Properties of Atomically Uniform Pb Films on Si

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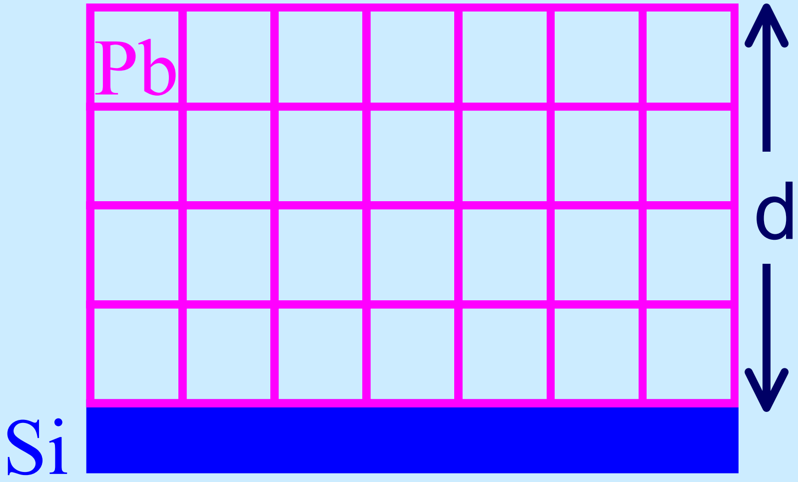
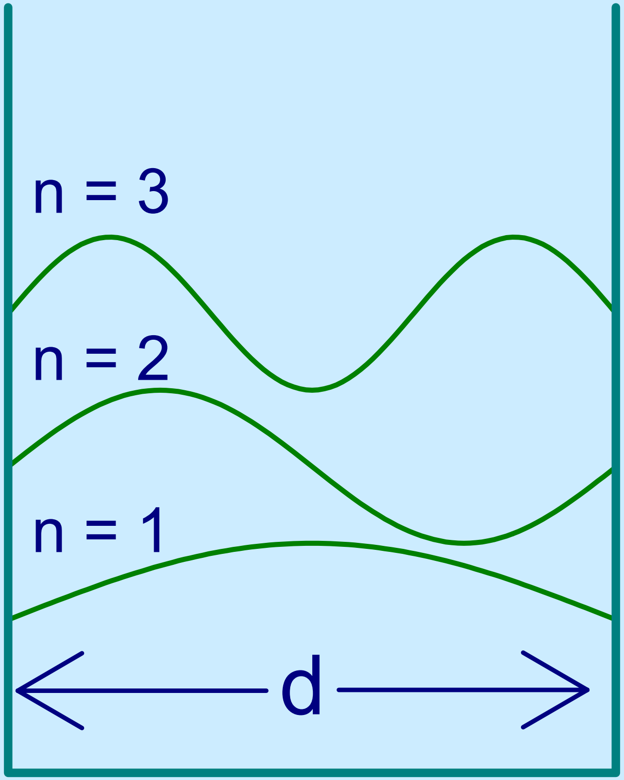
- Introduction
- Growth mode of Pb/Si(111)
- Bilayer Electronic Oscillations
- Dispersion in Pb/Si(111) films
- Thermal Stability of Pb/Si(111) films

Why Study Thin Films?

Physics reasons

- Confined systems
- Materials interaction, coupling
- Growth

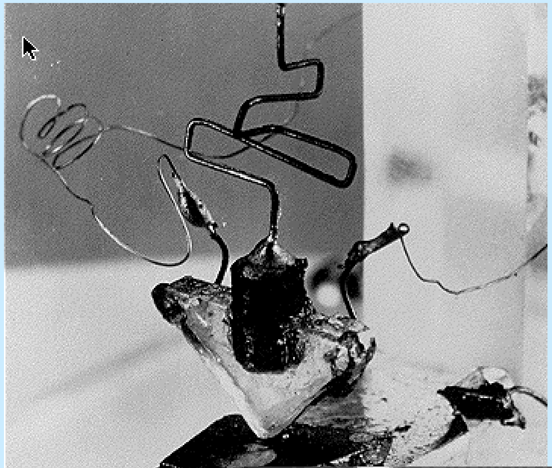




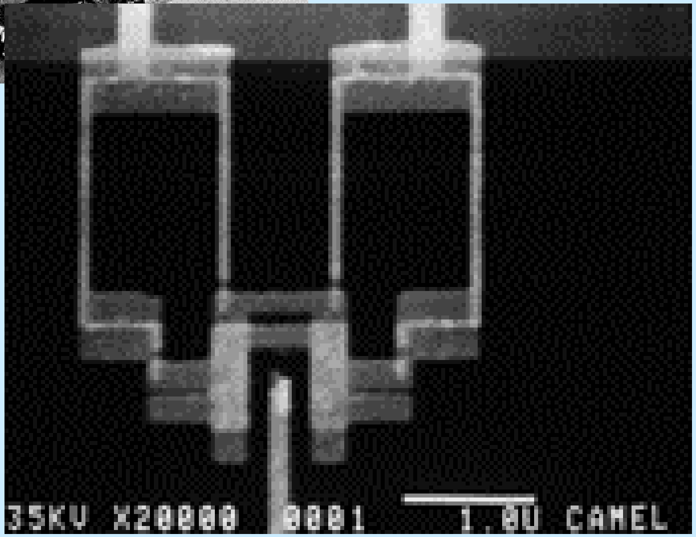
Why Study Thin Films?

Practical reasons

- What happens as electronics get smaller?
- Thermal stability



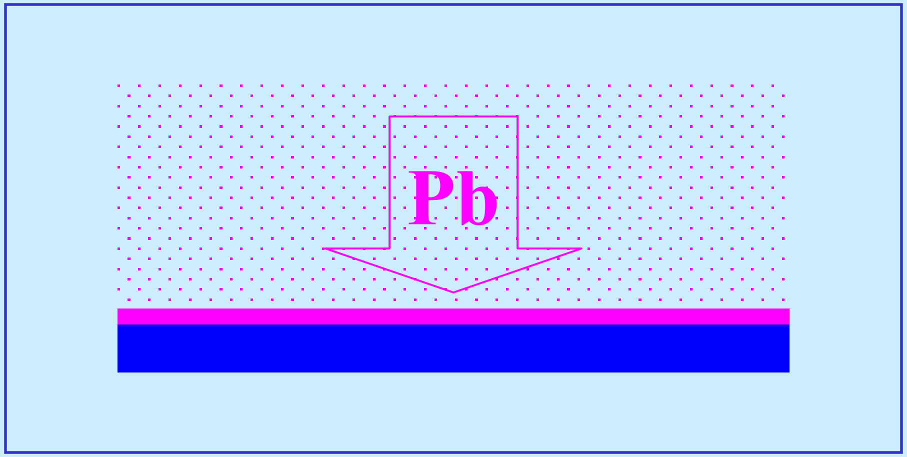
First transistor

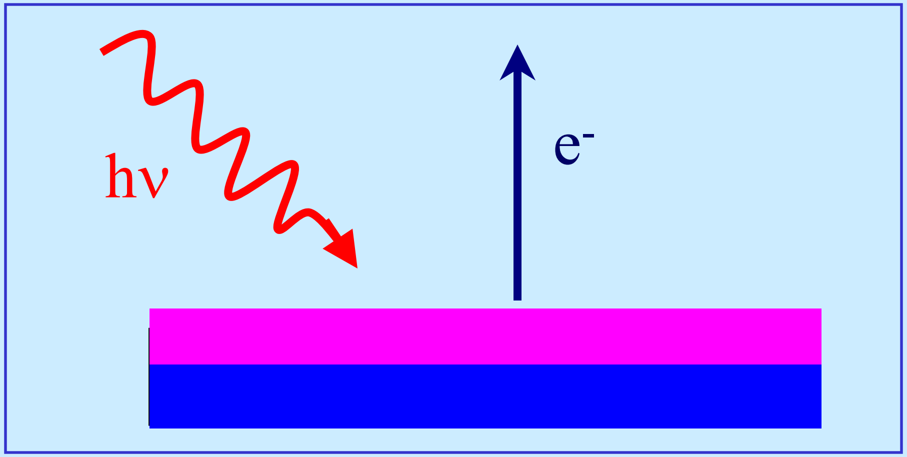


Newer transistor

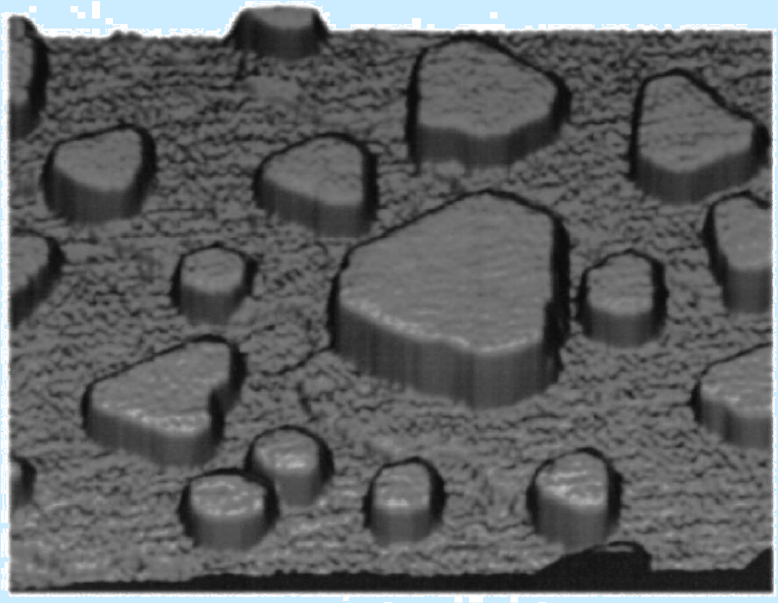
Our Experiment

1. Grow Pb films on 100 K Pb terminated Si with Molecular Beam Epitaxy (MBE).
2. Study sample with photoemission (photons in, electrons out)



