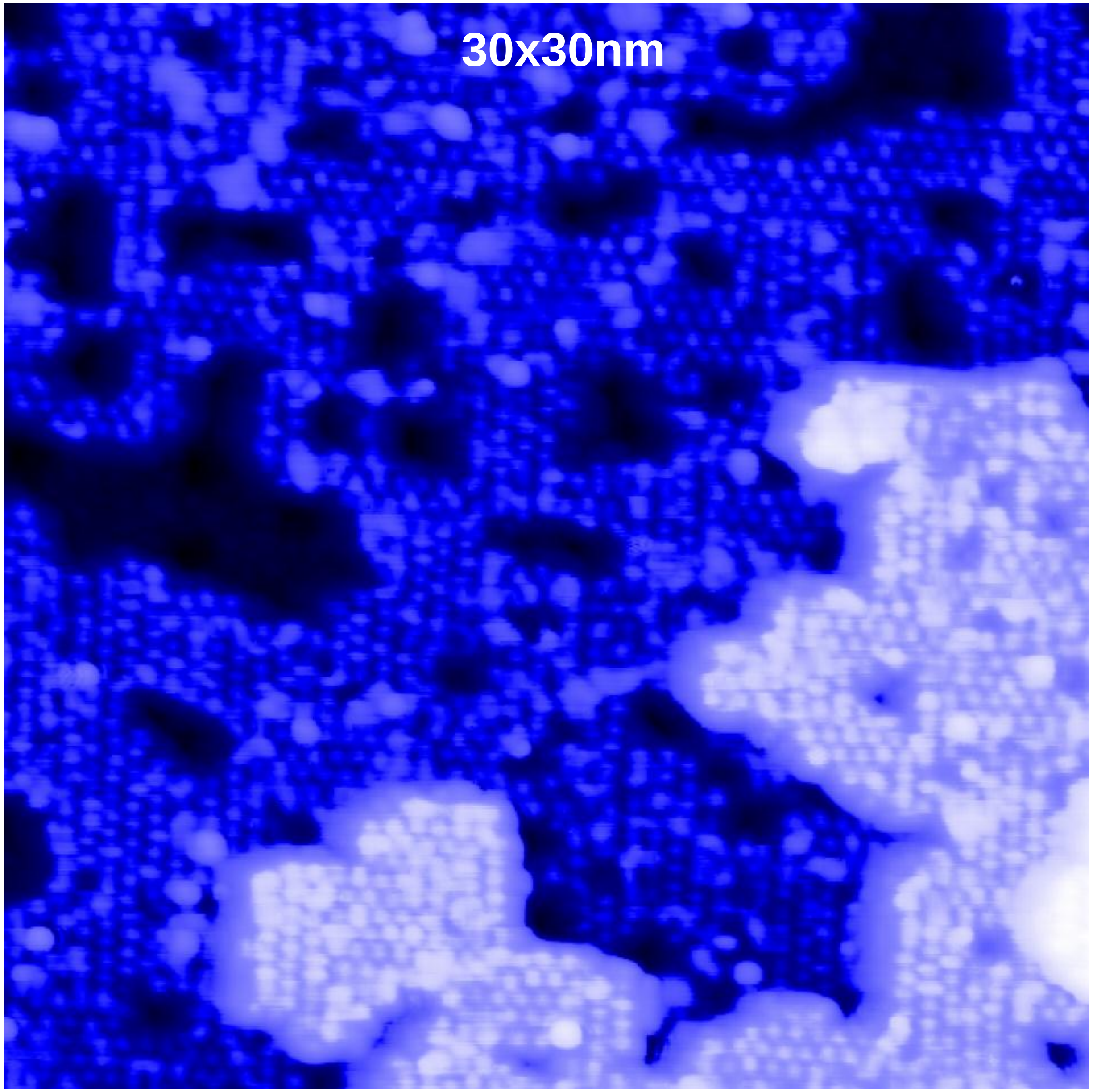






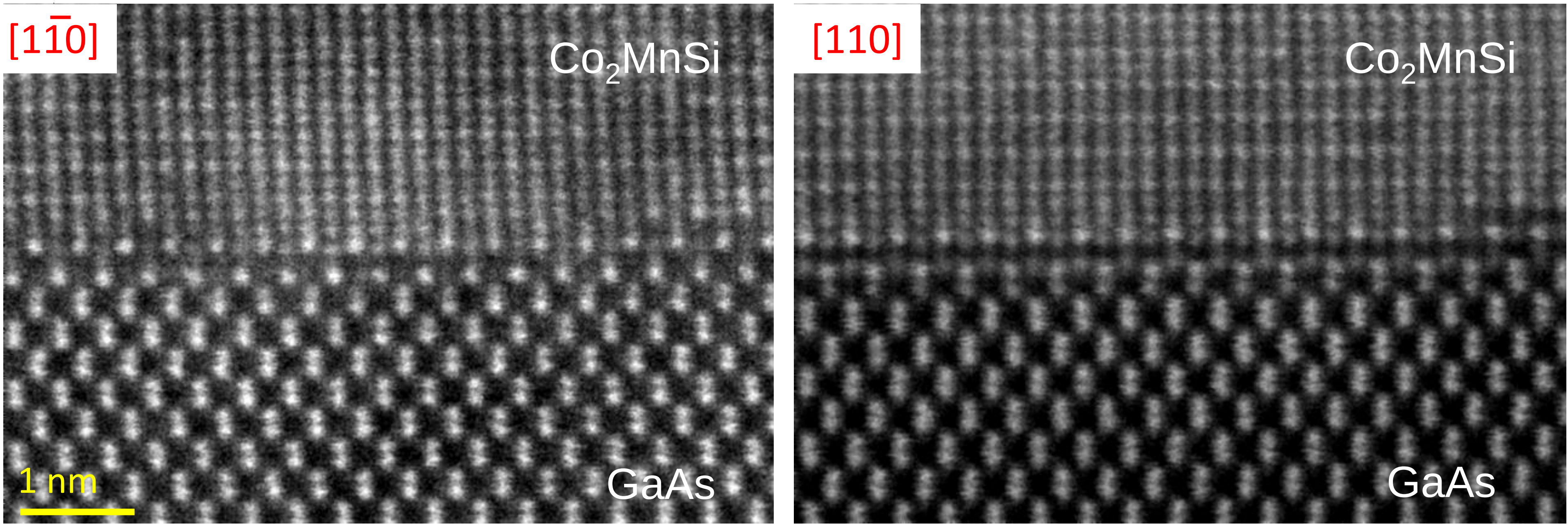
LDOS states features in STS spectra from GaAs region are present in spectra on Co_2MnSi islands

15.5nm Co_2MnSi/c(4x4) GaAs grown at 270° C



Cross-sectional HAADF-STEM

T_g 270° C



