

Creșterea și caracterizarea straturilor subțiri magnetice de Fe pe substraturi de Si(001) prin epitaxie din fascicul molecular

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The techniques employed are:

MBE chamber:

a) *preparation facilities*: (i) sample heating up to 1200 °C; cooling down to 77 K; (ii) evaporation from a 4-target e-beam evaporator; (iii) evaporation from a high temperature Knudsen cell (2000 °C); (iv) controlled gas adsorption and desorption; (v) monitor of thicknesses using a quartz microbalance.

b) *in situ characterization*: (i) LEED (Low Energy Electron Diffraction); (ii) RHEED (Reflection High Energy Electron Spectroscopy); (iii) AES (Auger Electron Spectroscopy); (iv) Quadrupole Mass Spectroscopy (thermal induced desorption, photodesorption).

STM chamber:

(i) sample preparation stage (heating, ion sputtering); (ii) tip preparation (ion sputtering); (iii) variable temperature (77 - 453 K) scanning tunneling microscopy; (iv) scanning tunneling spectroscopy (STS)

SARPES chamber:

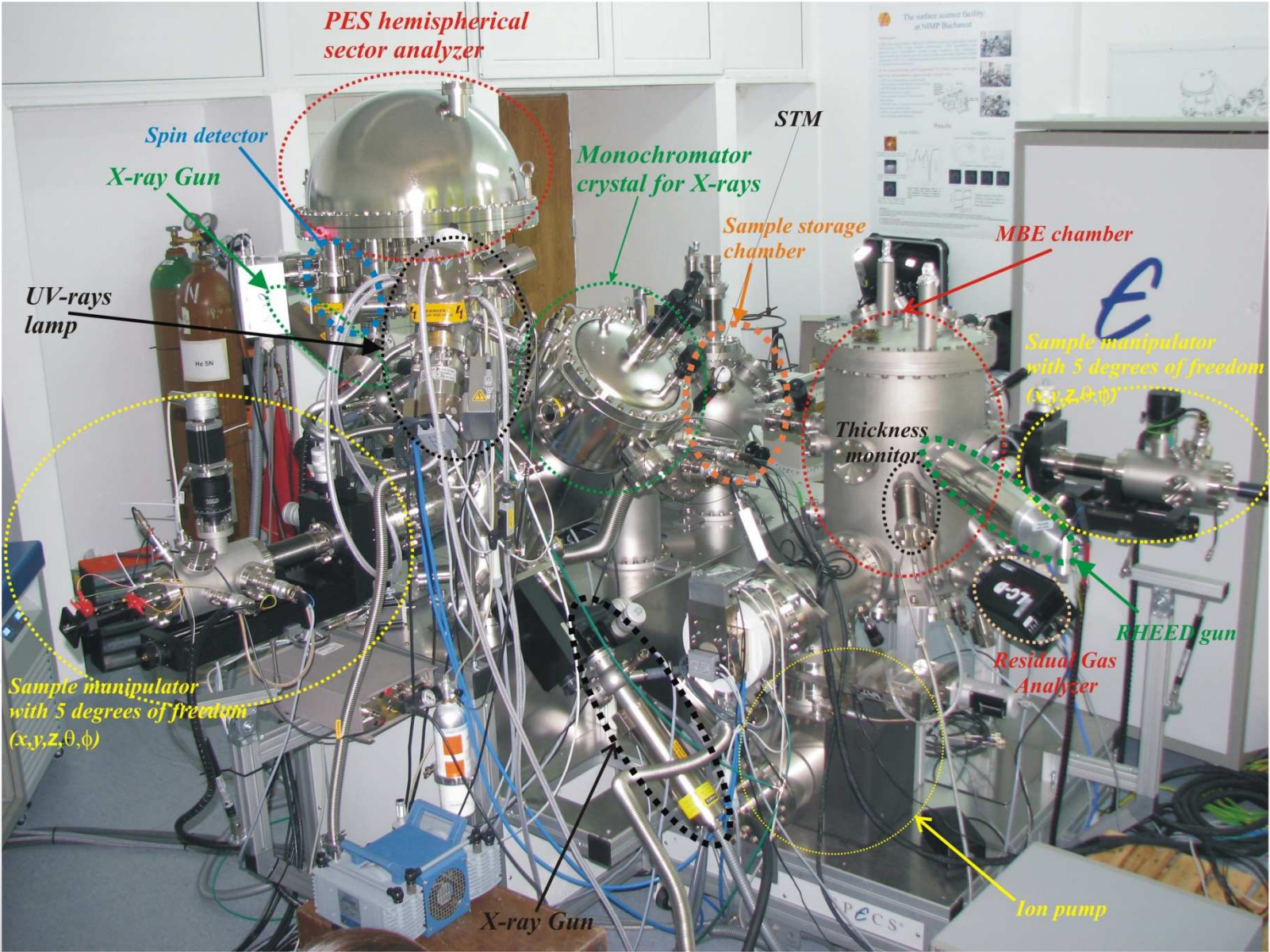
- (i) conventional X-ray photoelectron spectroscopy using a dual (Al/Mg K_{α}) anode;
- (ii) high resolution XPS using a monochromatized dual (Al K_{α} /Ag L_{α}) source;
- (iii) ultraviolet photoelectron spectroscopy (UPS He I, He II);
- (iv) angle-resolved XPS: x-ray photoelectron diffraction (XPD);
- (v) angle-resolved UPS (ARUPS): band structure, Fermi surface, etc.;
- (vi) spin-resolved UPS: spin-polarized density of states;
- (vii) angle- and spin-resolved UPS: spin-polarized band structure;
- (viii) remote-controlled ion sputtering: depth profiling;
- (ix) flood gun for sample neutralization.

Ex situ measurements:

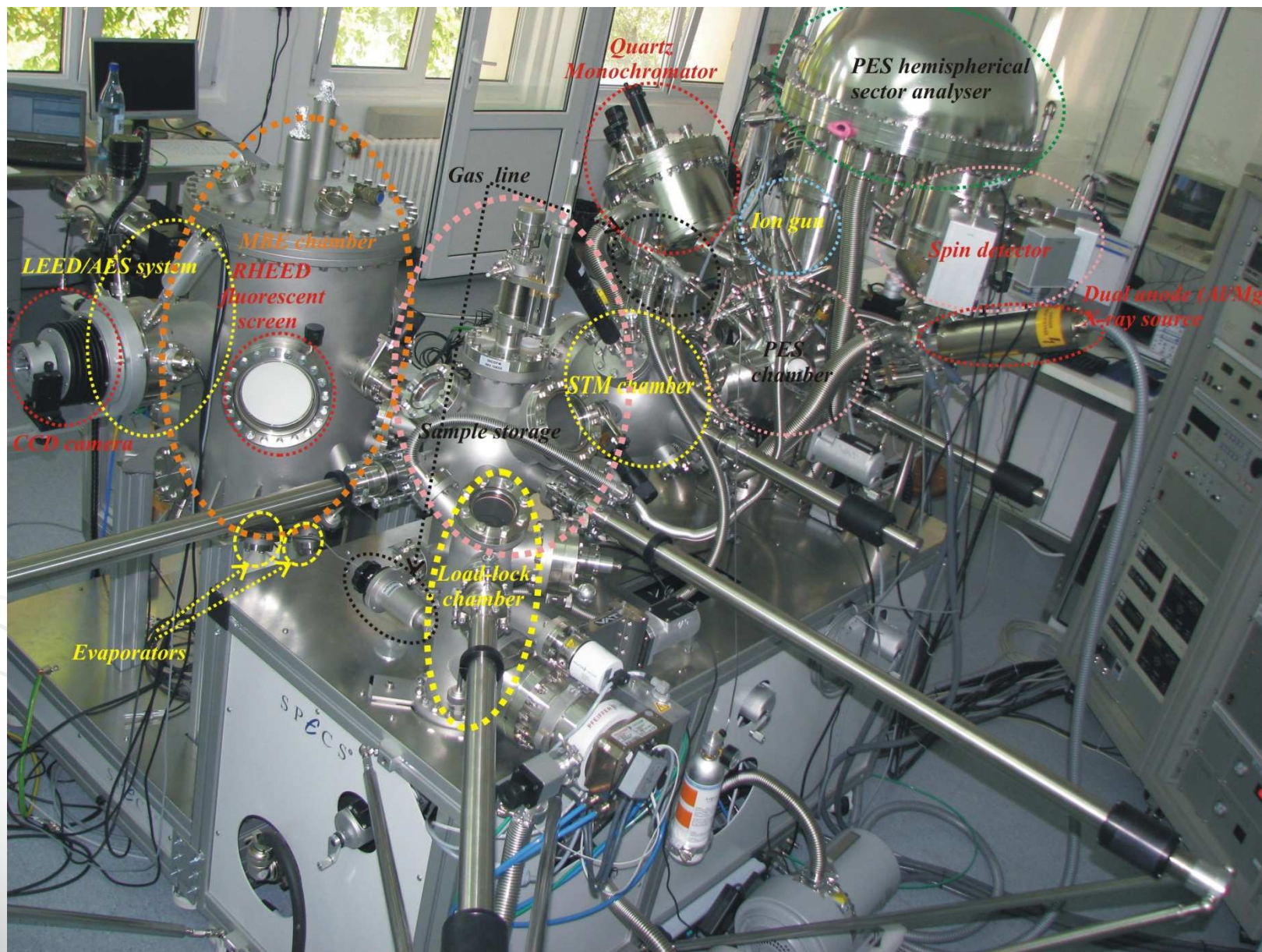
- (i) Extended X-ray absorption fine structure (EXAFS);
- (ii) X-ray absorption near-edge structure (XANES);
- (iii) Magneto-optical Kerr effect (MOKE);
- (iv) Mössbauer spectroscopy