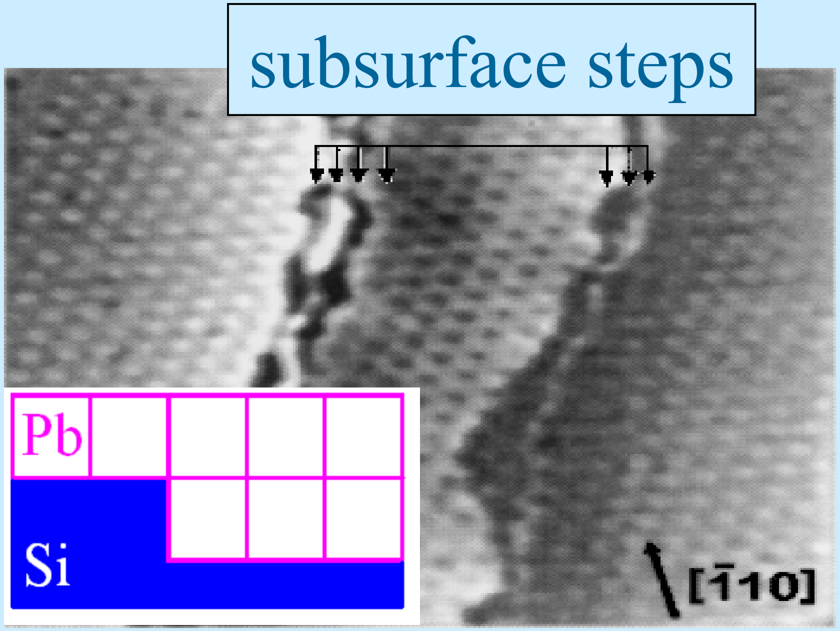


Pb/Si Previous Growth Work - STM



- 200 K growth
- Flat islands
- Preferred heights

Hupalo et al., PRB 2001



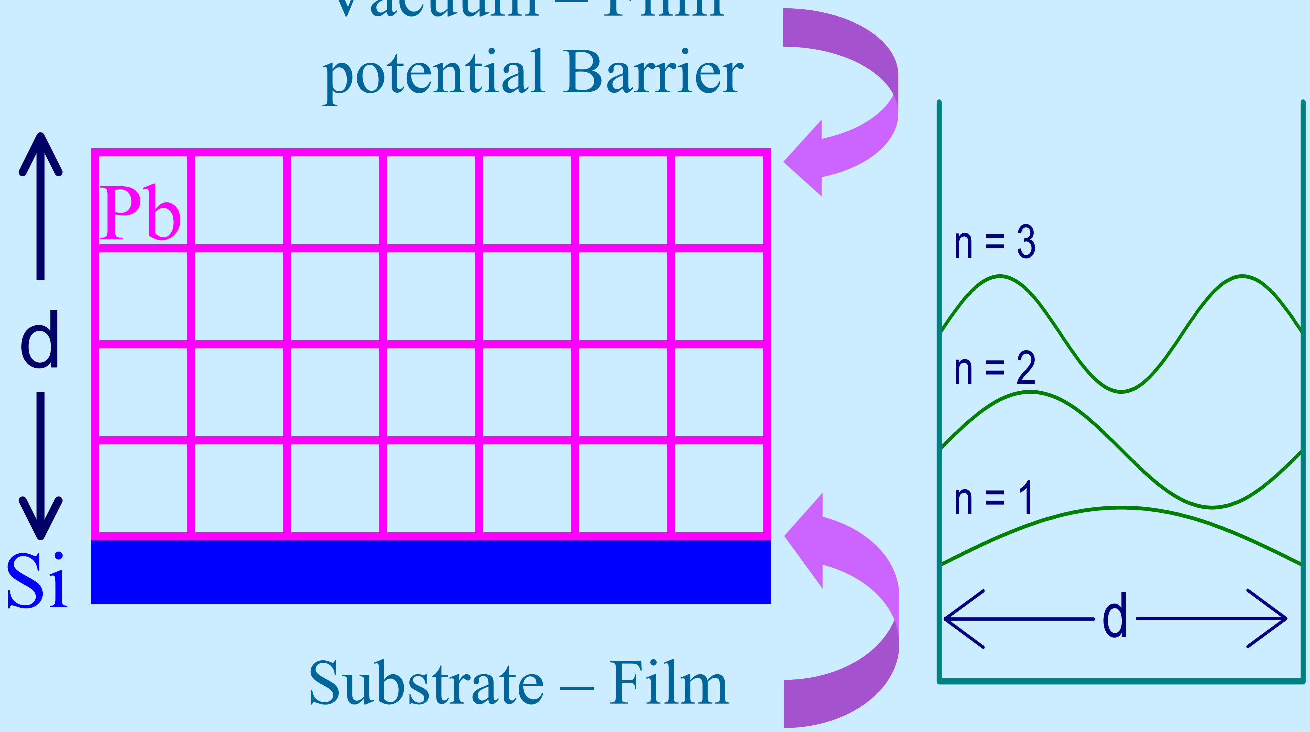
subsurface steps

- 77 K growth
- Flat surface islands (uneven substrate)

Altfeder, Narayanamurti, and Chen, PRL 2002

Quantum Well States

- Electron confined in film ⇒ Particle in a box states
- Need close to layer-by-layer growth to see states.

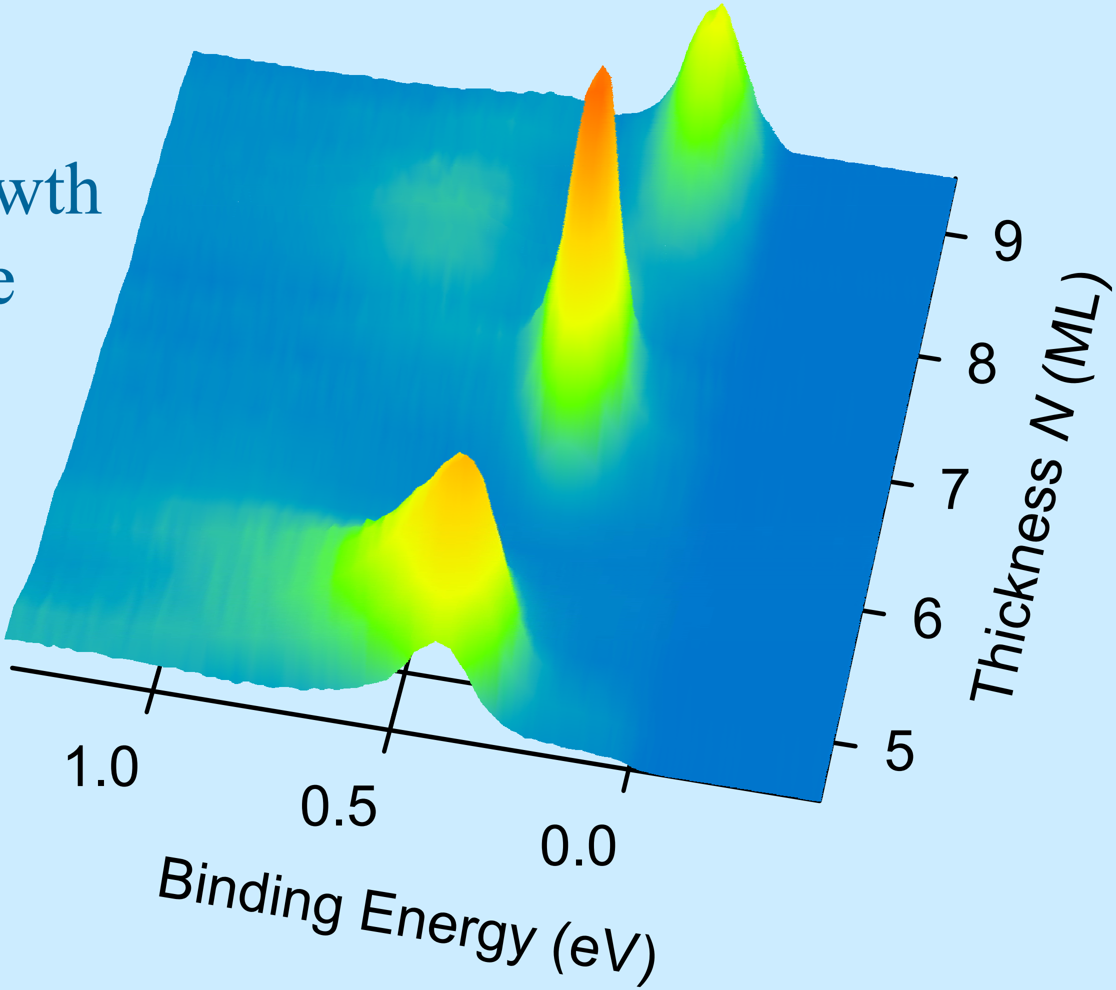


Vacuum – Film potential Barrier

Substrate – Film potential Barrier

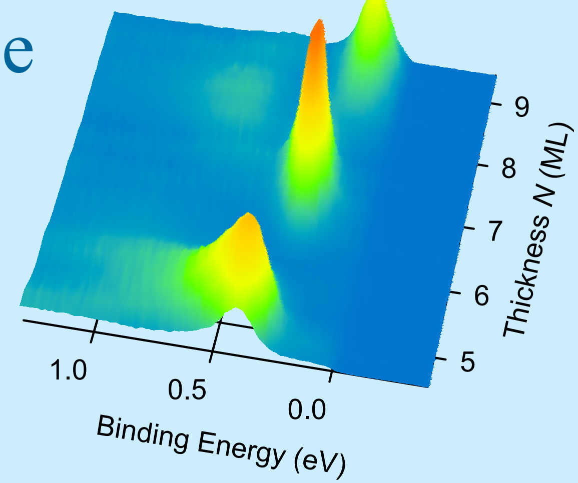
Pb/Si Layer by Layer Growth

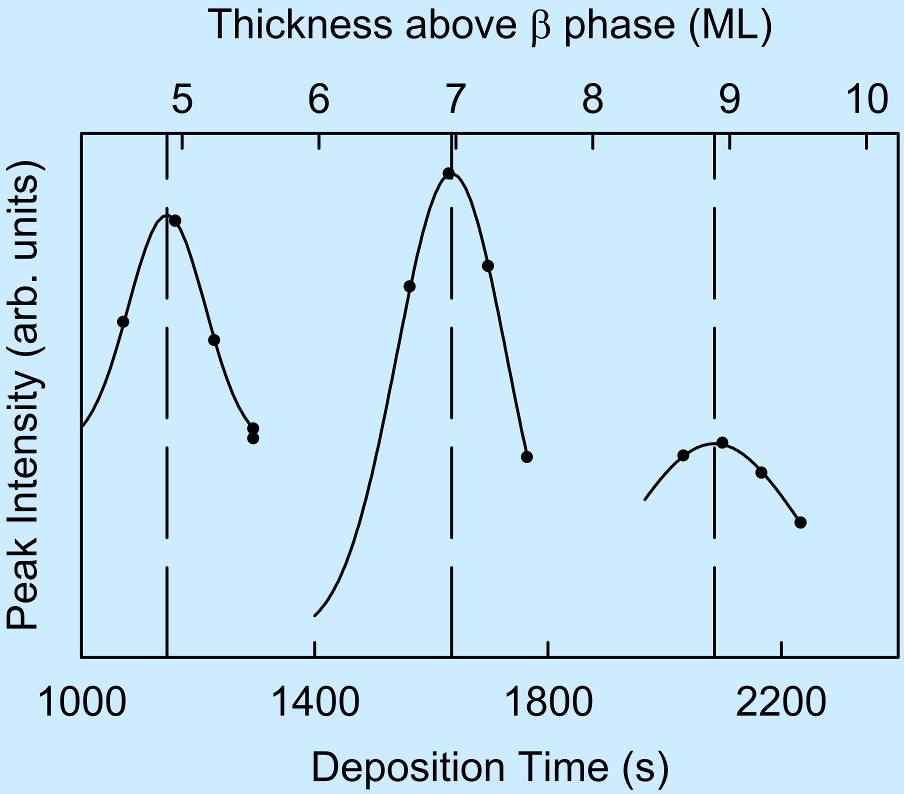
- Layer by layer growth despite large lattice mismatch
- Odd ML→sharp, intense peaks
  Even ML→broad shallow peaks



