Surface Modification of CaF$_2$

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Outline

- Introduction
- Background
  - Molecular Beam Epitaxy
  - Apparatus
  - Analysis
- CaF₂
  - Electron Irradiation
  - As Termination
Introduction

- What is Epitaxy/Epitaxial Growth?
  - The growth of one Crystal on another
- GaSe, AlSe, GaAs, TiO₂, CaF₂ on Si

- Various factors:
  - Lattice Match
  - Interface Chemistry
  - Surface Energy
Molecular Beam Epitaxy
The Chamber

Setup:

- Cryopump
- Growth
- Transfer Arm
- Crystal Monitor
- Evaporation cell
- Analysis
- LEED
- XPS/XPD
- UPS

• Growth Control —
  • Substrate Temp, $T_{\text{sub}}$
  • Cell flux, Cell Temp.
  • Growth time

• Analysis —
  • LEED
  • XPS/XPD
  • UPS

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The Chamber

- Growth Chamber
- Crystal Monitor
- Evaporation Cell
- UPS
- Analyzer
- XPS/XPD
- LEED
- Main Chamber
XPS

- Incident photons transfer energy to $e^-$ in the crystal
- Photo-electron energies are scanned

\[ KE(e^-) = h\nu - BE - \phi_{\text{inner}} \]
XPS

![XPS Graph]

- Ca LMM (Auger)
- F KVV (Auger)
- Ca 2s
- Ca 2p
- Shallow Cores
- Si 2p
- Si 2s

Photoemission Intensity vs. Binding Energy (eV)
Why $\text{CaF}_2$?

- Ionic Crystal
- Insulator with a great lattice match to Si (0.6% mismatch)
- Quantum wells, Confinement
Surface of CaF$_2$

- Stable in UHV
- No surface reconstruction
- F$^-$ termination is problematic
- Murphy’s Law of Epitaxy
  - “If A grows well on B, then B doesn’t grow well on A”
  - $\sigma$ (Si) $> 300\%\ \sigma$ (CaF$_2$)
e\textsuperscript{-} of at least $\sim 40$ eV are “shot” at the sample
**Knotek-Feibelman**

- $e^-$ of at least $\sim 40$ eV are "shot" at the sample
- A hole is created in the Ca 3p band
Knotek-Feibelman

- e⁻ of at least ~40 eV are “shot” at the sample
- A hole is created in the Ca 3p band
- An e⁻ from the F 2p decays into the hole
- e\(^{-}\) of at least \(\sim 40\text{eV}\) are “shot” at the sample
- A hole is created in the Ca 3p band
- An e\(^{-}\) from the F 2p decays into the hole
- An Auger e\(^{-}\) is ejected, leaving the F ion with a net 1+ charge
Post Irradiation
Surface of CaF$_2$ (post irradiation)

- Ca metal and CaF
- Very Reactive with residual gases in Chamber

Passivate Surface: As
The Question

- As works to passivate the surface
- Only sticks to Irradiated Surface
- Where is the As?
  - Surface, only 1/3 ML?
  - Diffused into Crystal?
Irradiation with As

![Graph showing photoemission intensity vs. binding energy (eV) with peaks labeled Ca 3s, Ca 3p, As 3d, and F 2s.]
The Answer

- Irradiated CaF$_2$ allows for 1 ML of As to be deposited
- Annealing induces diffusion into the Crystal
- When Annealed in As, ML remains
Summary

- MBE allows for controllable growth of Thin CaF$_2$ Films
- XPS is a relatively fast way to analyze the composition of Thin Films
- ESD, while increasing the Surface energy, creates a highly reactive surface
- As for the As?
  - ML on surface diffuses down with annealing
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