Using synchrotron radiation at Hasylab, DESY, Hamburg (long-term project running)

The setup (I)

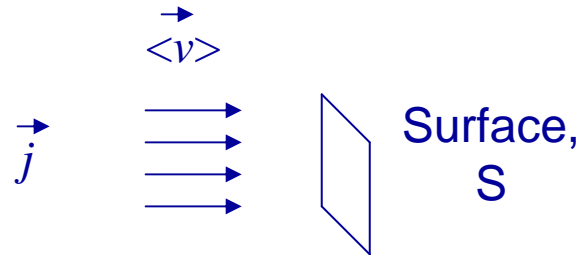


The setup (II)



Ultrahigh vacuum basics

Contamination rate of a reactive surface (metals/semiconductors)



flux of molecules
from residual gas

$$\vec{j} = n \langle \vec{v} \rangle$$

$$\langle v \rangle \approx \sqrt{\frac{3k_B T}{m}} \quad \text{from Maxwell-Boltzmann statistics}$$

≈ 492 m/s for N_2 (mass = 28 a.m.u.) @ 273 K

$$n = \frac{P}{k_B T} \quad \text{from the Boltzmann equation}$$

$\approx 2.65 \times 10^{16}$ mol./m³ for $P = 10^{-4}$ Pa $\approx 10^{-6}$ mbar and $T = 273$ K

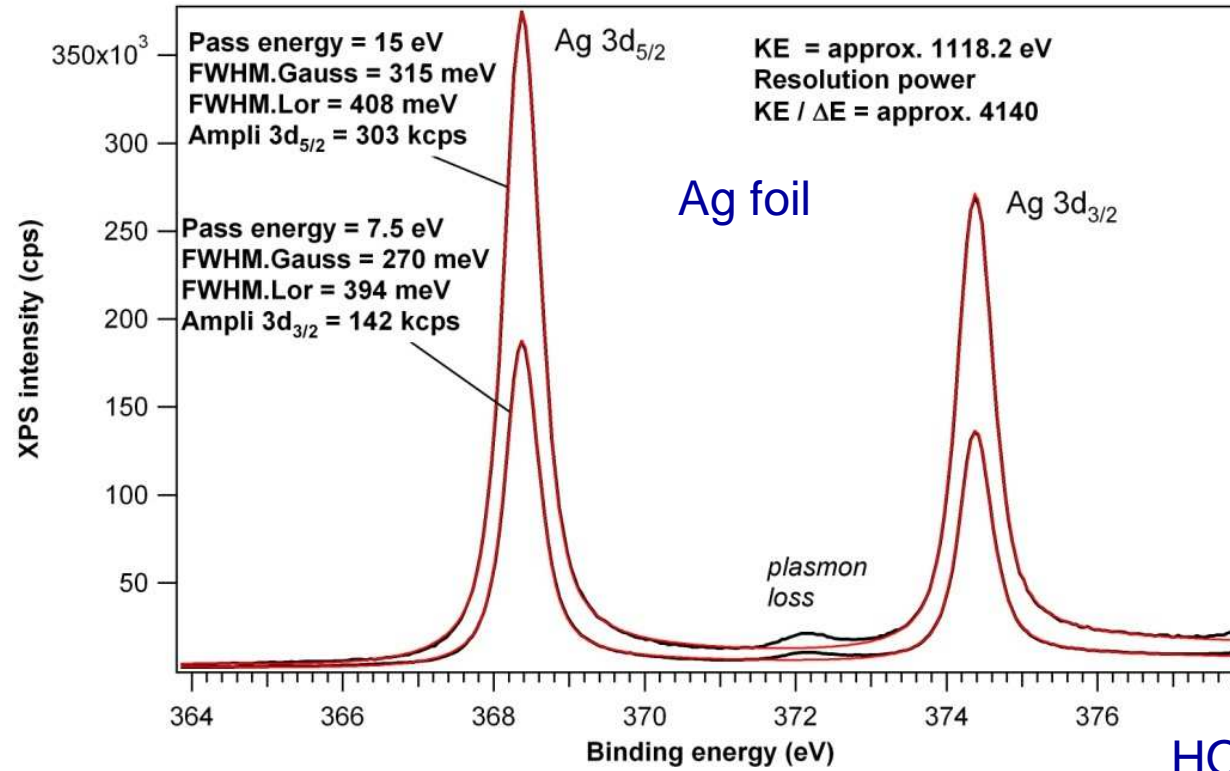
● Contamination dynamics: $\frac{\partial N}{\partial t} = j \cdot S \approx \frac{N_r}{\tau_c} = \frac{\sigma_r S}{\tau_c} = \frac{\text{Number of reactive sites}}{\text{Contamination time}}$

σ_r = surface density of contamination sites ≈ 1 site / $4 \text{ \AA}^2 = 2.5 \times 10^{19}$ sites / m²

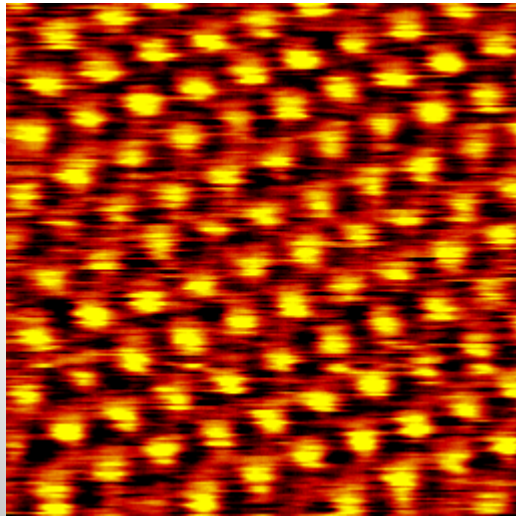
$$\tau_c = \frac{\sigma_r}{j} = \frac{\sigma_r}{n \langle v \rangle} \approx \frac{2.5 \times 10^{19}}{2.65 \times 10^{16} \times 492} \approx 1.9 \text{ sec.}$$

VERY FAST CONTAMINATION

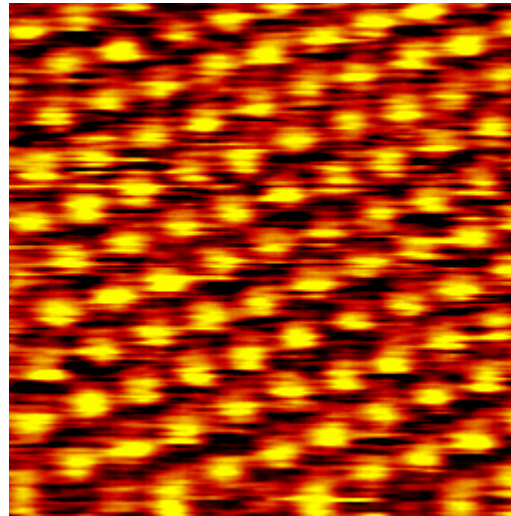
Performances:



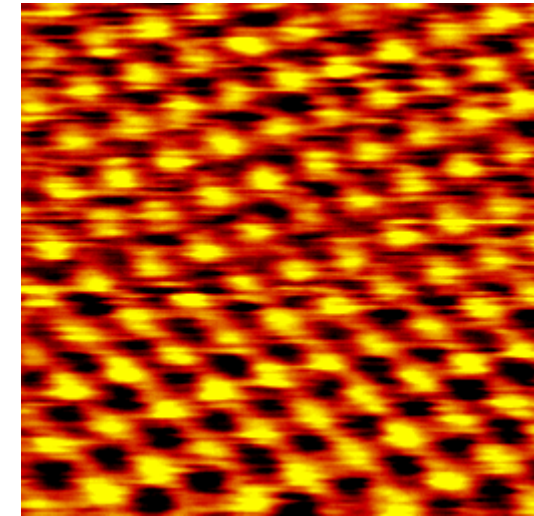
FOV=20 nm



$V_t=630,5$ mV



$V_t=712,9$ mV



$V_t=883,8$ mV

Atomic structure of the reactive Fe/Si(111)7x7 interface

Why Fe/Si?