- Co_2MnSI growth initiated by ½ML MnSi

A. Rath, F. Shi, P. Voyles

HAADF-EELS-STEM Co_2MnSi/GaAs(001) interface

MnSi-initiated sample

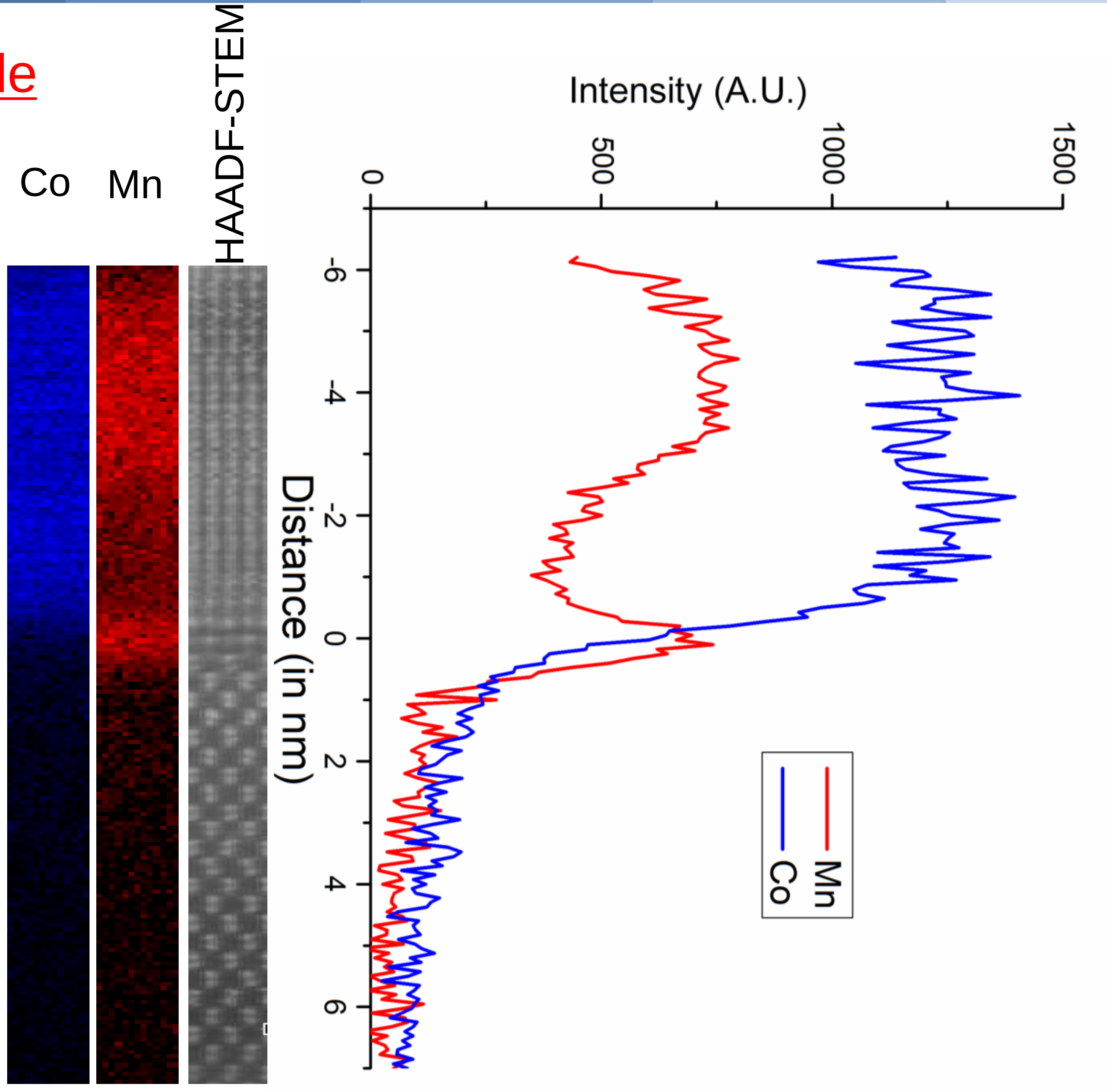
STEM-EELS mapping

shows the Mn-rich interface

and diffusion of Mn

into the GaAs

Mn_2As-like formation at the interface?