Film Thickness Determination

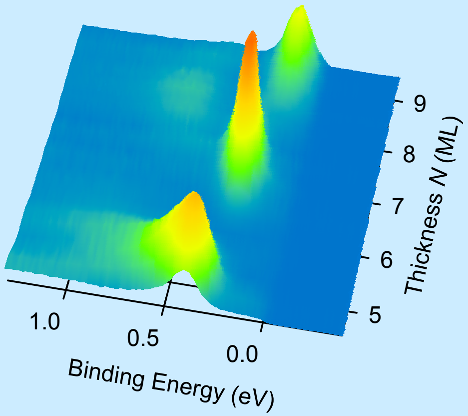
- Deposition time between 1st and 3rd major peak is 4 ML
- Seconds/ML gives total thickness of film
- Initial substrate α or β phase

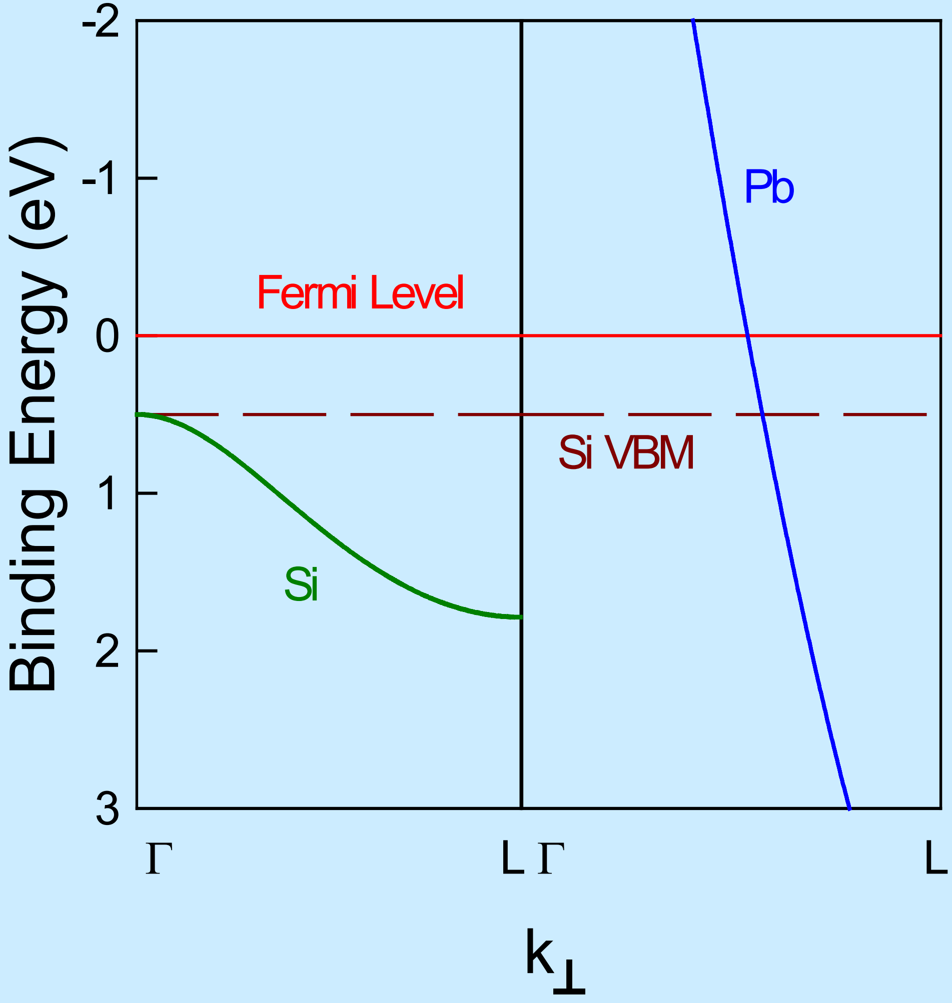




Quantum Well Confinement

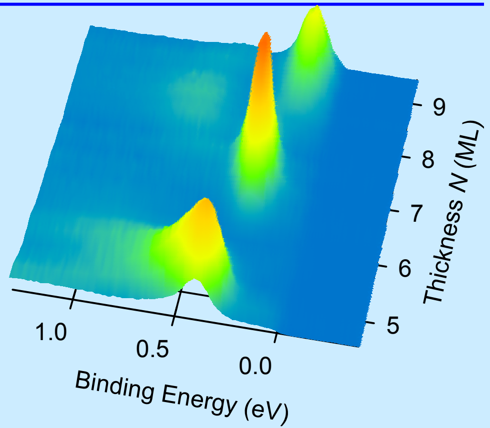
- Sharp peaks - Good confinement between Si VBM and Fermi Level
- Broad peaks - Partial confinement below Si VBM

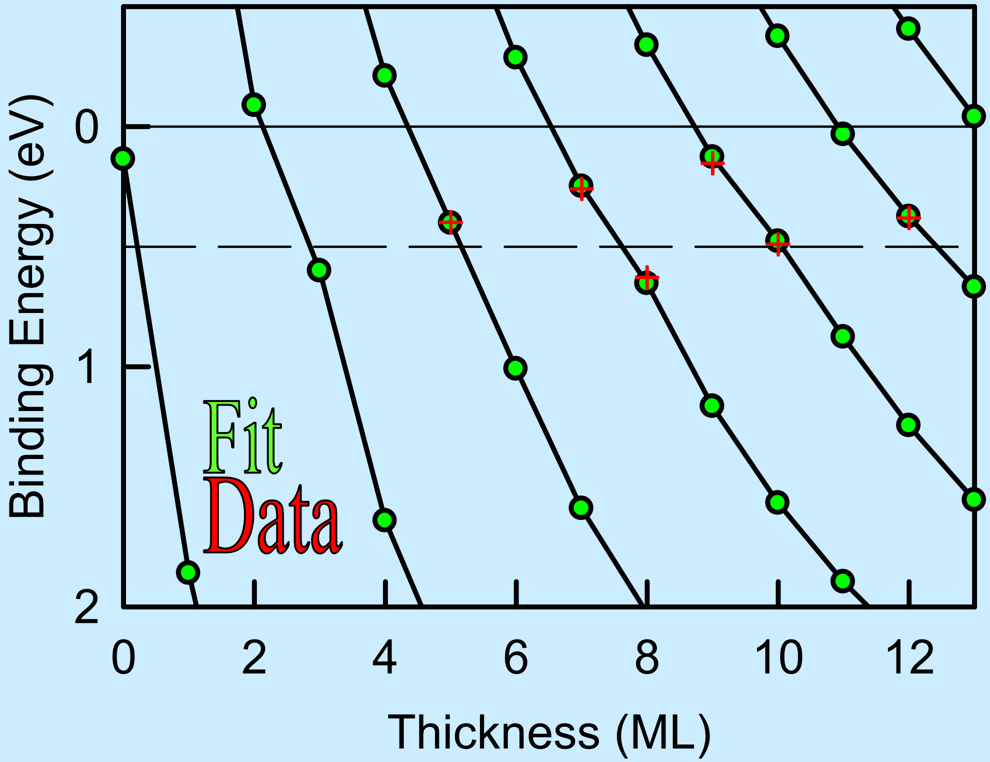




Film Electronic Structure

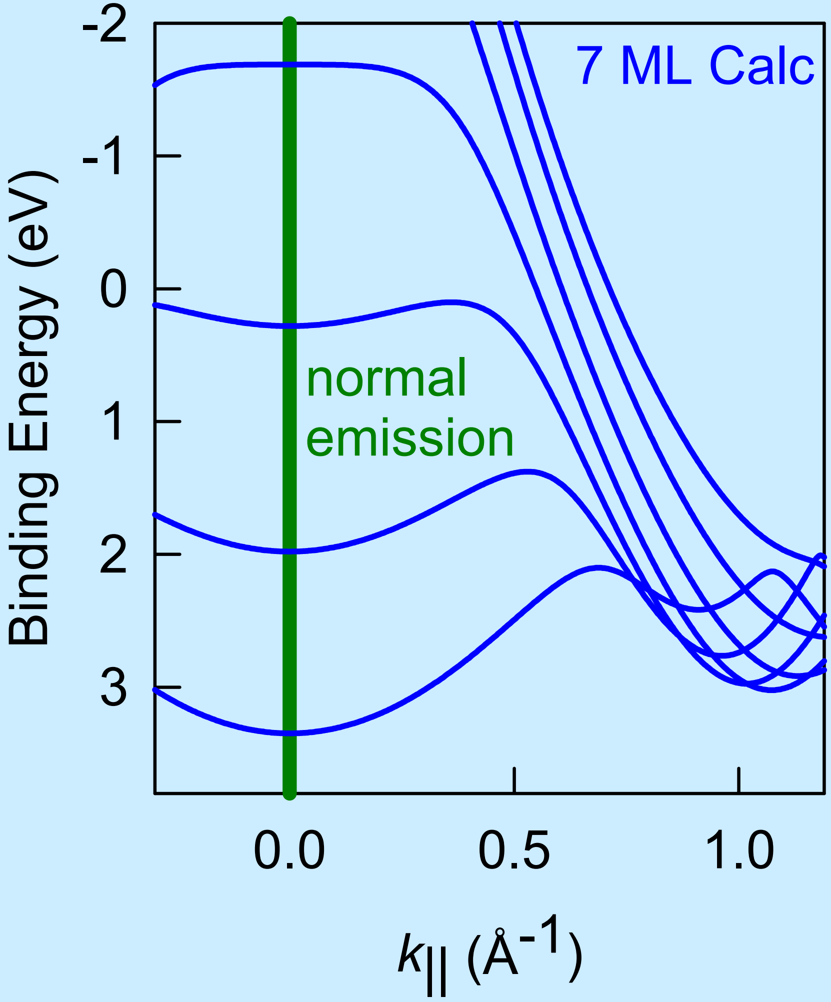
$$\underbrace{2k(E)d}_{\text{phase change in film}} + \underbrace{\phi_V(E)}_{\text{at vacuum}} + \underbrace{\phi_I(E)}_{\text{at interface}} = 2\pi n$$