A. Mascaraque

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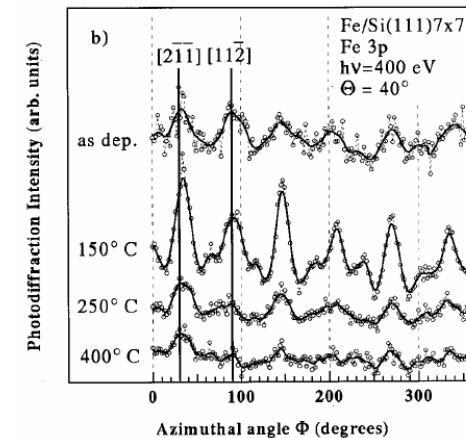
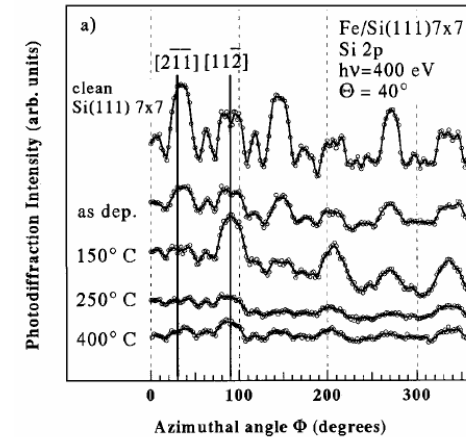
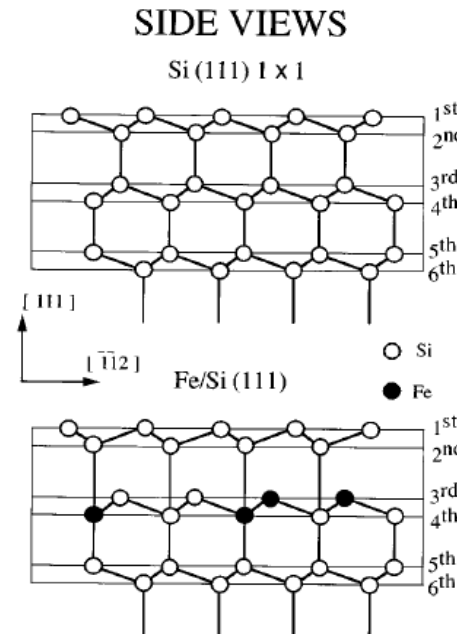
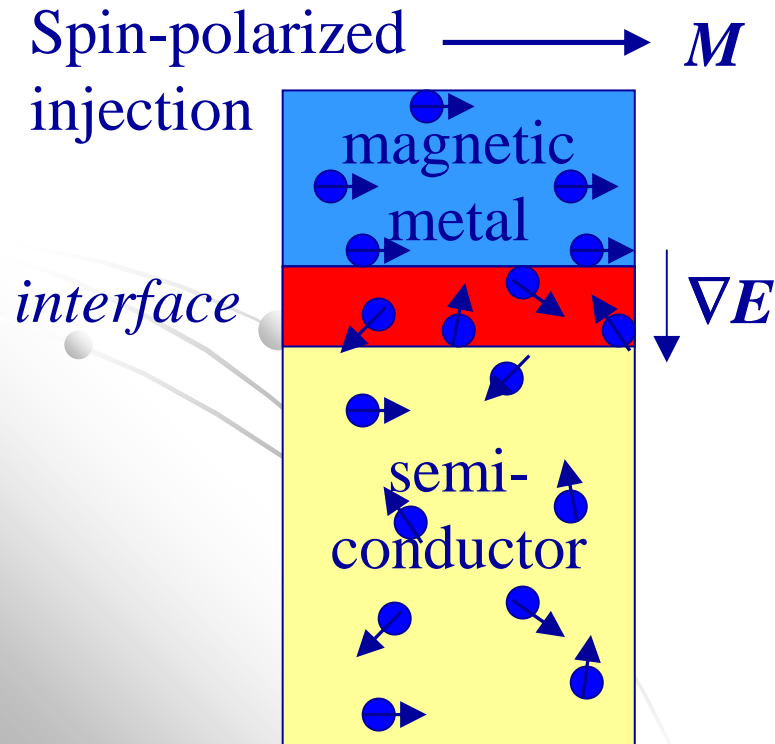
J. Avila, C. Teodorescu, and M. C. Asensio

*LURE, Bâtiment 209D, Université Paris-Sud, F-91405 Orsay, France
and Instituto de Ciencia de Materiales, CSIC, 28049 Madrid, Spain*

E. G. Michel

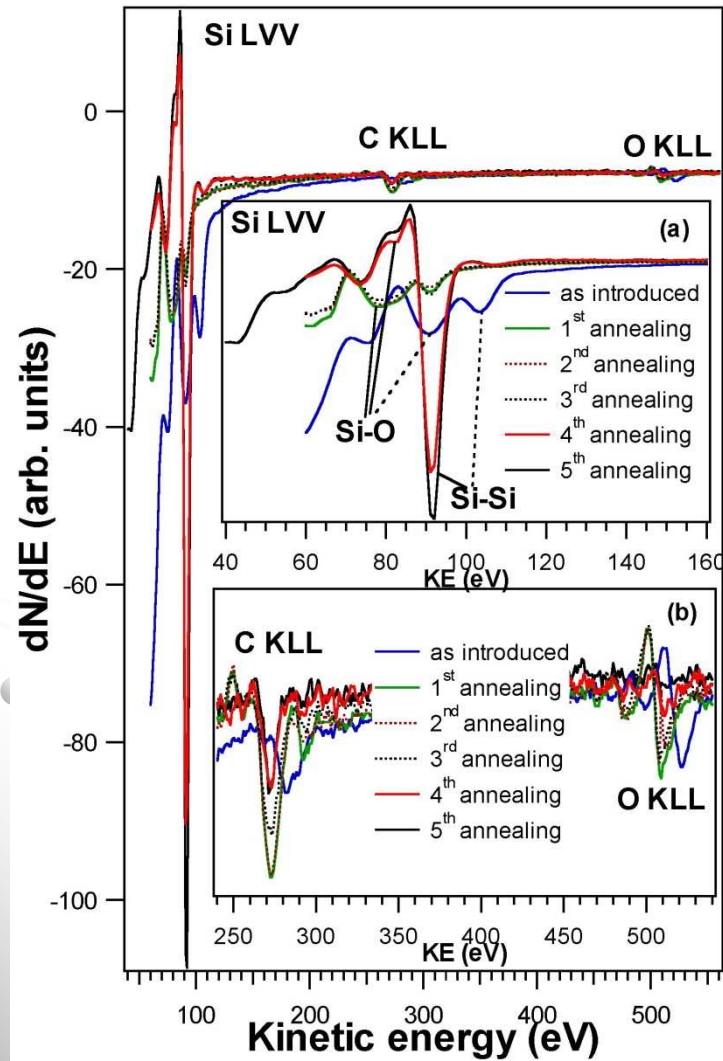
*Departamento de Física de la Materia Condensada and Instituto Universitario de Ciencia de Materiales "Nicolás Cabrera,"
Universidad Autónoma de Madrid, 28049 Madrid, Spain*

(Received 24 October 1996)



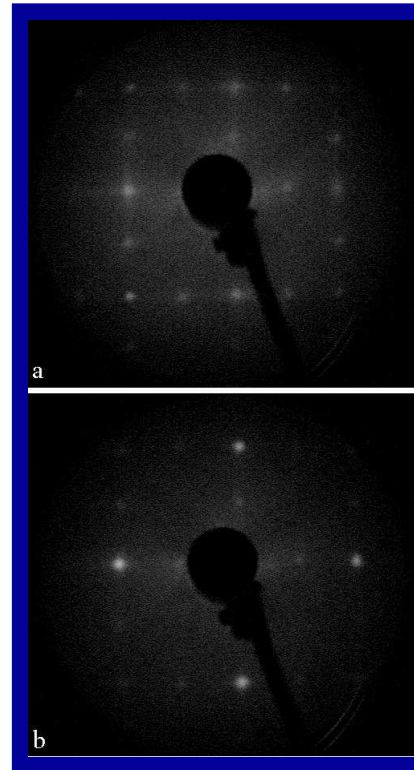
Result #1: Cleaning of Si(001) samples and study of the subsequent contamination (I)