J. L. Hilton et al., JAP **102,** 063513 (2007)

Atomic-Resolution EELS: **MnSi**

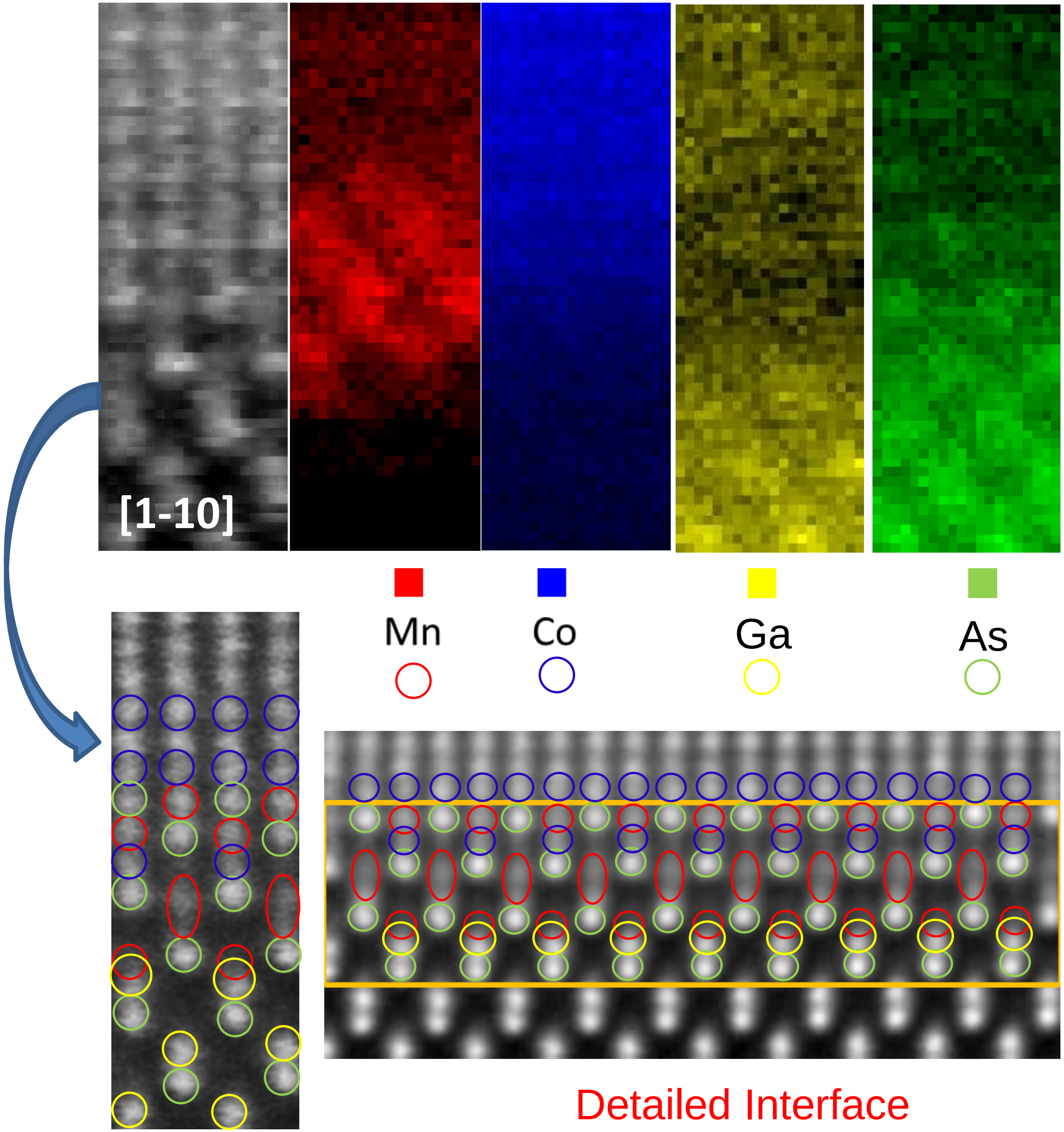
Mn atoms are six atomic layers

away from the CMS layer and distributed

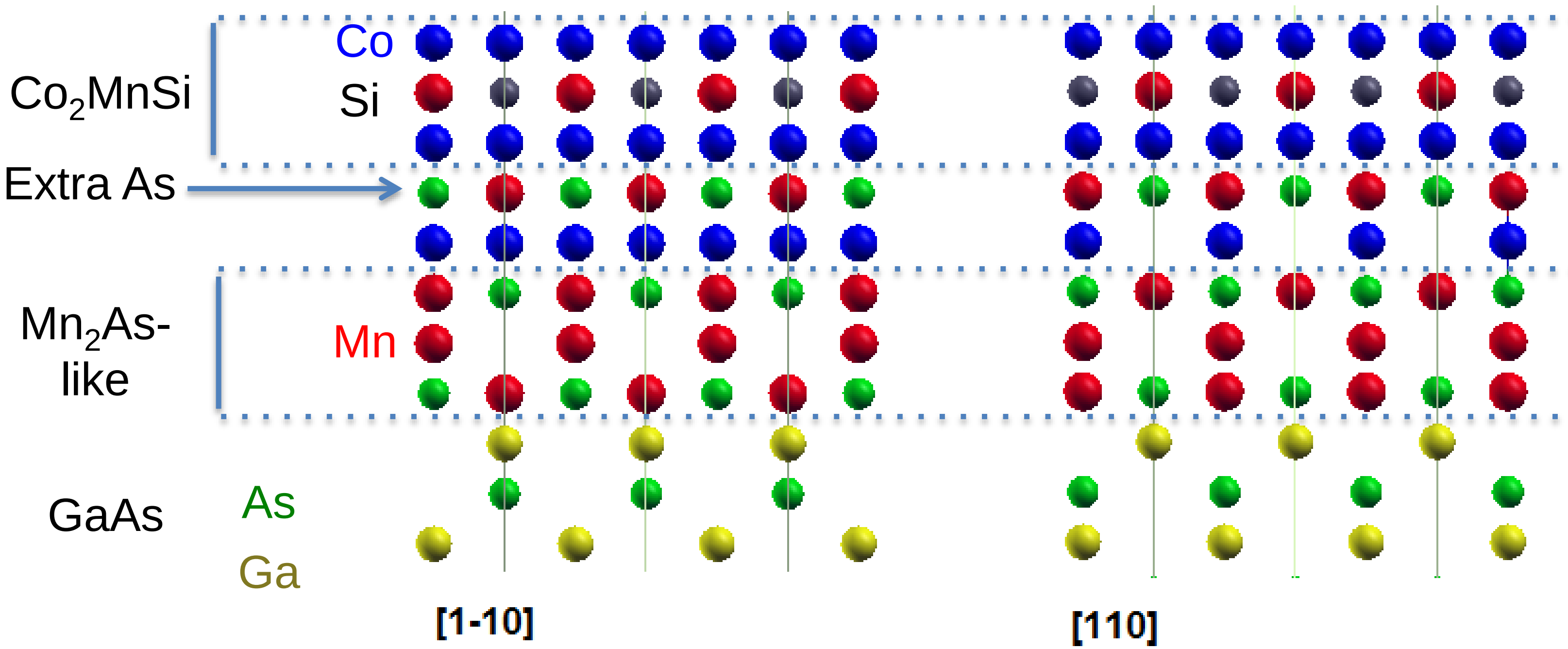
inside the GaAs. Similarly, As atoms are