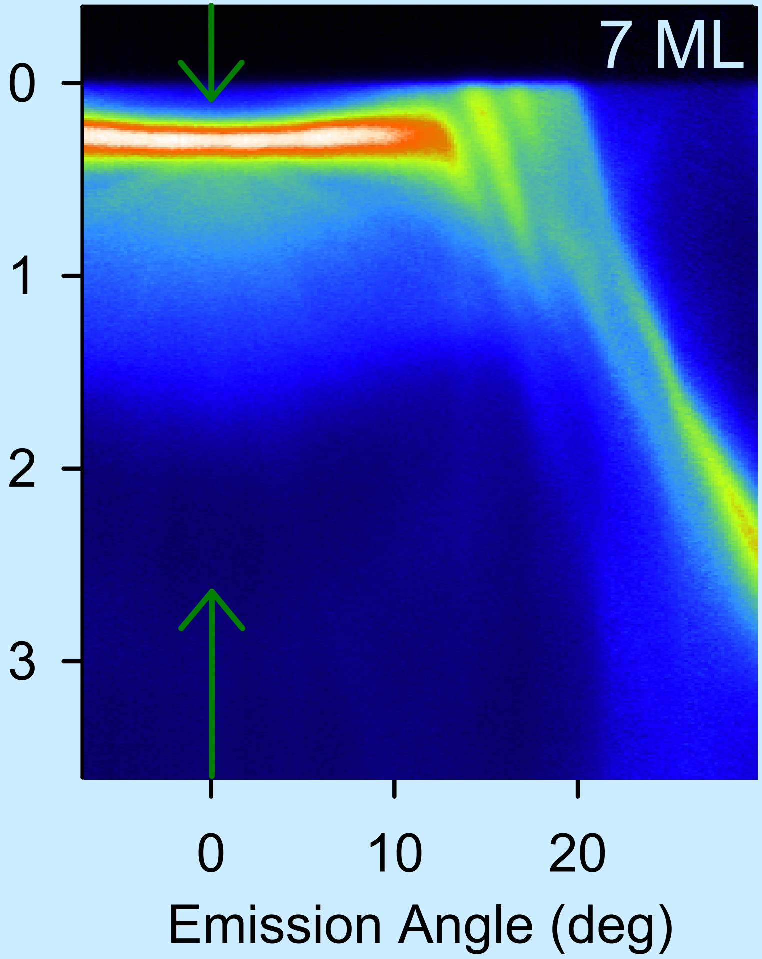




- Bohr-Sommerfeld model
- Theoretical form for boundary phase shifts
- One parameter fit

Off Normal Spectroscopy



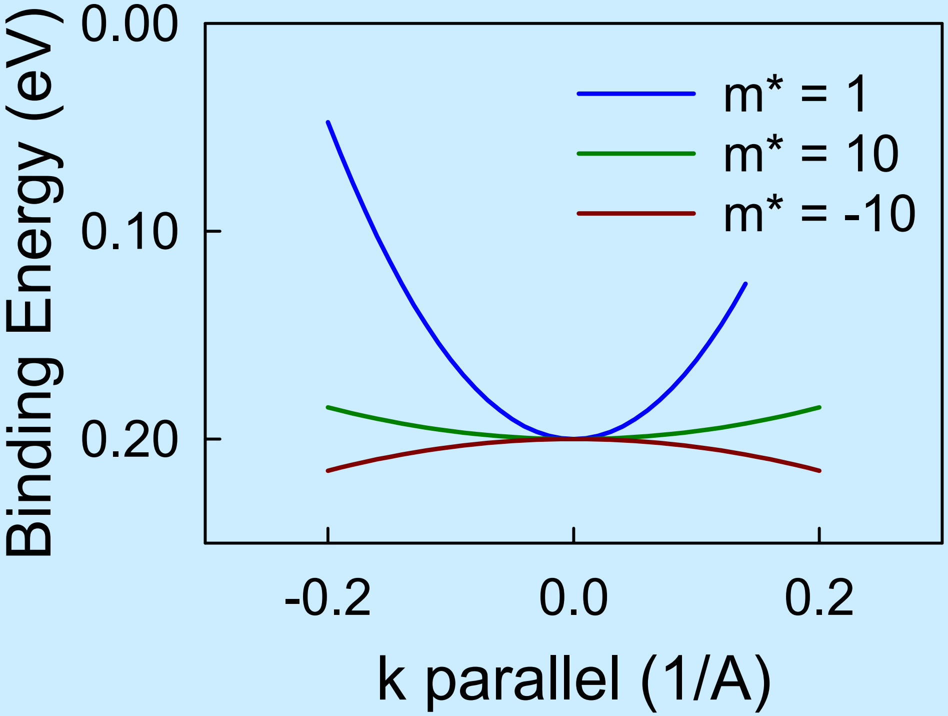


Effective Mass Refresher

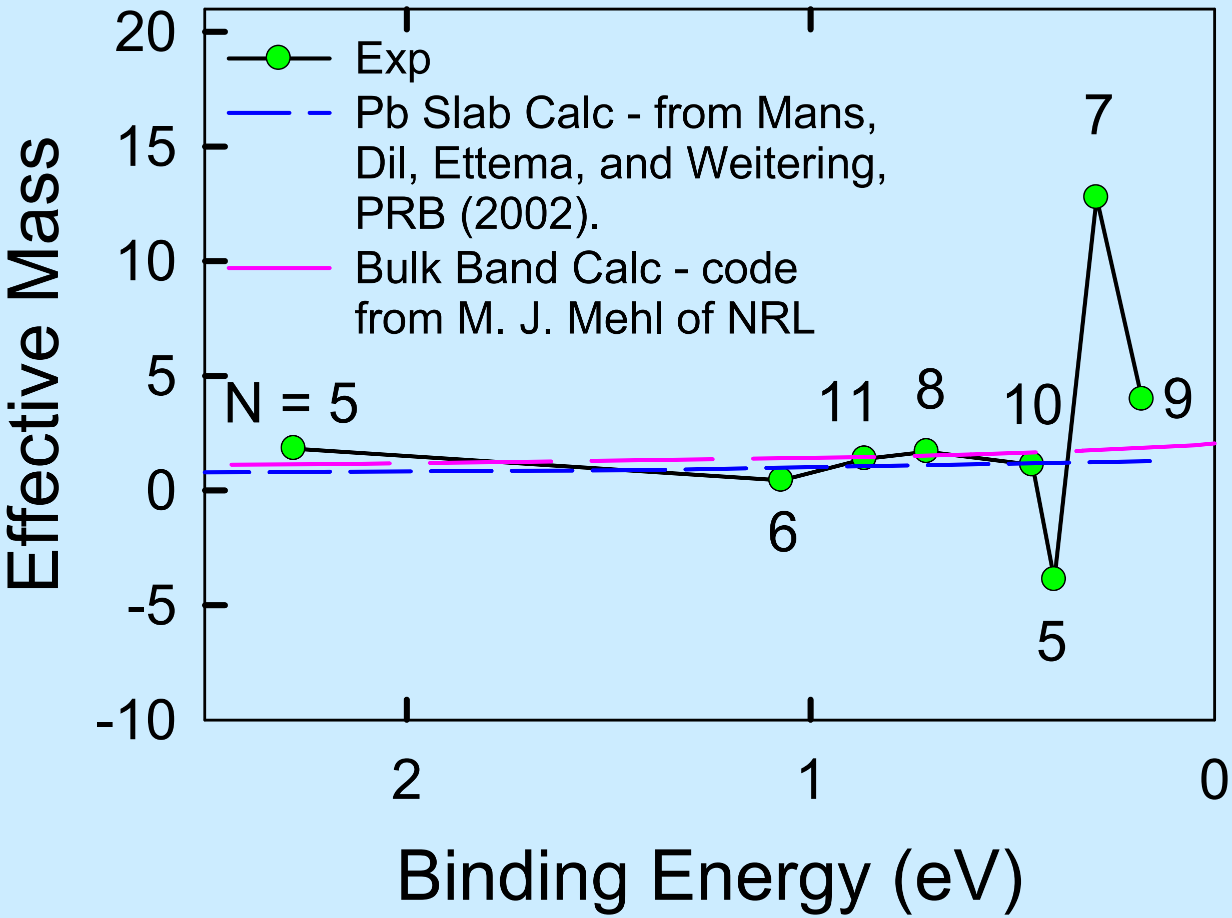
- Curvature of energy band near high symmetry direction

$$E \sim \frac{\hbar^2 k_{||}^2}{2m_e}\frac{1}{m^*}$$

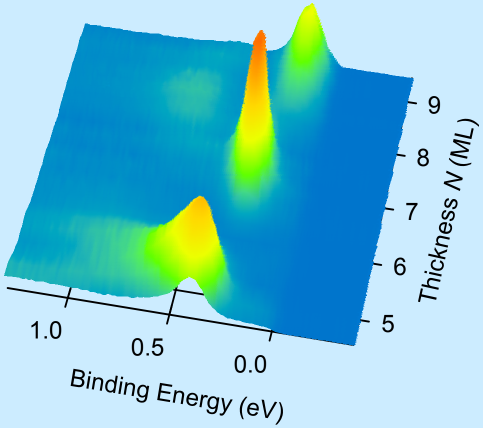
- Curved band ⇒ low m*
- Flat band ⇒ high m*