Auger electron spectroscopy



LEED

56 eV



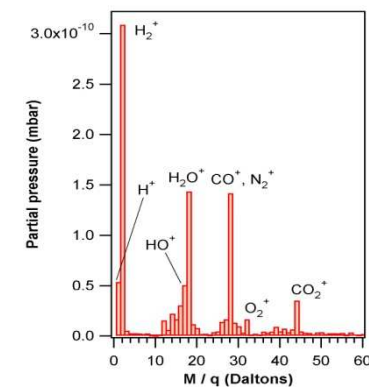
44 eV

Residual gas analysis

RHEED



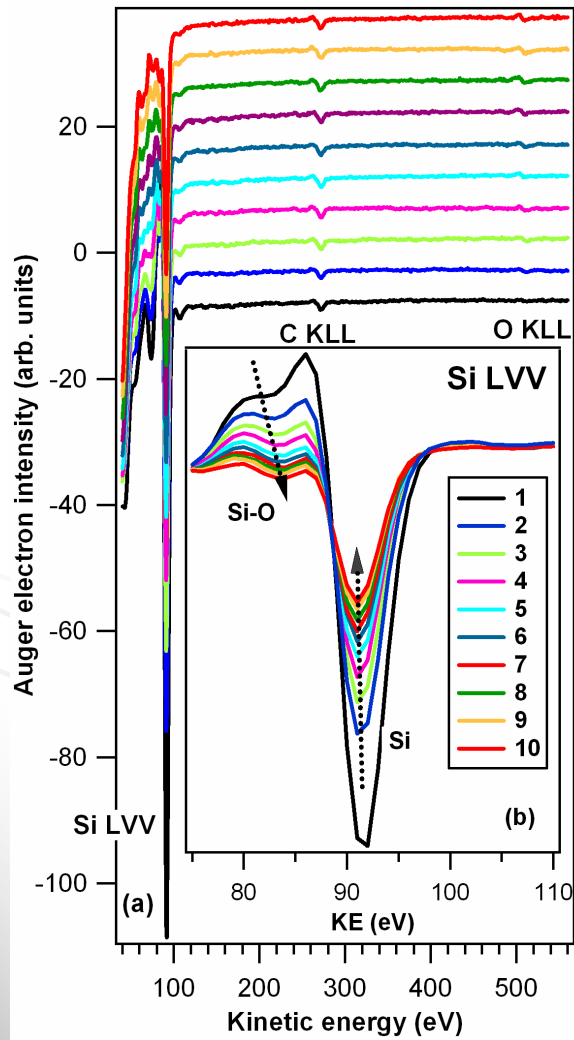
25 keV



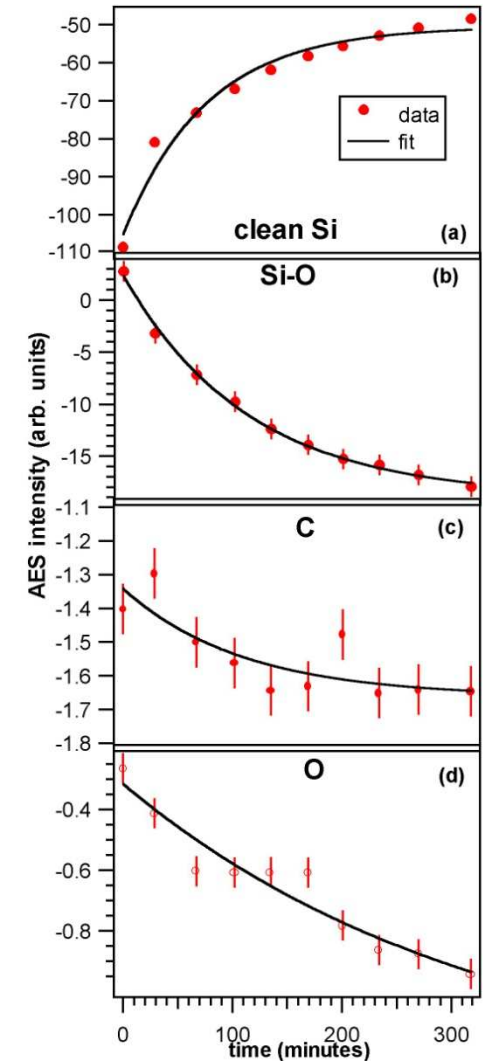
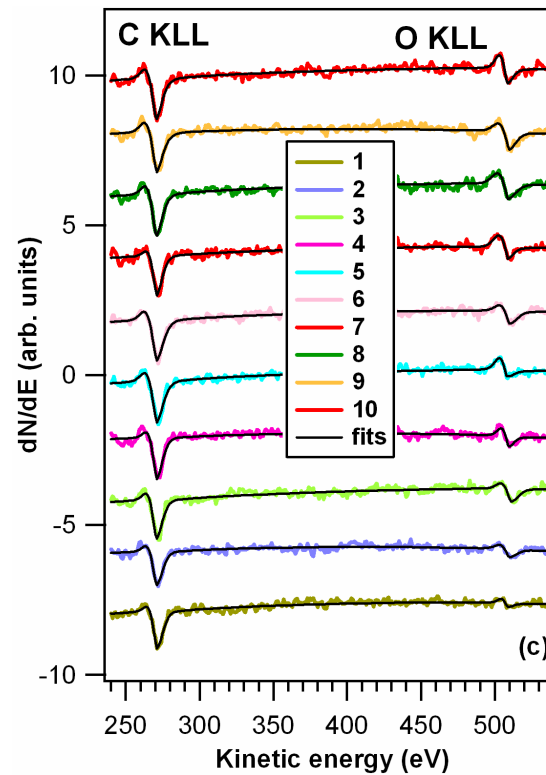
Gheorghe et al., Rom. J. Phys., submitted (2010)

Result #1: Cleaning of Si(001) samples and study of the subsequent contamination (II)

$P_{\text{mes.}} \approx 1 \times 10^{-9}$ mbar.



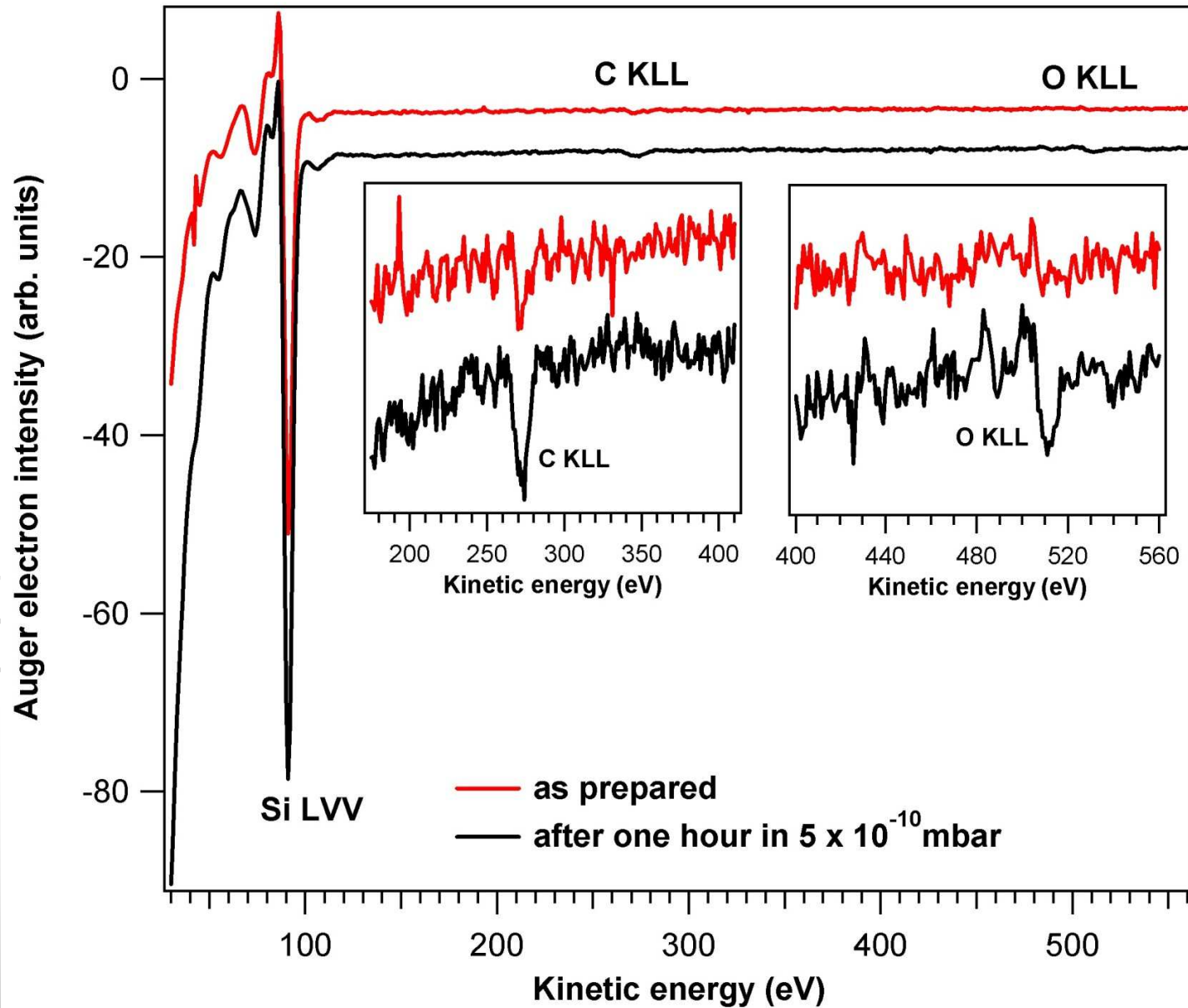
Auger electron spectroscopy



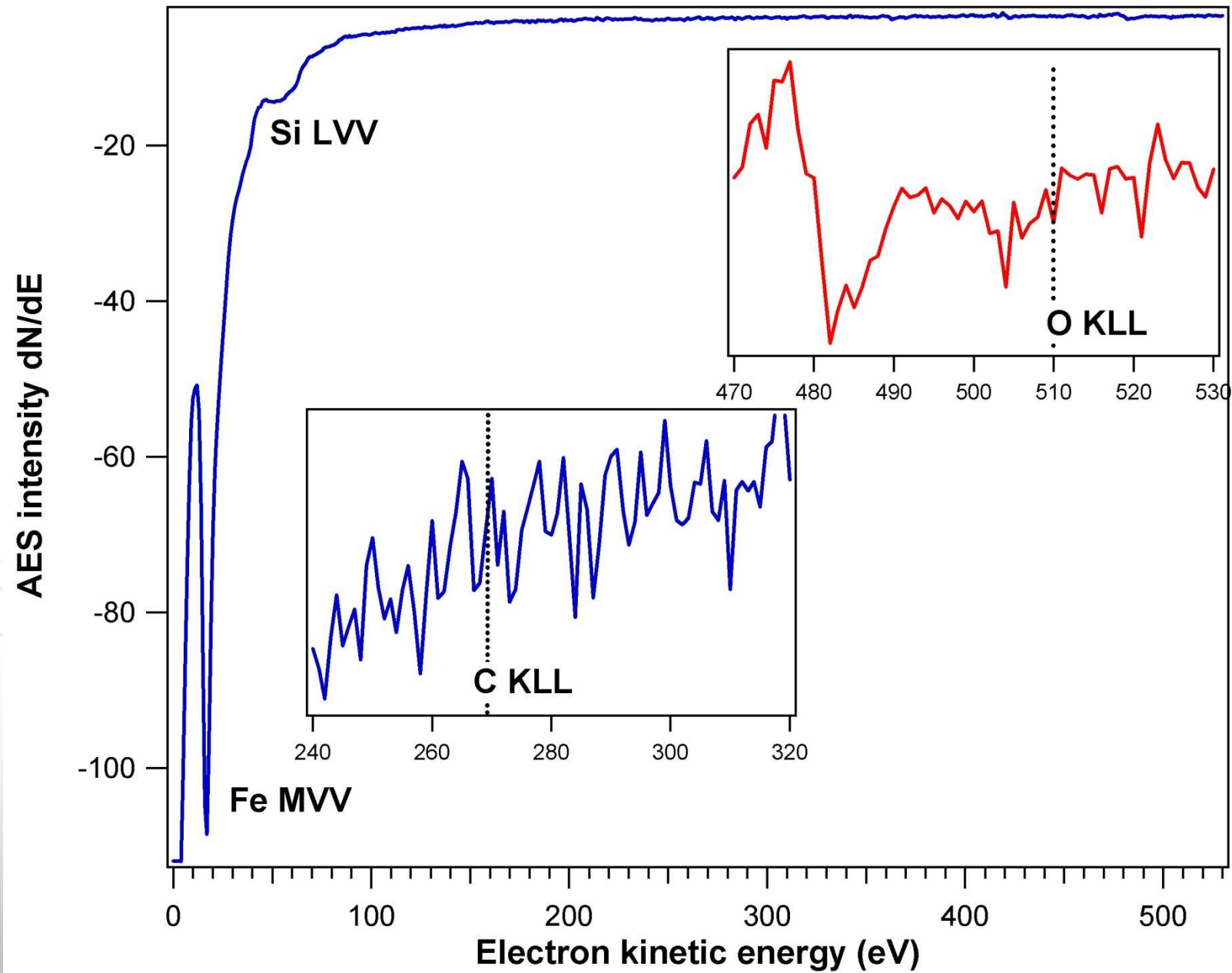
Gheorghe et al., Rom. J. Phys., submitted (2010)