six planes away from GaAs and distributed inside CMS layer

Unable to detect Si

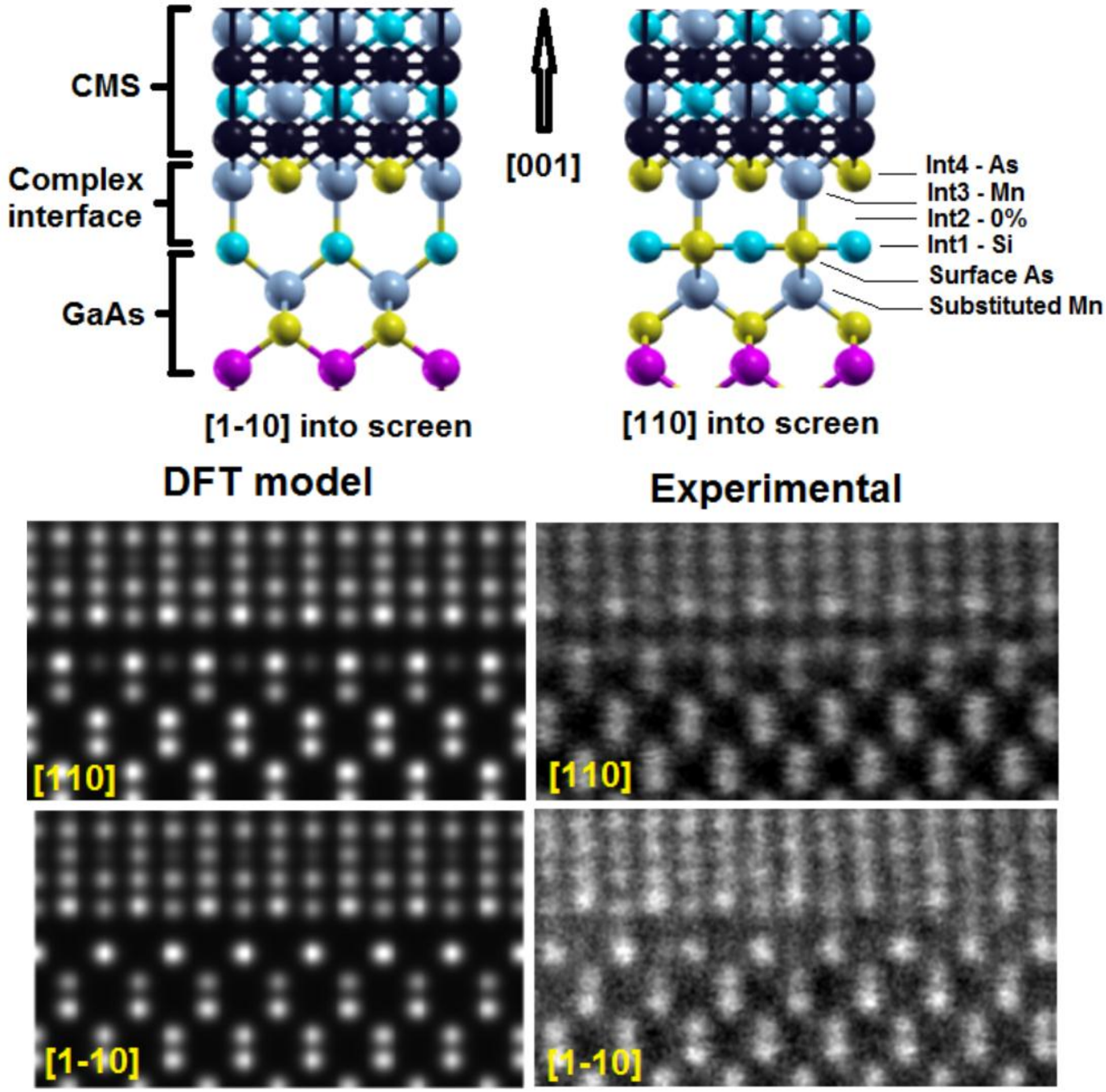


Theoretical model of interface before relaxation



Comparison of Theory and Experiment

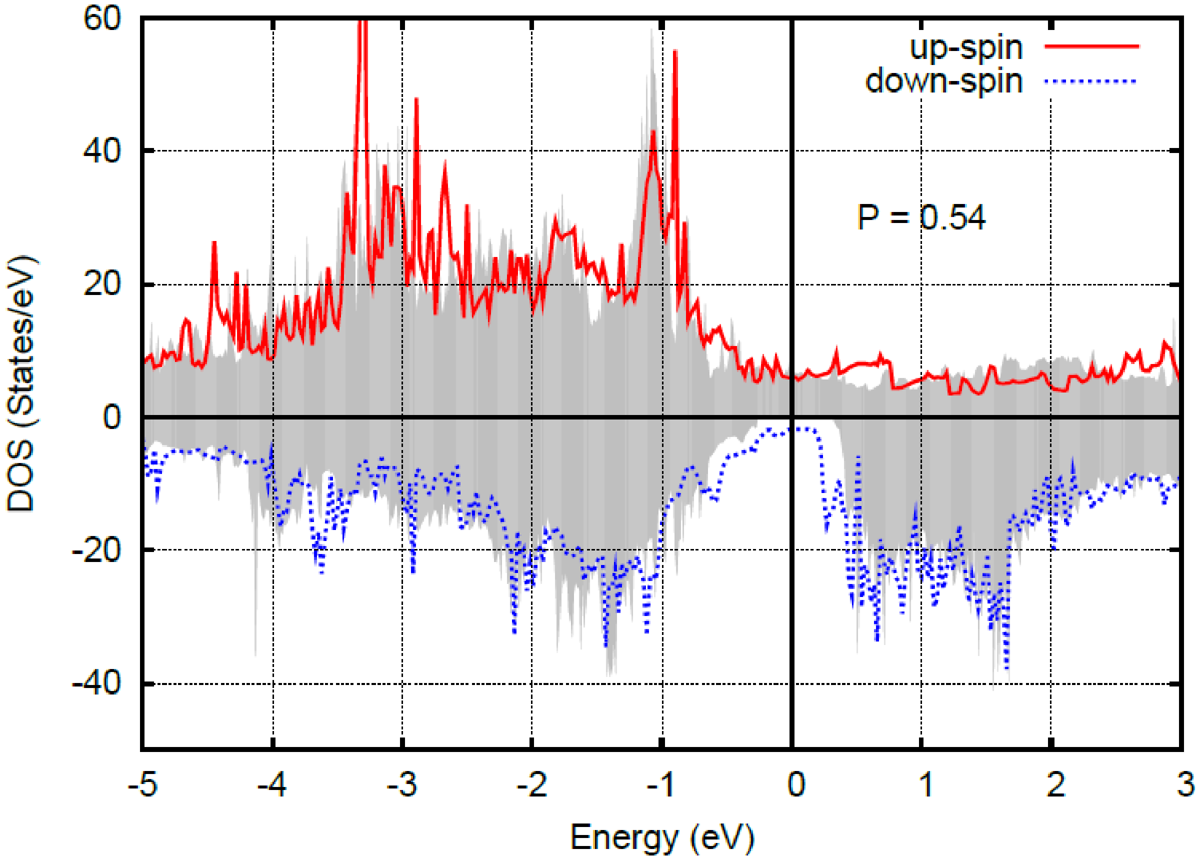