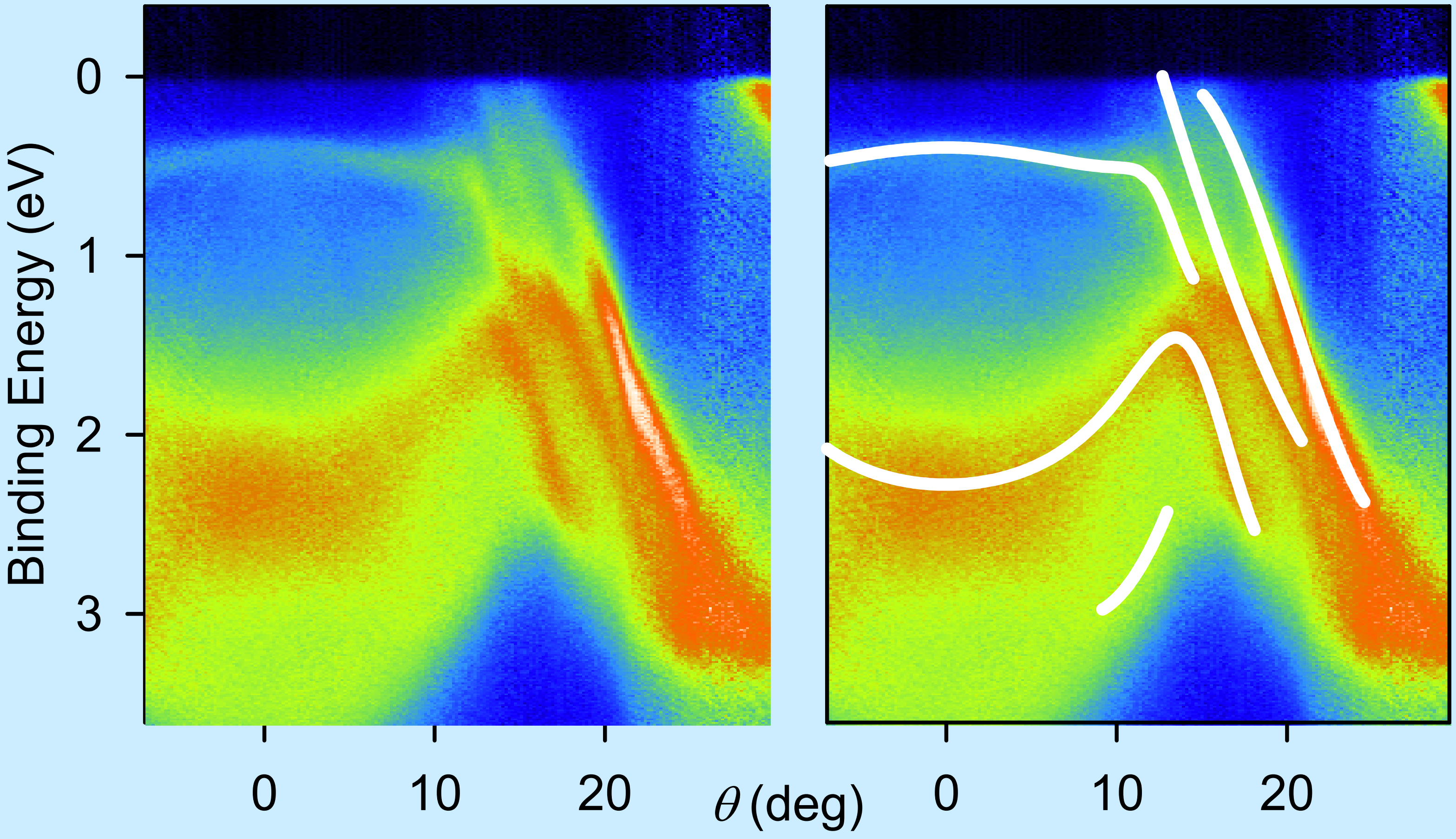
Effective Mass Measurements



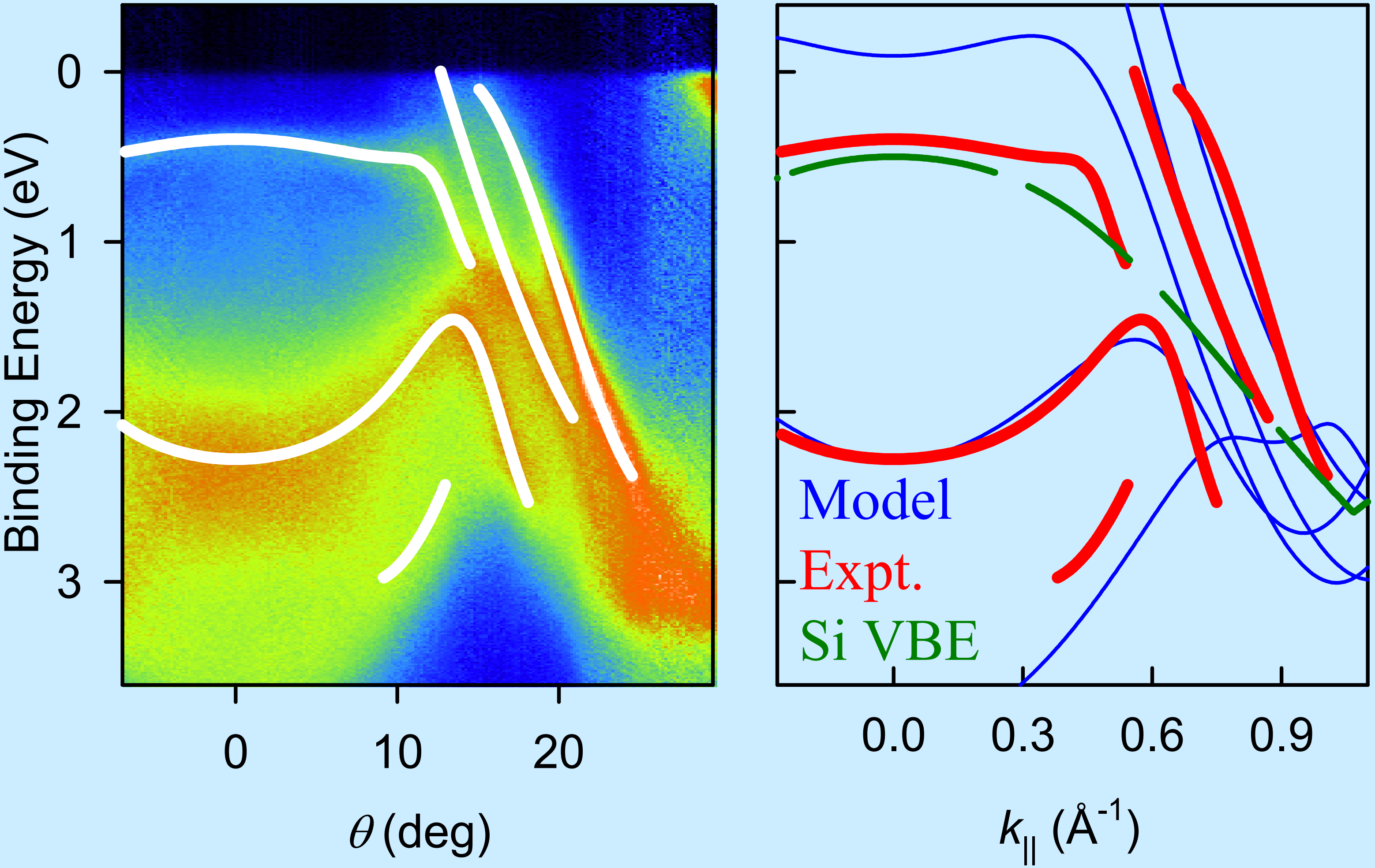
- Theory good at high BE
- Aberrant effective mass near Si VBM