Clean Si(001) - (III)

C contamination < 1.2 % of one ML!
O contamination < 0.3 % of one ML!

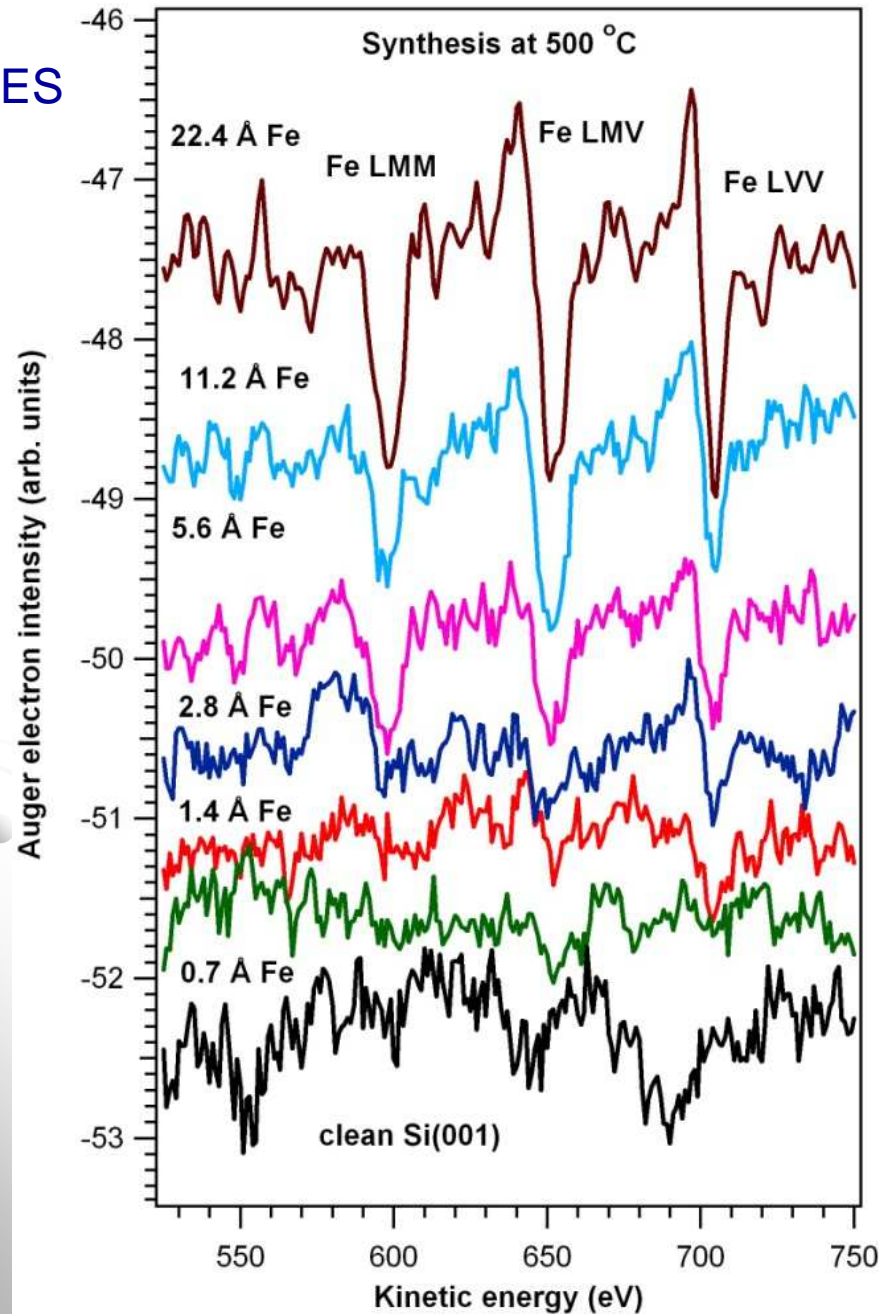


Result #2: Growth of Fe on Si(001) (I)



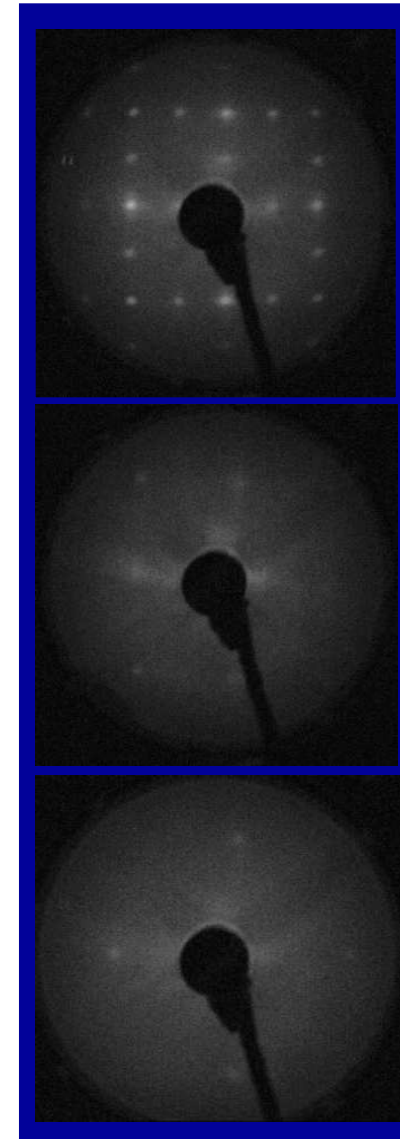
Result #2: Growth of Fe on Si(001) (II)

AES



$T_s = 500 \text{ }^\circ\text{C}$

LEED, 56 eV



Si(001)

