Electronic Structure of Fe Atomic Chains on a Pt(997) Surface

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Outline

UHV setup

STM and LEED

Research applications

Fe nanowires on Pt templates

Fe nanoparticles on Silicon
(by high pressure sputtering)

Conclusions
The UHV chamber: $10^{-10}$ Torr

![Diagram of UHV chamber components]

- **Load manipulator**
- **LEED**
- **Sample manipulator**
- **Load block**
- **Main chamber**
- **STM**
- **Mech Pump**
- **Turbo Pump**
- **Ion Pump**
The UHV chamber: $10^{-10}$ Torr
LEED (check substrate quality)
STM
Omicron STM

- Computer controlled
- Sensitive Pt-Ir tip
- 0.1 nm resolution
- Can be used as STS (scanning tunneling spectroscopy)
UHV setup steps

Fully installed and functional at $10^{-10}$ Torr

1. Main chamber + load block
2. STM
3. LEED
4. Vertical manipulator
5. Load manipulator
UHV baking process

1. Mechanical pump >1h (mTorr)
2. Turbo pump >4h then check ion gauge (μTorr)
3. Pressure down to 10^-7-10^-8 Torr in about 2 days
4. Bake for two days (80°-120°C) and cool down
5. Run the TSP (titanium sublimation pump) to clean the ion filament
6. Ready at 10^-10 Torr!
Samples: Pt (997) substrates for Fe deposition

Motivation

- Pt (997) can be used as an efficient, low cost template for bottom-up fabrication of nanostructures.
- One-dimensional atomic chains can be used as nanowires for electronics applications.
Samples: Pt (997) substrates for Fe deposition

1. Start with Pt(997) substrates (a stepped surface that can be kept clean for a few minutes under UHV).

2. Anneal at 900°C and use oxygen to remove surface carbon.

3. Sputter with Ar gas and anneal again.

4. Use LEED to check surface quality.

5. Do STM and photoemission spectroscopy.

6. Deposit Fe by molecular beam epitaxy (MBE).

7. Do STM and photoemission spectroscopy.
The stepped Pt(997) surface is cut at $6.5^\circ$ from the (111) surface.
LEED pattern (148eV) of clean Pt(997) surface
STM image of the clean Pt(997) surface
STM image of Fe atomic chains on Pt(997)
Angular resolved photoemission spectrum of Pt(997) surface

Ayieta et al. (JVST, 2007)
Angular resolved photoemission spectrum of Fe atomic chains on Pt(997) surface
Photoemission Process

\[ E_{\text{kin}} = \hbar \omega - E_B - \Phi \]

\[ E_{\text{kin}} = \hbar \omega - \Phi \]

for \( E_B = 0 \)
Other measurements

1. Energy distribution curves and band structures

2. Hysteresis loop and magnetization vs. Fe coverage (ML)

3. Characterization of Fe nanoparticles from high pressure sputtering (Material Letters, 2008)
EDC and Band Structure for 70eV
Band Structure of Clean Pt(997) for 70eV
Hysteresis Loop and Magnetization vs. Fe coverage (ML)
Characterization of Fe nanoparticles from high pressure sputtering
Sputtering chamber

- Operates at $10^{-3}$ Torr
- Plasma deposition (makes highly uniform films)
- 4 sputtering guns which can deposit nanoparticles
AFM Images of Fe nanoparticles on Silicon (at IUPUI, Decca’s Lab)
Gun pressure calibration

![Graph showing gun pressure vs. particle size. The x-axis represents particle size in nanometers (nm), ranging from 0 to 3000, and the y-axis represents gun pressure in mTorr, ranging from 0 to 120. Data points are represented as green diamonds.](image-url)
X-ray scattering from Fe nanoparticles
(at IUPUI, Swope’s Lab)
TEM of Fe nanoparticles on Si wafer (at Argonne, IL)
Conclusions

• Vaccum chamber instrumentation has been successfully set up and used for manufacturing of Fe nanowires and nanoparticles.

• STM and LEED reveal the stepped structure of Pt(997) and that Fe atomic chains are formed along step edges.