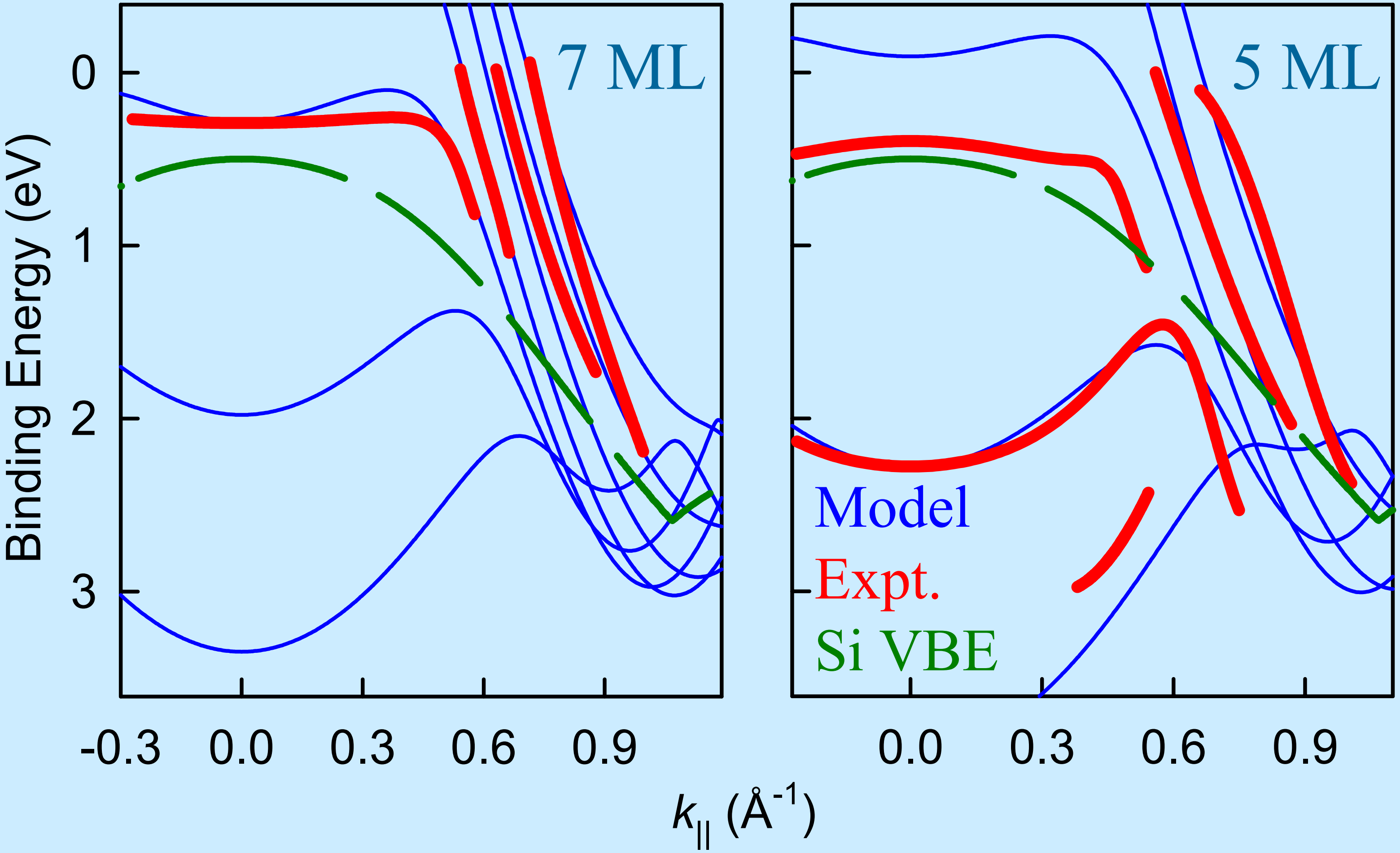
Dispersion Measurement – 5ML



Dispersion Measurement – 5ML

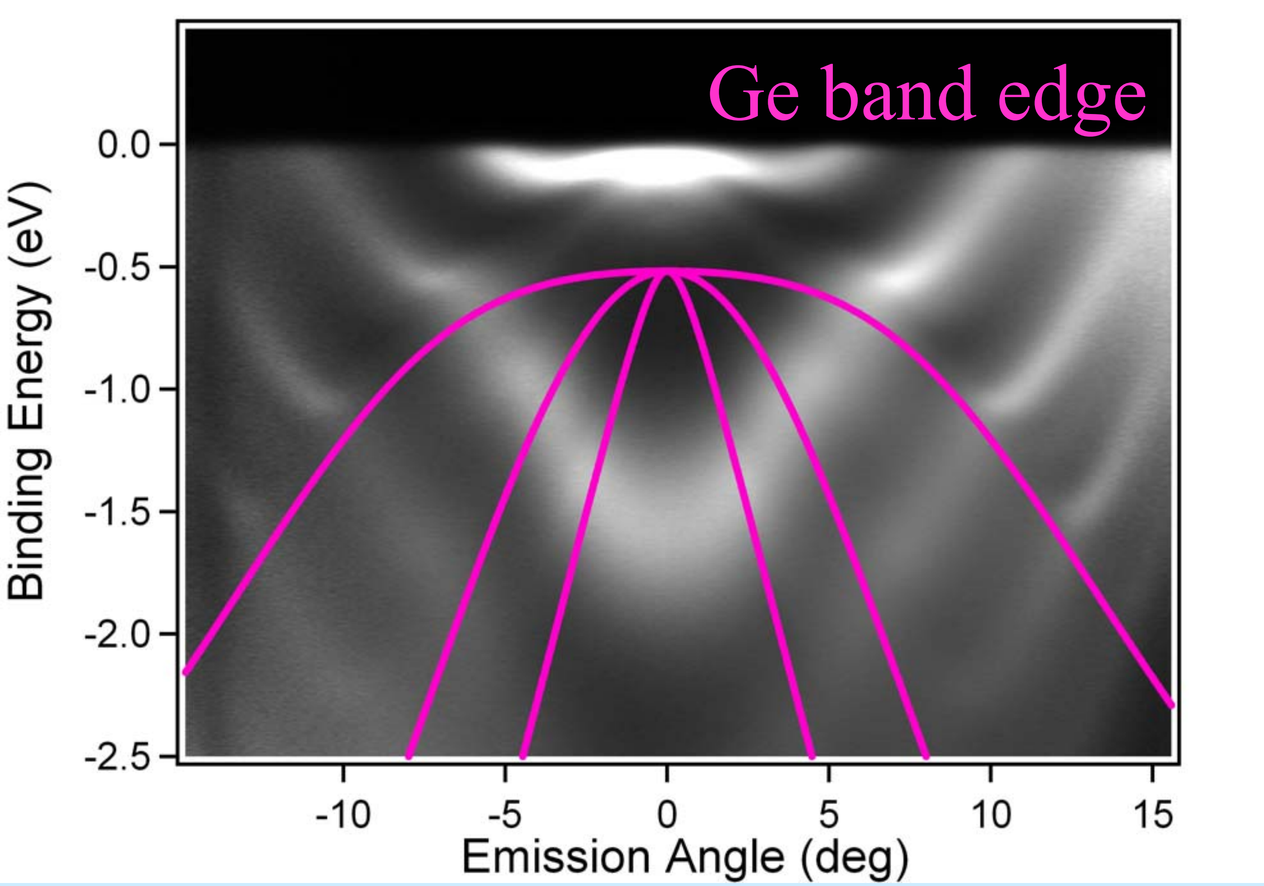


Si Band Edge Effect - Anticrossing

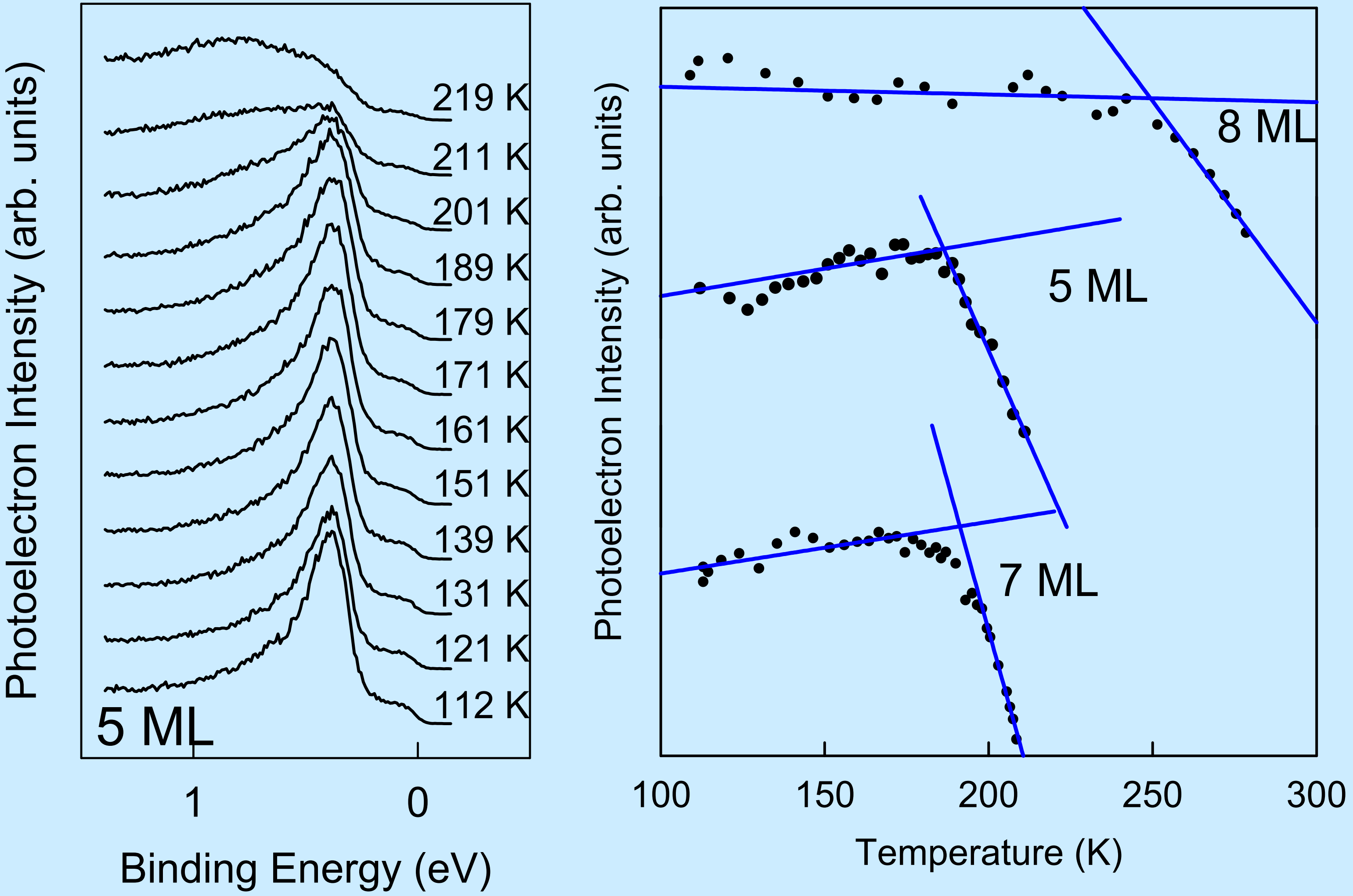


New Anticrossing Observations

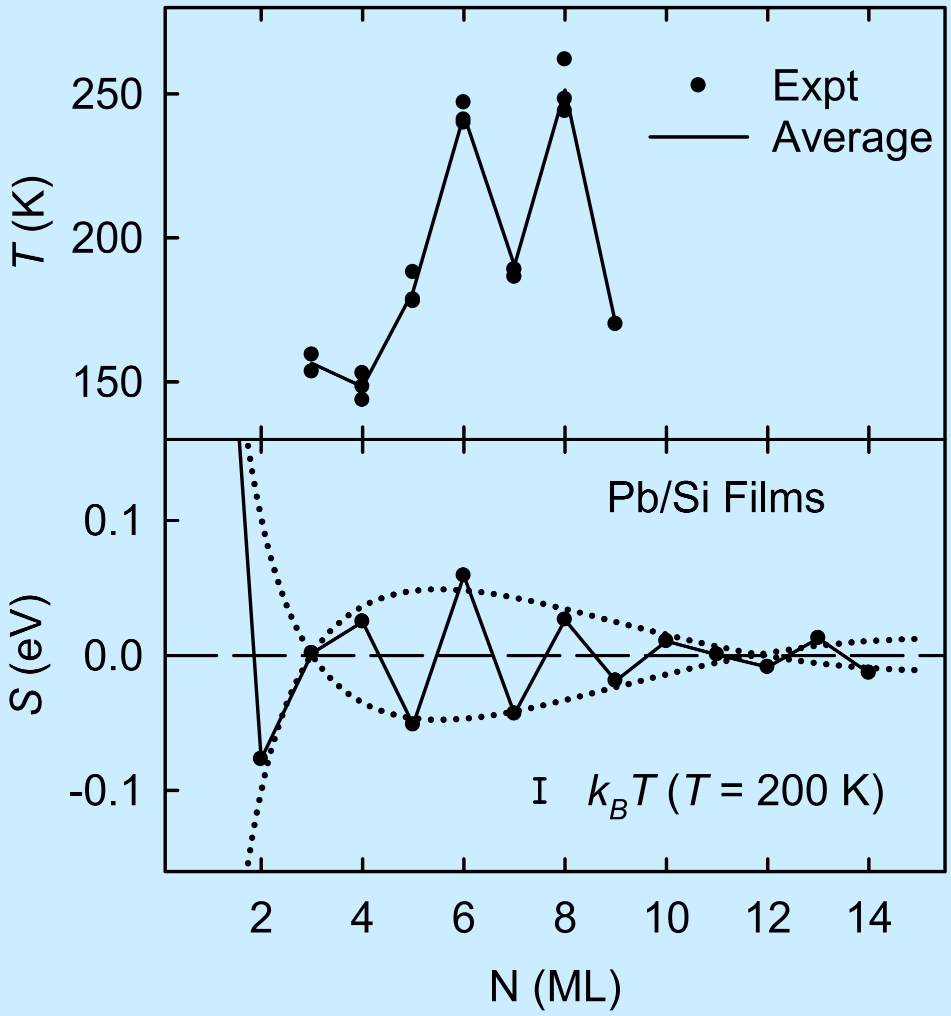
8 ML Ag/Ge(111) S.-J. Tang et al. PRL 96, 216804