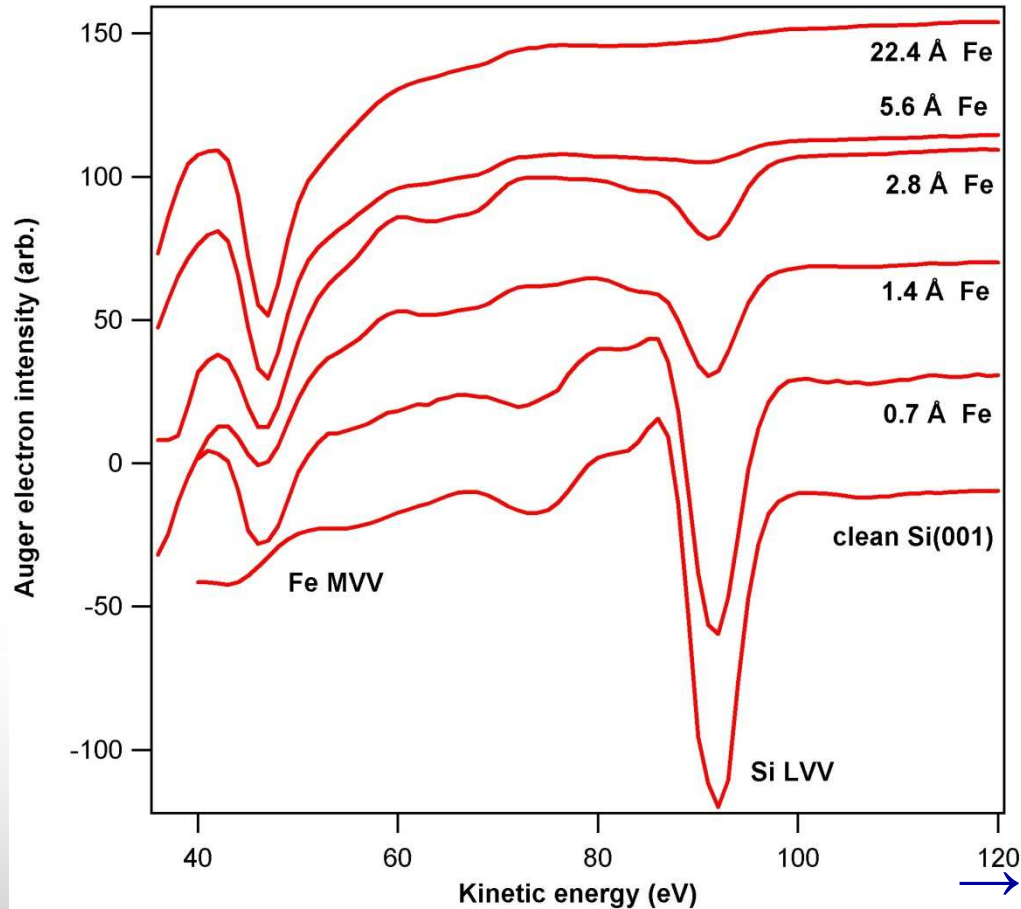
0.7 Å Fe

2.8 Å Fe

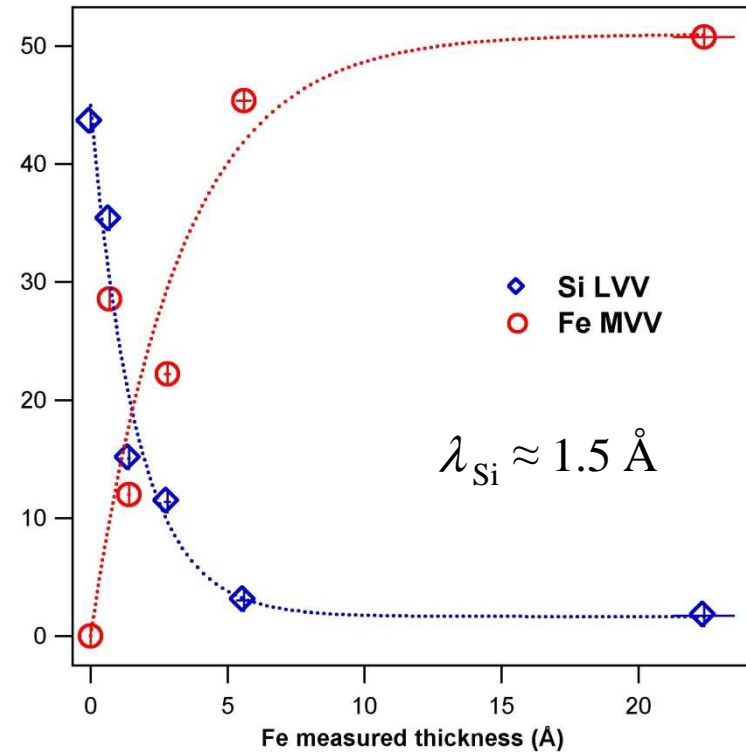
RT deposition -> no LEED

Result #2: Growth of Fe on Si(001) (III)

Deposition at room temperature (300 K)



λ = electron inelastic mean free path ($\approx 5-6 \text{ \AA}$)



$$I^{(\text{Si})} = I_0^{(\text{Si})} \exp(-\theta / \lambda)$$

$$I^{(\text{Fe})} = I_0^{(\text{Fe})} [1 - \exp(-\theta / \lambda)]$$

$$\rightarrow \theta_{\text{real}} \approx 3 \times \theta_{\text{measured}}$$

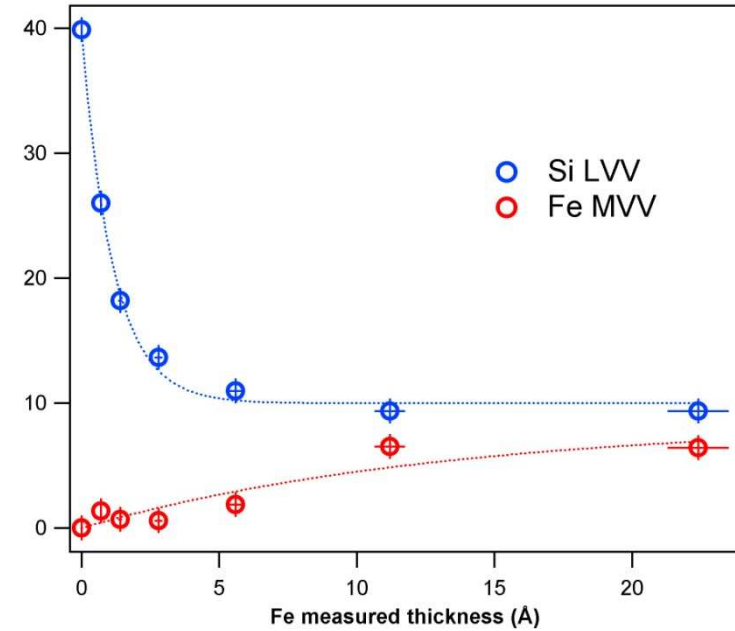
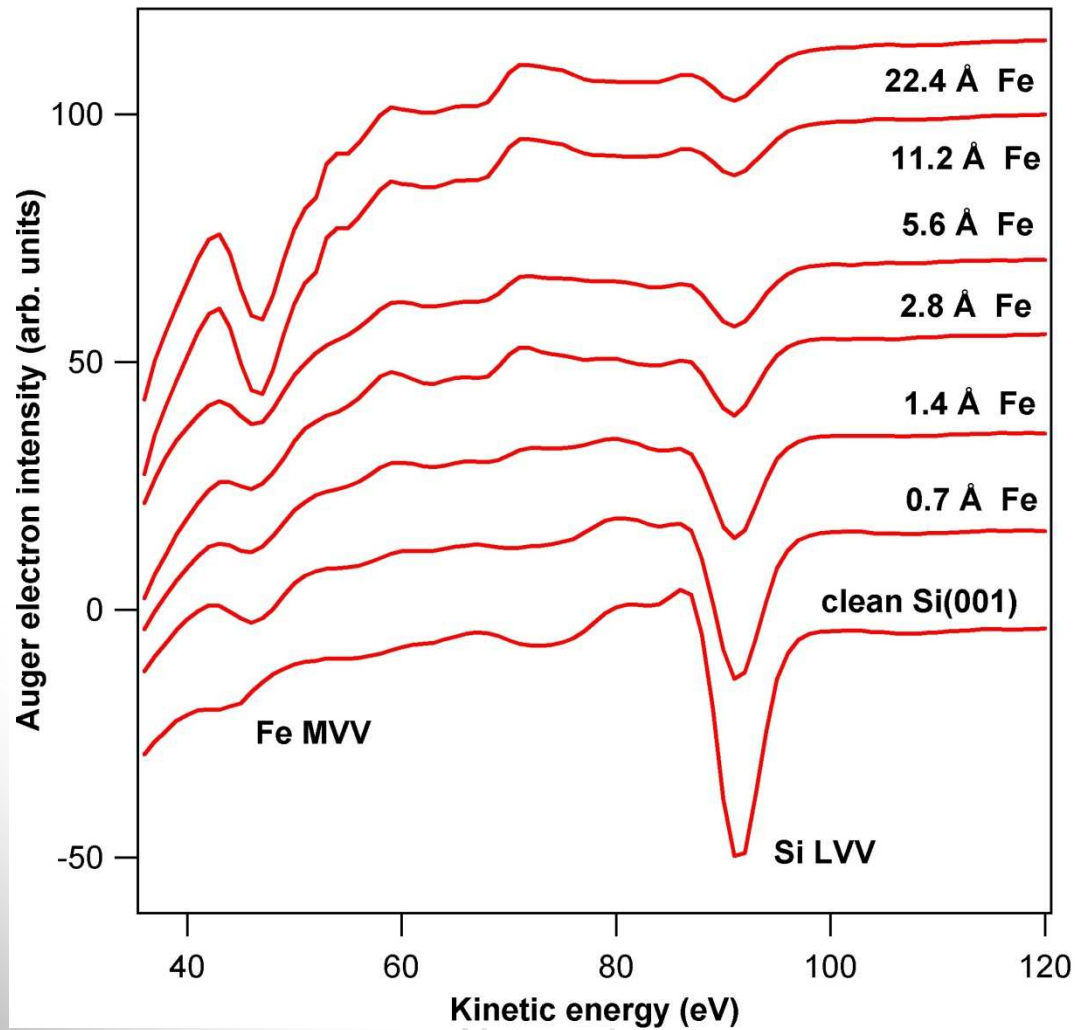
→ no (few) reactivity at interface

→ no diffusion of Si into Fe

→ no long range order (LEED)

Result #2: Growth of Fe on Si(001) (IV)