Model #90



C. Sivakumar
W. Butler

A. Rath
P. Voyles

Interface effect on the density states

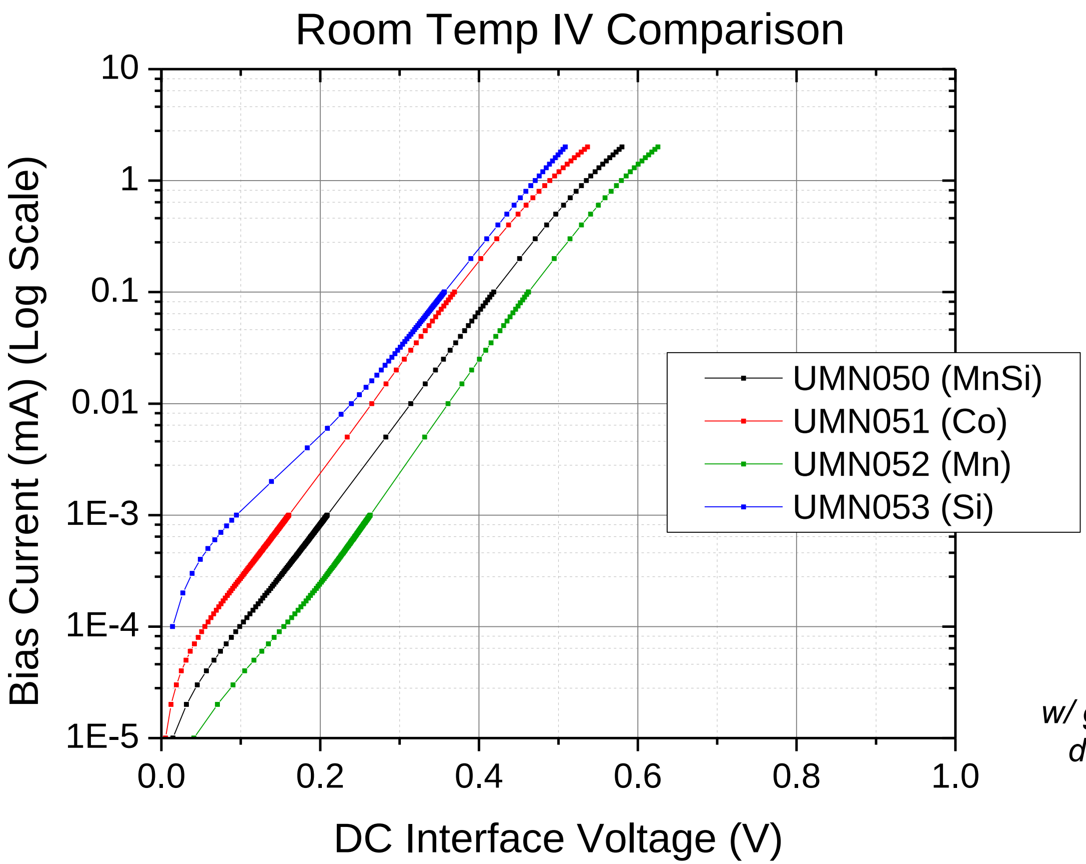


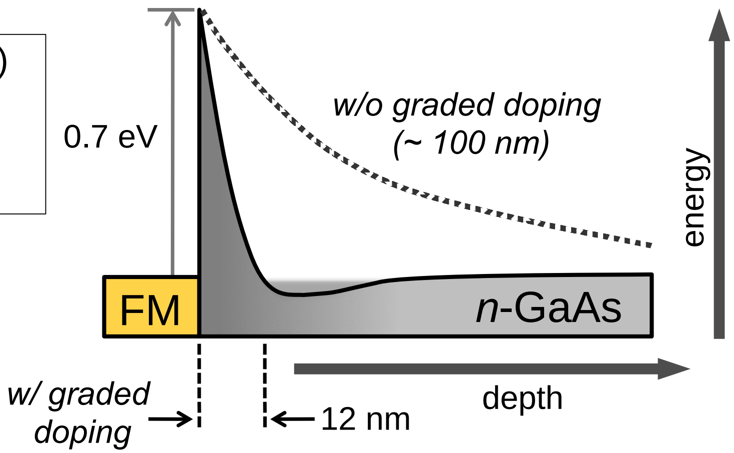
Red and blue   Model #90 (best-fit model) DOS