Measuring Thermal Stability



Thermal Stability



- 5-9 ML has bilayer oscillation as predicted
- Low ML unusually unstable

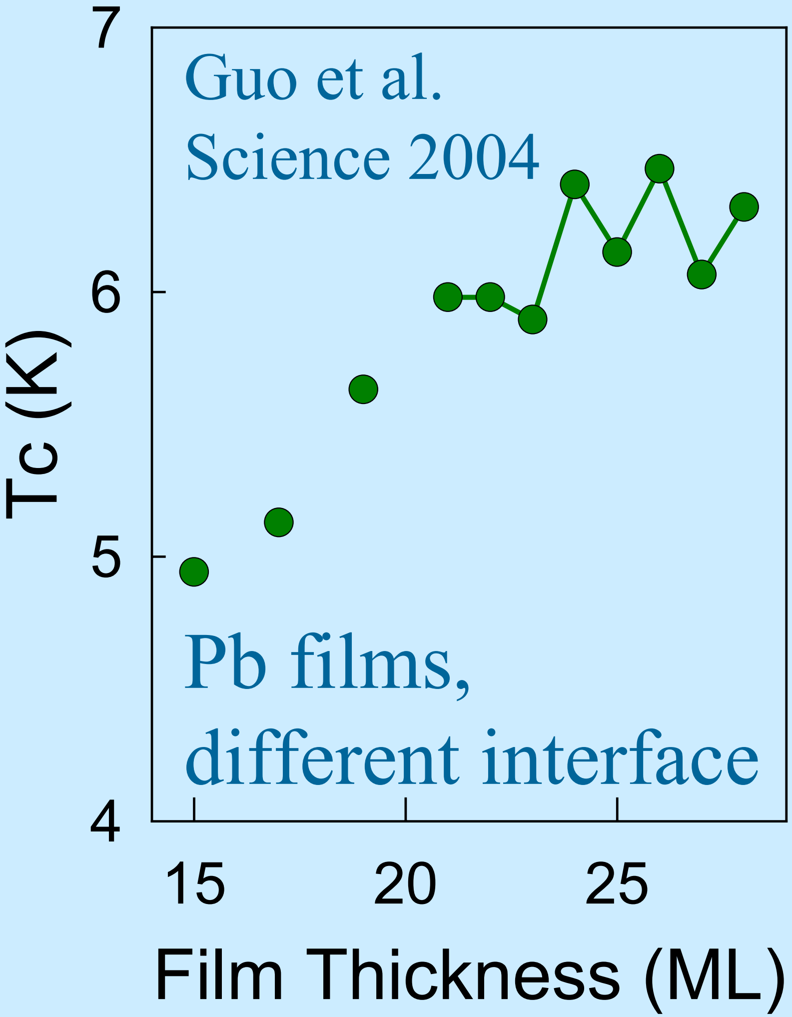
Calculation

- S = 2nd derivative of Surface Energy

$$S = \frac{E(N+1) + E(N-1)}{2} - E(N)$$

- Si lattice is compressed to match Pb lattice

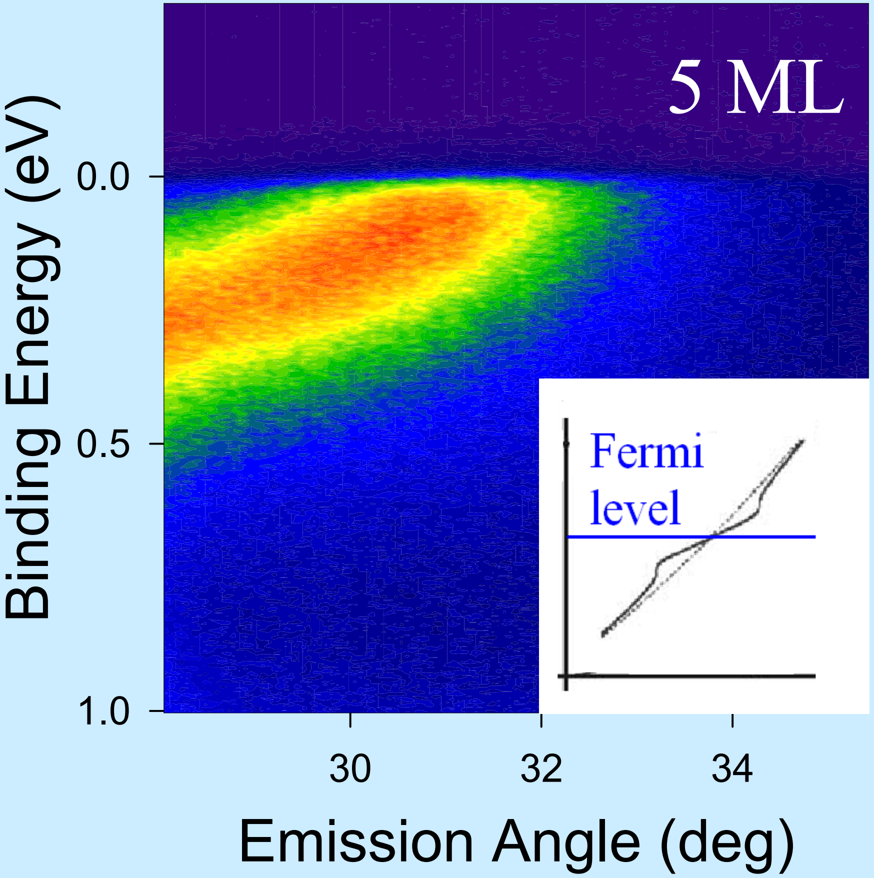
Next: Electron-Phonon Coupling



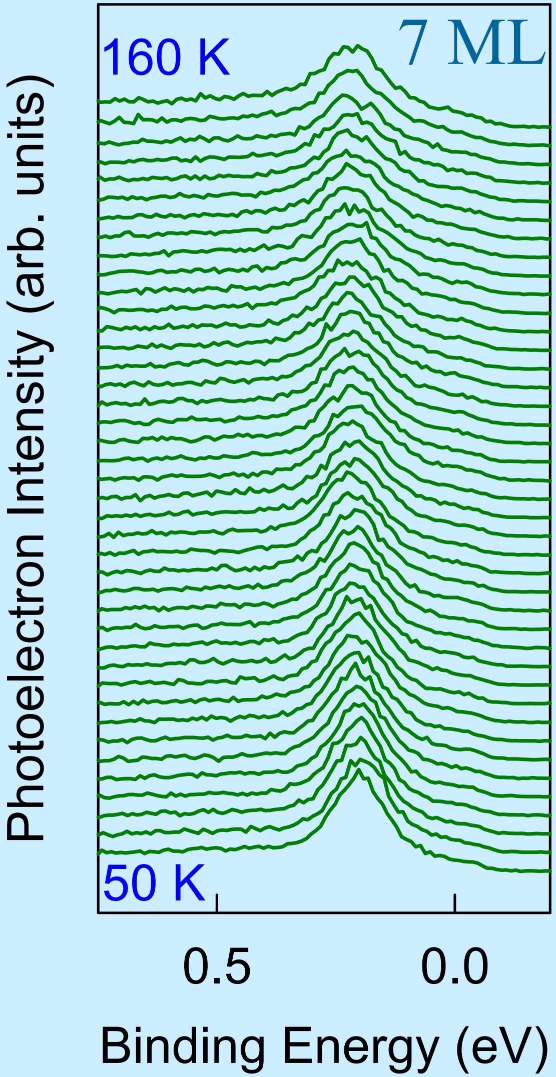
Guo et al.
Science 2004

Pb films,
different interface

Tc ~ electron-phonon coupling
near Fermi level



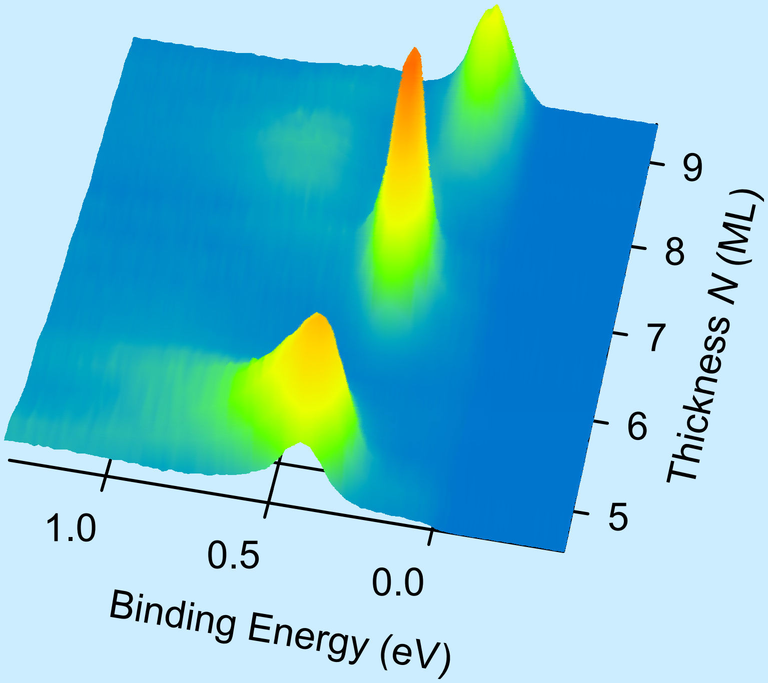
Next: Electron-Phonon Coupling



- Electron-Phonon coupling from peak width change with temp
- Peak position moves, how much oscillates

Summary

- Atomically uniform films
- Bilayer electronic oscillations
- Quantum well sub-band dispersion
- Thermal stability of films shows even-odd oscillations



Backups follow

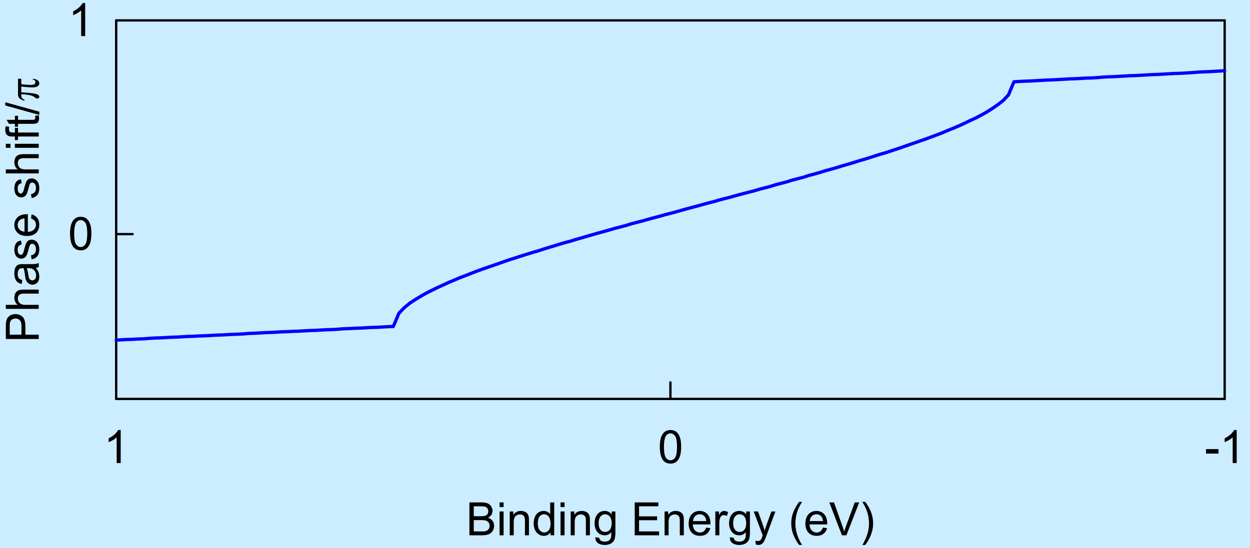
Phase Shift

$$\phi_{\text{Pb/Si}} = \text{Re}\left[-\cos^{-1}\left(2\frac{E-E_L}{E_U-E_L}-1\right)\right]+\phi_0$$

from N. V. Smith,
Phys. Rev. B **32**,
3549 (1985).

$$\phi_{\text{Pb/Vacuum}} = A\left[\text{Re}\left[-\cos^{-1}\left(2\frac{E-L}{U-L}-1\right)\right]+B\right]$$