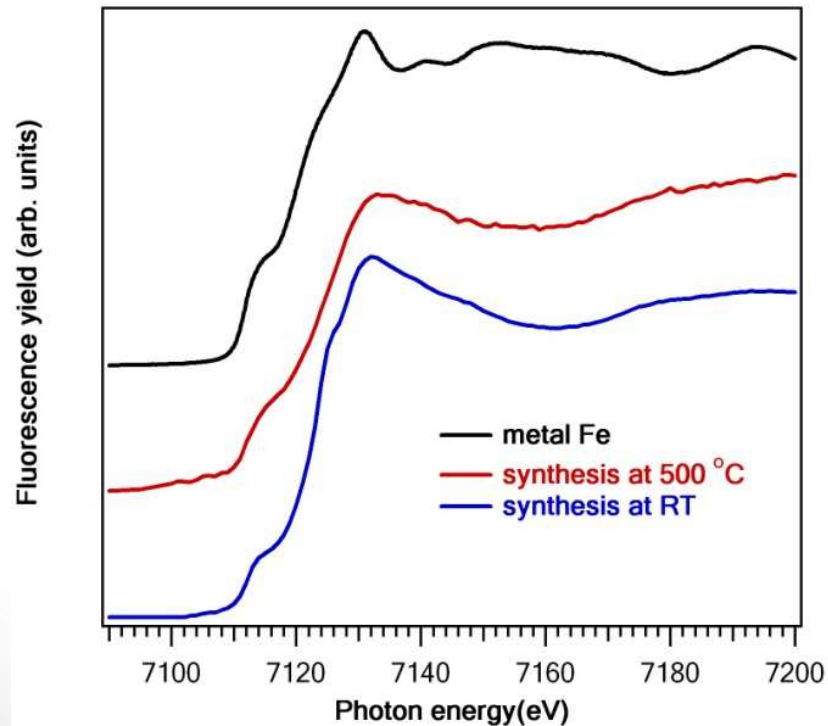
Deposition at 500 °C



- reactivity at interface
- formation of $\text{FeSi}_{1.18}$ (mixture of FeSi and FeSi_2)
- long range order (LEED)

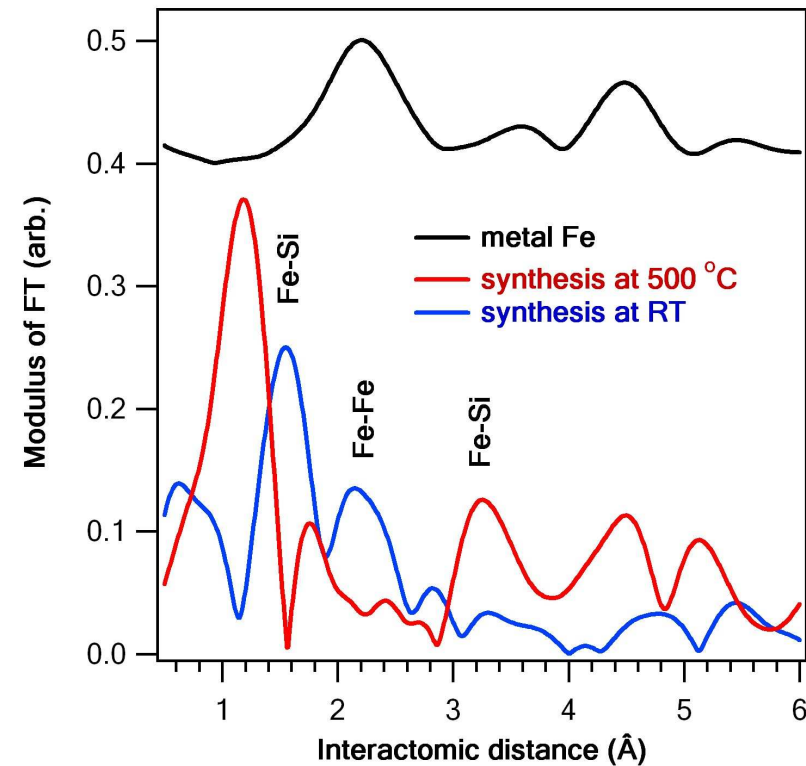
Result #2: Growth of Fe on Si(001) (V)

X-ray absorption near-edge spectroscopy (XANES)



Capped samples (with Au or Cu)

Extended X-ray absorption fine structure (EXAFS)

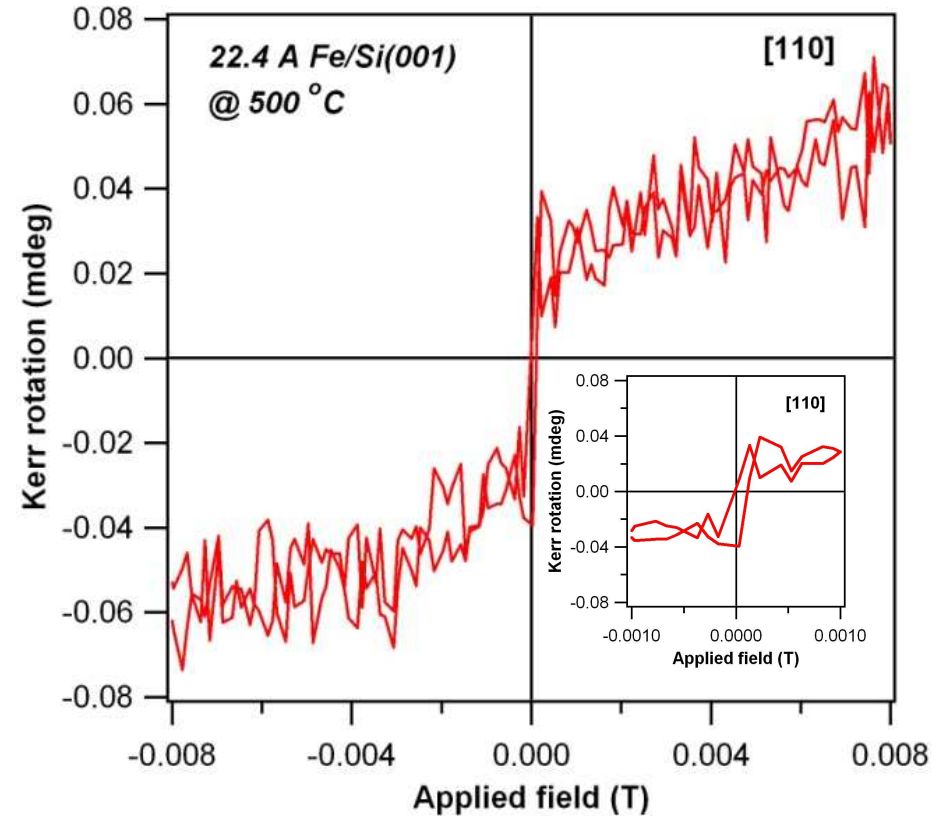
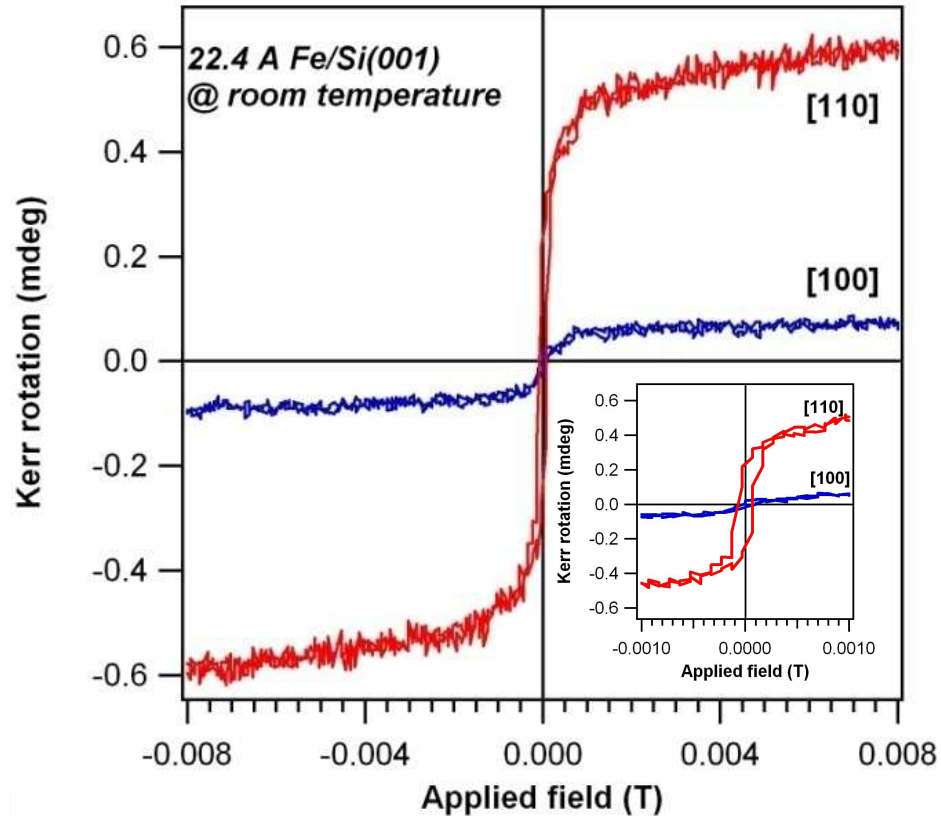


$$\chi(k) \equiv \frac{\mu(k) - \mu_0(k)}{\mu_0(k)} = \sum_j \frac{N_j}{kR_j^2} |f_j(\pi, k)|^2 \exp(-2\sigma_j^2 k^2) \exp(-R_j / \lambda(k)) \times \sin[2kR_j + \phi_j(k) + \delta_1'(k)]$$

$$k = \sqrt{\frac{2m(h\nu - E_0)}{\hbar^2}}$$

Result #2: Growth of Fe on Si(001) (VI)

Magneto-optical Kerr effect (MOKE)



- formation of (ferromagnetic) iron silicide;
- disordered Fe films show enhanced magnetism;
- disordered Fe films show uniaxial anisotropy;
- magnetism \uparrow when reactivity \downarrow .