• 3d-5d hybridization in Fe-Pt interact and exchange splitting as observed in double peaks in photoemission data.
Conclusions

- Fe nanoparticles were created using a high pressure magnetron technique.
- X-ray diffraction shows that the Fe nanoparticles adopt a body centered cubic structure.
- HRTEM shows that an iron oxide layer covered the Fe cores and forms a core shell structure.
- AFM image give average size of samples created under different pressures.
Acknowledgments

Lab members:
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Dr. Ricardo Decca, Merrell Johnson (AFM)
Dr. Jeff Swope (X-ray)

CAMD, Louisiana State Univ:
Dr. Yaroslav Losovyj (Photoemission spectroscopy)
Hysteresis Loop and Magnetization Vs Fe coverage (ML)
Interaction between Pt(997) and Fe atoms

**Fe:** 1s\(^2\) 2s\(^2\) 2p\(^6\) 3s\(^2\) 3p\(^6\) 4s\(^2\) 3d\(^6\)

**Pt:** 1s\(^2\) 2s\(^2\) 2p\(^6\) 3s\(^2\) 3p\(^6\) 3d\(^{10}\) 4s\(^2\) 4p\(^6\) 4d\(^{10}\) 4f\(^{14}\) 5s\(^2\) 5p\(^6\) 5d\(^9\) 6s\(^1\)
Sputtering chamber
SPUTTERING CHAMBER
Expansion of free Energy of V.S.

\[ f(\theta) = f(0) + \frac{b(d)}{d} = f(0) + b(d) \frac{\tan \theta}{h} \]

\[ f(\theta) = F.E.V.S. \]

\[ b(d) = \beta + g(d) \]

\[ f(0) = F.E.L.I \]
Dependence of $g$ on $d$

\[ g(d) \rightarrow d^{-2} \]

\[ g(d) \rightarrow d^{-3} \]
Kinetic Energy of a Free Particle

\[ E = \frac{\hbar^2 \kappa^2}{2m} \quad \text{and} \quad E = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \]

\[ \kappa_\parallel = \sqrt{\left(\frac{2mE}{\hbar^2}\right)} \sin \theta \quad \text{and} \quad \kappa_\perp = \sqrt{\left(\frac{2mE}{\hbar^2}\right)} \cos \theta \]
EQT: Intensity and Free path

\[ I_z = I_0 e^{-\frac{z}{\lambda \cos \theta}} \rightarrow \text{Beer – Lambert's} \]

\[ \hbar \omega = E_{kin} + \Phi + |E_B| \]

\[ P_{||} = \hbar k_{||} = \sqrt{2m_e E_{kin}} \sin \theta \]

\[ P_{\perp} = \hbar k = \sqrt{2m_e E_{kin}} \cos \theta \]
Probability of transition

\[ w_{fi} \alpha \frac{2\pi}{\hbar} |\langle f \mid H'_{\text{int}} \mid i\rangle|^2 \partial(E_f - E_i - \hbar \omega) \]

\[ H'_{\text{int}} \equiv \frac{e}{2m} (A \bullet P_{op} + P_{op} \bullet A) \equiv -\frac{e}{m} A \bullet P_{op} \]

\[ I(E, \hbar \omega) \alpha \sum_{i, f, G} |M_{fi}|^2 \partial(E_f - E_i - \hbar \omega) \partial(k_f - k_i - G) \]

\[ |M_{fi}|^2 \alpha |A \bullet \langle f \mid P_{op} \mid i\rangle|^2 \]
Binding Energy Versus K Parallel Vector
Energy Distribution Curve (EDC)
EDC and Band Structure for 40eV
EDC and Band Structure for 70eV
EDC and Band Structure for 60eV
Derivative Band for 70eV
Derivative Band 60eV

\[
E - E_F (\text{eV}) \quad K (\text{Å}^{-1})
\]
Derivative Band for 40eV
Derivative Band for 21.5eV
Hysteresis Loop and Magnetization Vs Fe coverage (ML)
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Gun Pressure vs Size

![Graph showing the relationship between gun pressure (mTorr) and particle size (nm).]
Sample Angle $2\theta$ vs Intensity

Fe bcc (11)
Fe bcc (20)
Fe bcc (21)
Si (400)
Conclusion

• Iron nanoparticles were created using a high pressure magnetron technique
• X-ray diffraction shows that the nanoparticles created adopt a body centered cubic structure
• HRTEM showed that an iron oxide layer covered the Fe cores and forms a core shell structure.
• AFM image give average size of samples created under different
The Load Block and Manipulator
Sputtering Power Source, TSP and Ion Gauge
Manipulator and Sample Holder
Ceramic Sample Holder
Main conclusions

1. Fe atomic chains are good because
2. Growing Fe chains on Pt is excellent because
3. The method of surface analysis works or not
4. We learn the following interesting physics:
The UHVchamber, LEED unit