Greyscale DOS is for an ideal abrupt termination of MnSi/As in CMS/GaAs (001)

$Co_2MnSi/GaAs(001)$ Room Temperature I-V

Influence of initiation layer





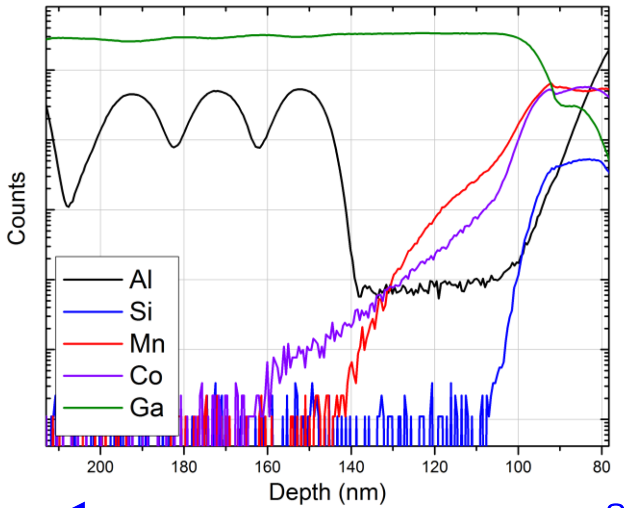
- Schottky barrier height change?
- Mn indiffusion?