After four months of operation of the MBE-STM-SARPES system:

Submitted/accepted papers:

1. M. Verziu, J. El Haskouri, D. Beltran, P. Amoros, D. Macovei, N.G. Gheorghe, C.M. Teodorescu, S.M. Coman, V. I. Parvulescu, *Mesoporous Tin-Triflate Based Catalysts for Transesterification of Sunflower Oil*, **Topics in Catalysis**, accepted (2009);
2. Ionel Stavarache, Ana-Maria Lepadatu, Nicoleta G. Gheorghe, Marius A. Husanu, George Stan, Dan Marcov, Adrian Slav, Gheorghe Iordache, Tionica F. Stoica, Vladimir Iancu, Valentin S. Teodorescu, Cristian M. Teodorescu, Magdalena Lidia Ciurea, *Structural investigations of Ge nanodots embedded in SiO₂*, **J. Nanopart. Res.**, submitted (2009);
3. Andrei N. Parvulescu, Davide Mores, Eli Stavitski, Cristian M. Teodorescu, Pieter C.A. Bruijninx, Robertus J.M. Klein Gebbink and Bert M. Weckhuysen, *Chemical Imaging of Catalyst Deactivation during Biomass Conversion Processes: The Etherification of Biomass-based Alcohols with Alkenes over H-Beta Zeolites*, **J. Am. Chem. Soc.**, submitted (2010);
4. P. Palade, G.A. Lungu, Thermodynamic destabilization of Li-N-H system by Si addition, **J. Alloys Compds.**, almost accepted (2010);
5. N.G. Gheorghe, G.A. Lungu, M.A. Husanu, *Successful cleaning and study of contamination of Si(001) in ultrahigh vacuum*, **Rom. Rep. Phys.**, submitted (2010).

+ Other 5 papers in work: own results on Fe/Si(001) plus four in collaboration with V.I. Pârvulescu, G. Filoti, A.C. Gâlcă, G. Stan

Team composition:

Dan Macovei, S.R. I

Cristian-Mihail Teodorescu, S.R. I

Marius-Adrian Husanu, Researcher

George-Adrian Lungu, A.R.

Nicoleta Gheorghe, A.R.

Eugenia Holdean, T I

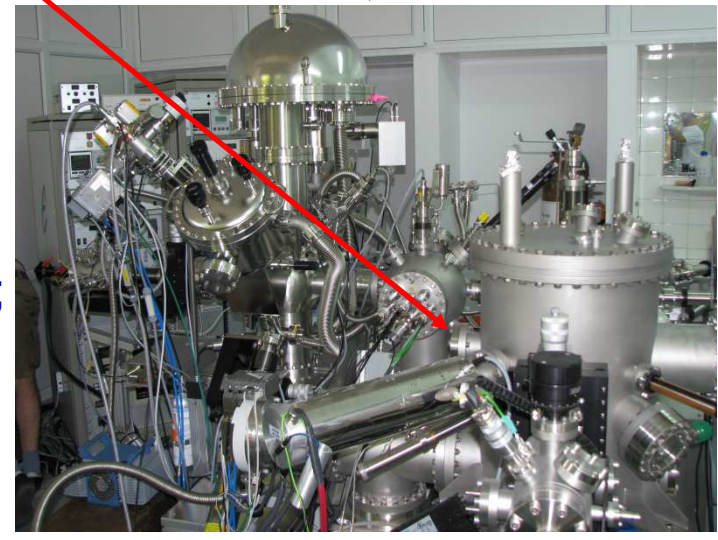
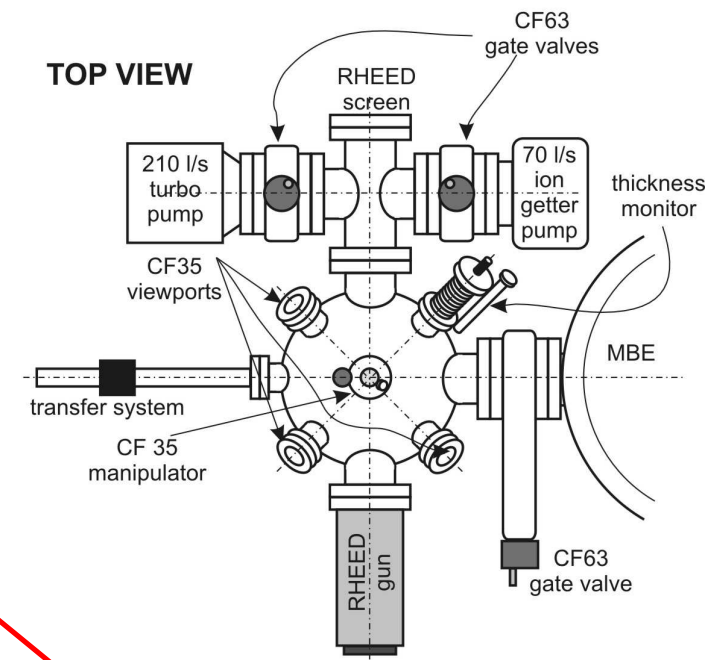
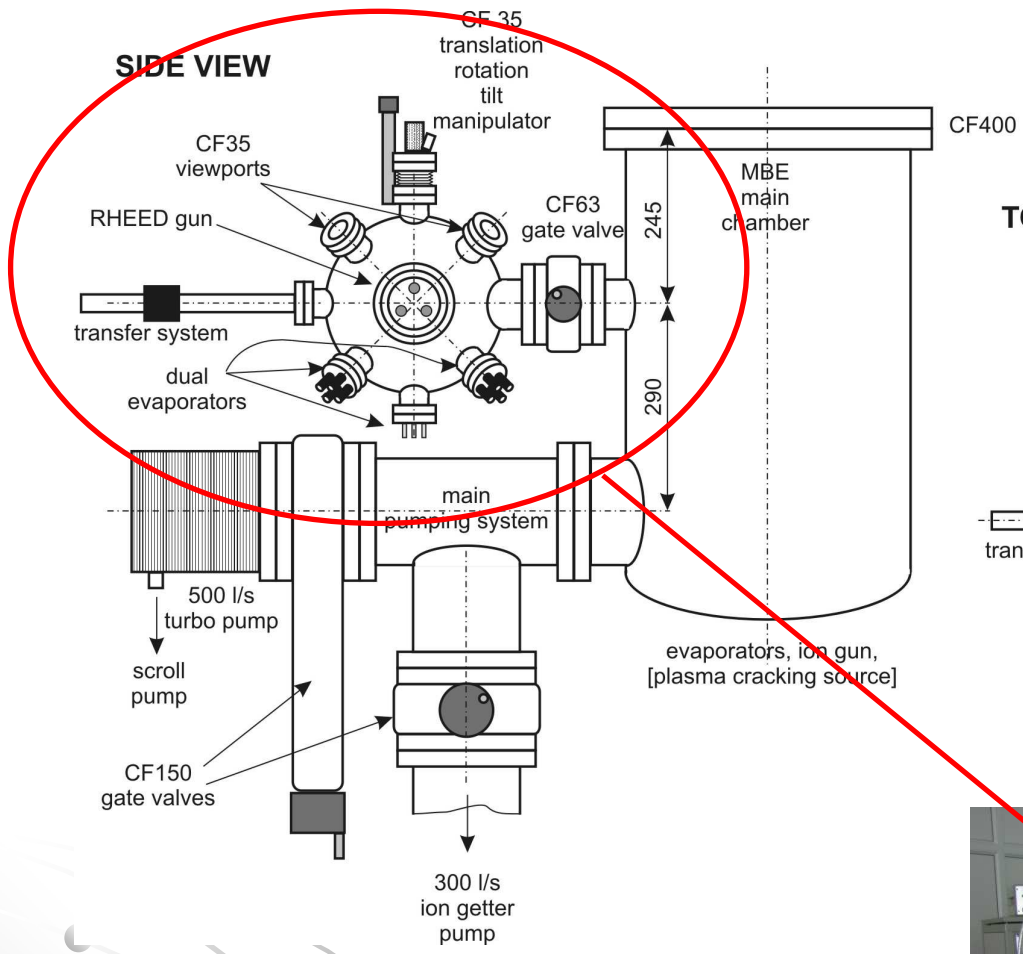
Doina Vântur, T II

Adi Segal, student, T II part time

+ Ruxandra Costescu , will be hired as S.R. III from March 2010

→ setup of a reintegration grant (RP)

1. Setup of an MBE annex for III-V semiconductors.
 2. Theoretical studies of (a) indirect exchange mediated by a 2DEG;
(b) transport coefficient and Wiedemann-Franz law in two dimensions.
 3. Synthesis of III-V systems.
 4. Synthesis of metals/III-V systems.
 5. Synthesis of 2DEG heterostructures doped with magnetic ions.
 6. Synthesis of "rolled-up nanotubes".
 7. Thermal conduction properties by time-domain thermoreflectance measurements.
- 10 papers intended



Total price of the setup: Eur 50,000

- 5 evaporators (Ga, In, As, Al, 3d metals);
- thickness monitor;
- heating evaporator;
- possibly a RHEED.

Other research foreseen in 2010:

(1) Completing the work on Fe/Si(001):

- spin-resolved photoemission: high impact research;
 - high resolution XPS;
 - photoelectron diffraction on Fe/Si(001) (Fe and Si core levels).
- direct comparison between EXAFS and photoelectron diffraction (never done).

(2) Mn/Si(001) and (3) Mn/Ge(001):

- Auger electron spectroscopy, LEED, RHEED, MOKE, EXAFS, XANES;
- spin-resolved PES;
- high-resolution XPS. Etc.

7-9 papers intended



Vă mulțumesc!