Backside SIMS to probe ferromagnet/semiconductor reactions

Is Mn compensating the n-type Shottky contact?

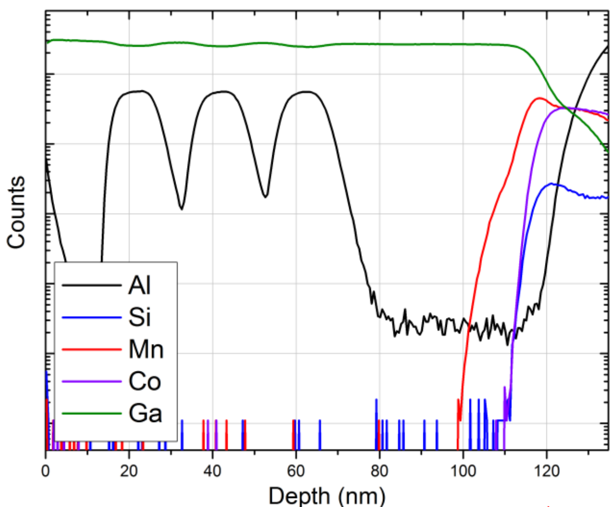
Frontside

(false profile)



Sputter direction

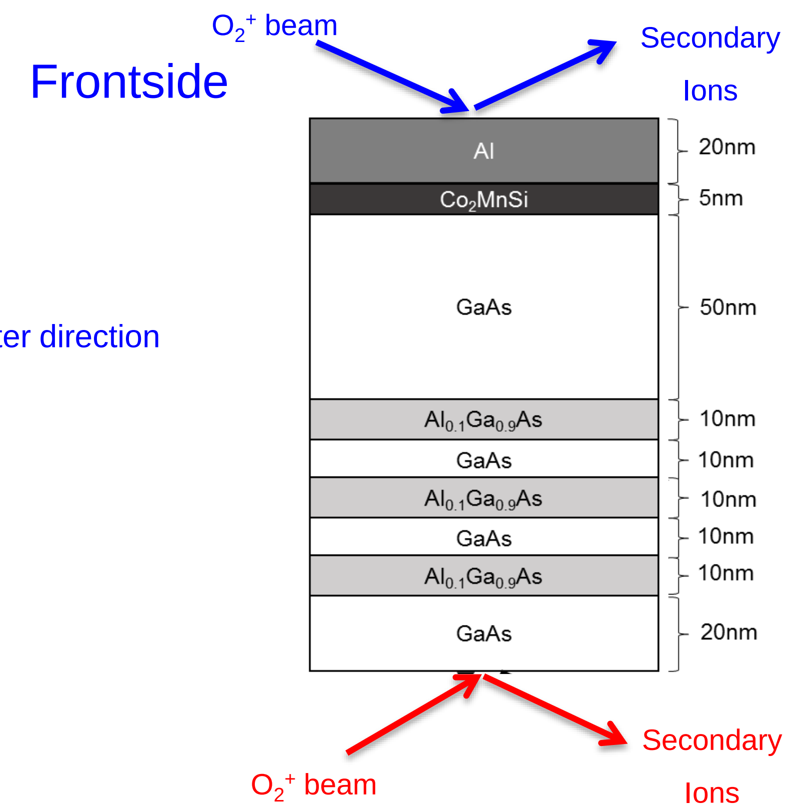
Backside



Sputter direction

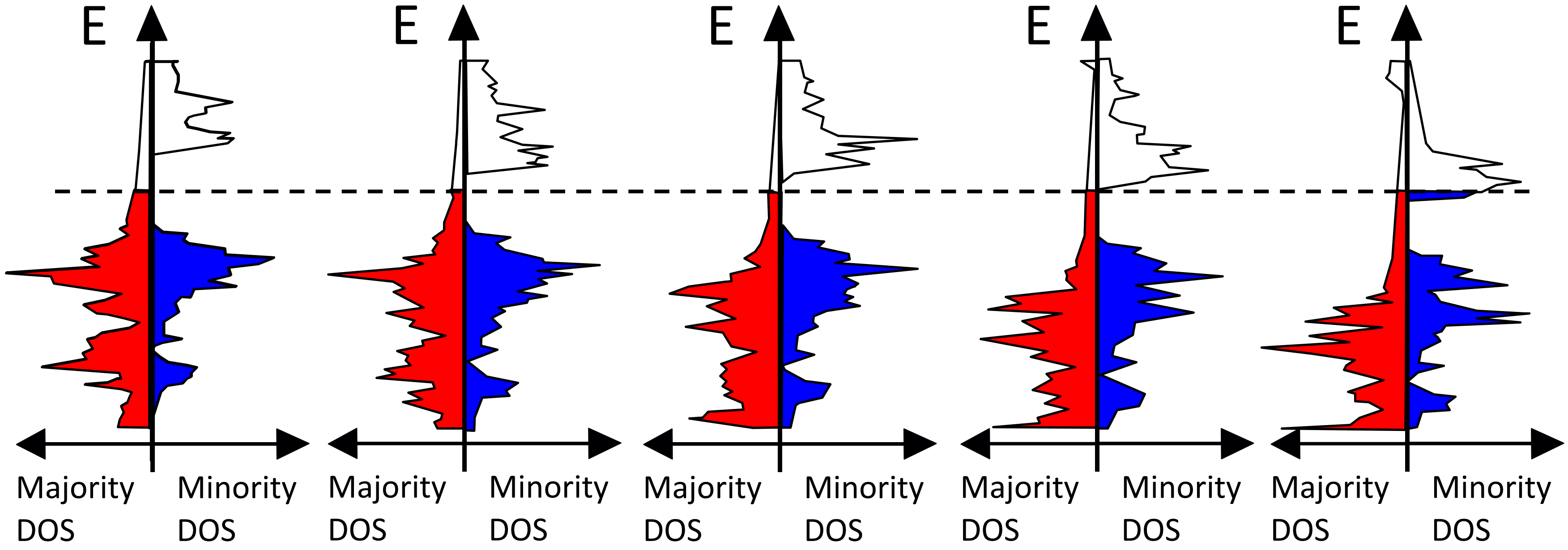
Backside SIMS

- Reduces knock-on of Co, Mn, and Si into GaAs



Ebina et al., Appl. Phys. Lett. **104,** 172405 (2014)

Tuning the Heusler Fermi Level

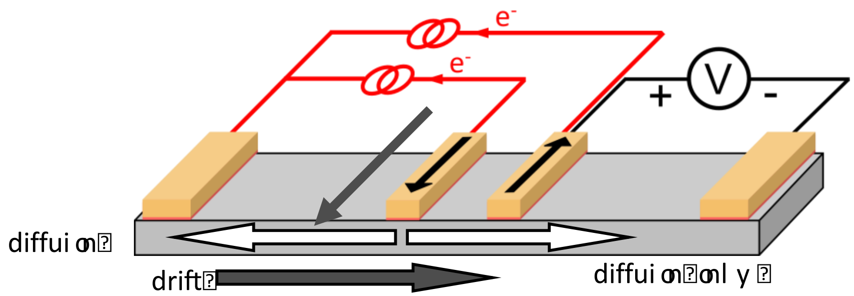


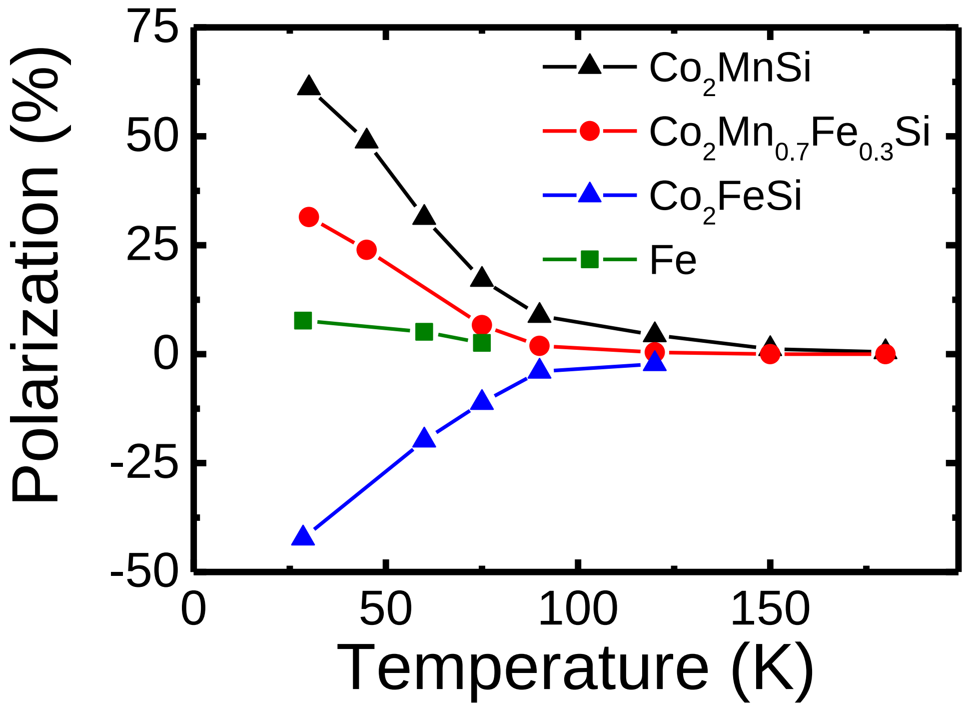
Co_2MnSi $Co_2Mn_{0.5}Fe_{0.5}Si$ Co_2FeSi

- Co-doping Co_2MnSi with Fe increases the Fermi level

  - Co_2MnSi – 0.06% mismatch to GaAs
  - Co_2FeSi – 0.09% mismatch to GaAs

$Co_2Mn_{1-x}Fe_xSi$: comparison with Fe





- Polarizations determined by “biased detector technique”
- Sign change in going from Co_2MnSi to Co_2FeSi

Summary

- Demonstrated high quality MBE growth of Heusler compounds and integration with III-V semiconductors
- Demonstrated high spin polarization in GaAs
- Opposite sign of spin polarization for Co_2MnSi and Co_2FeSi
- Spin polarization can be tuned using $Co_2Mn_{1-x}Fe_xSi$
- Detailed interfacial structure is complicated – feedback between experiment and theory is essential for developing a consistent model of the interfacial atomic structure
- Strong evidence for Mn indiffusion into the GaAs