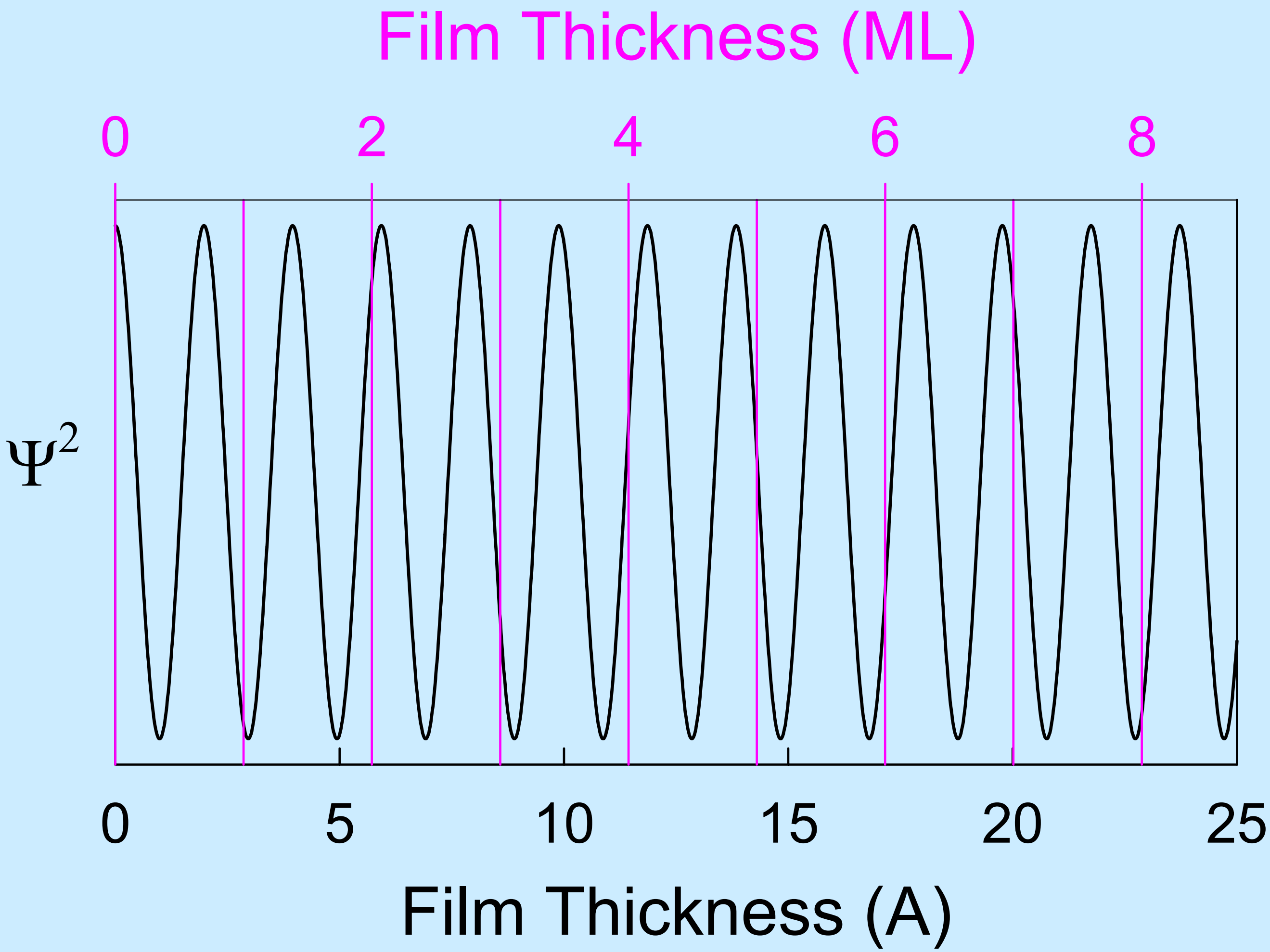
A, B, U, L fit to phase
shift in C. M. Wei,
M. Y. Chou, PRB
66, 233408 (2002).



Bilayer Oscillations

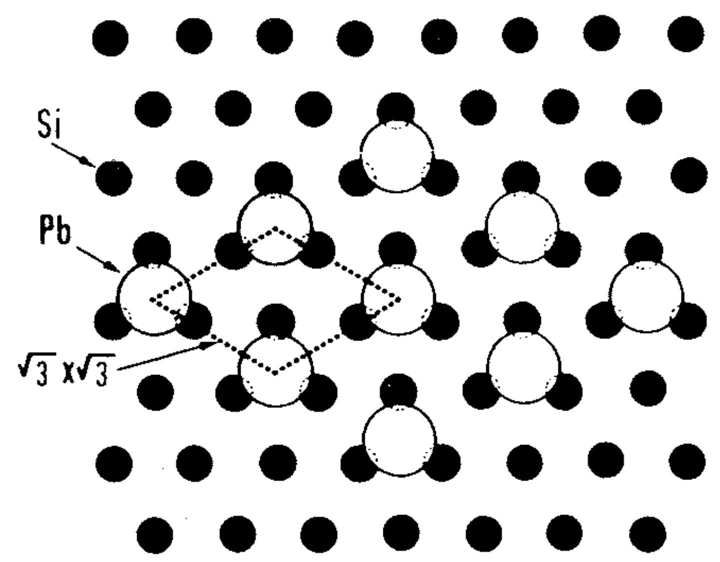
$\lambda_F = 0.691\ t_o$

- Charge near surface alternates max or min each layer
- Not perfect so beating

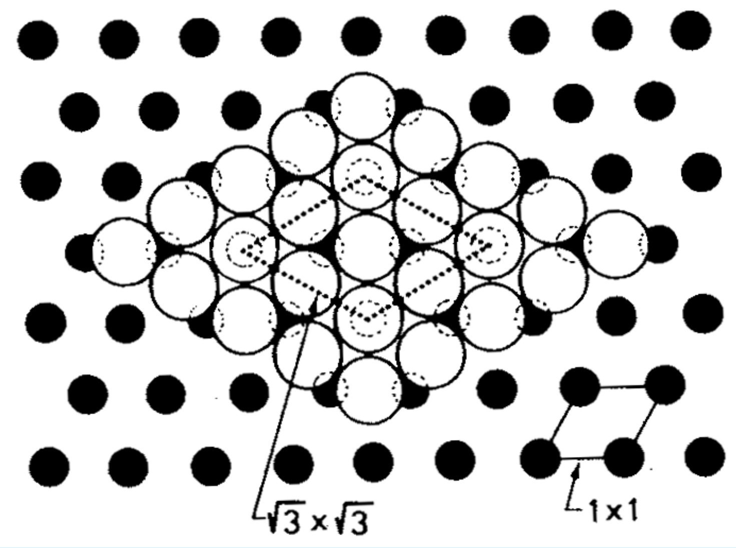


√ 3x √ 3 Pb/Si(111) Surface

- β: 1/3 ML Pb/Si



- α: 4/3 ML Pb/Si



Illustrations from Saitoh et al. Surface Science **154**,394 (1985).

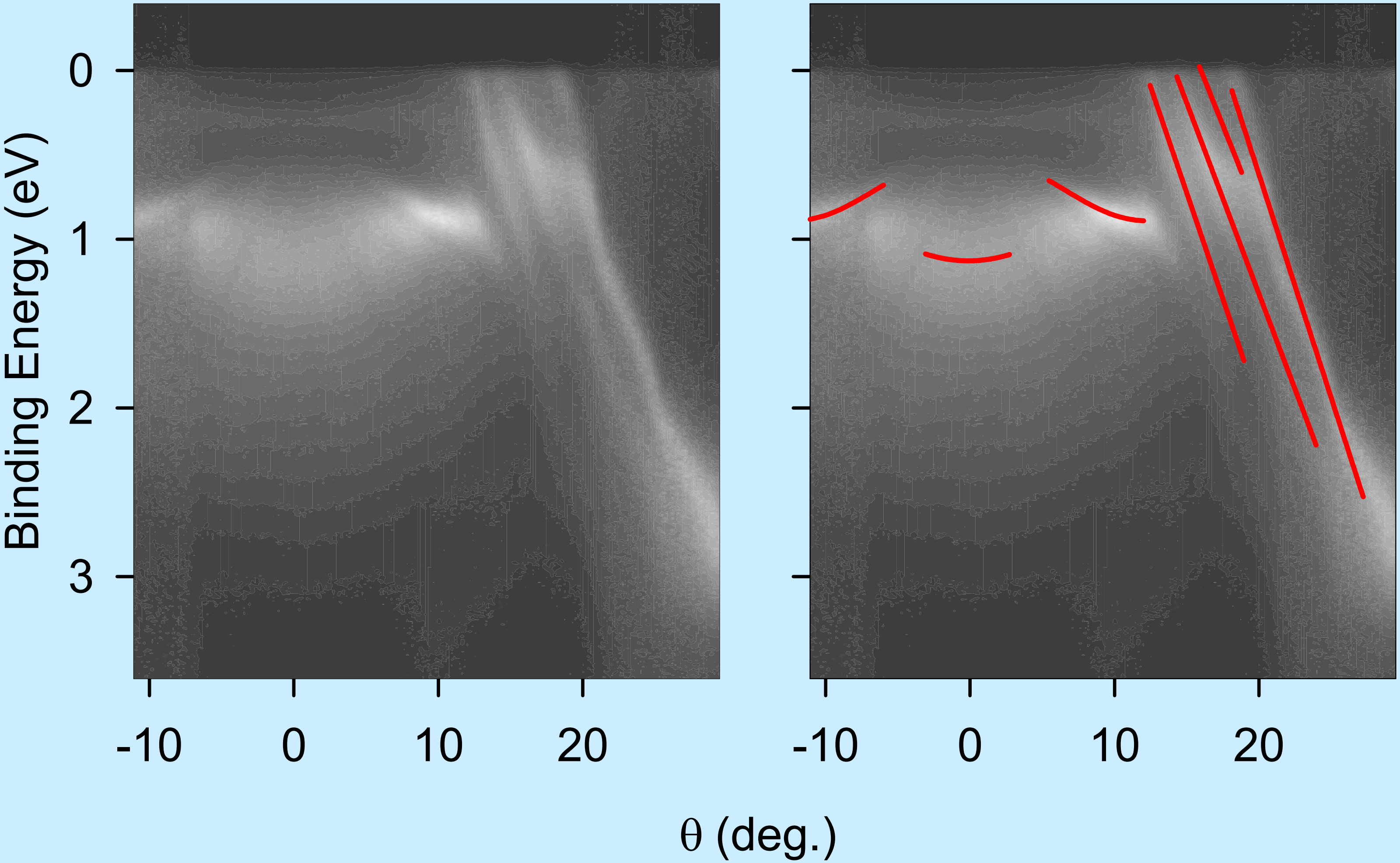
Number of Q.W. States

$$\underbrace{2Nk(E)t}_{\text{phase change in film}} + \underbrace{\phi_V(E)}_{\text{at vacuum}} + \underbrace{\phi_I(E)}_{\text{at interface}} = 2\pi n$$

Now suppose $n = N + \tilde{n}$. Then

$$\begin{aligned} 2Nkt + \phi &= 2\pi(N + \tilde{n}) \\ 2N(k - k_L)t + \phi &= 2\pi\tilde{n} \end{aligned}$$

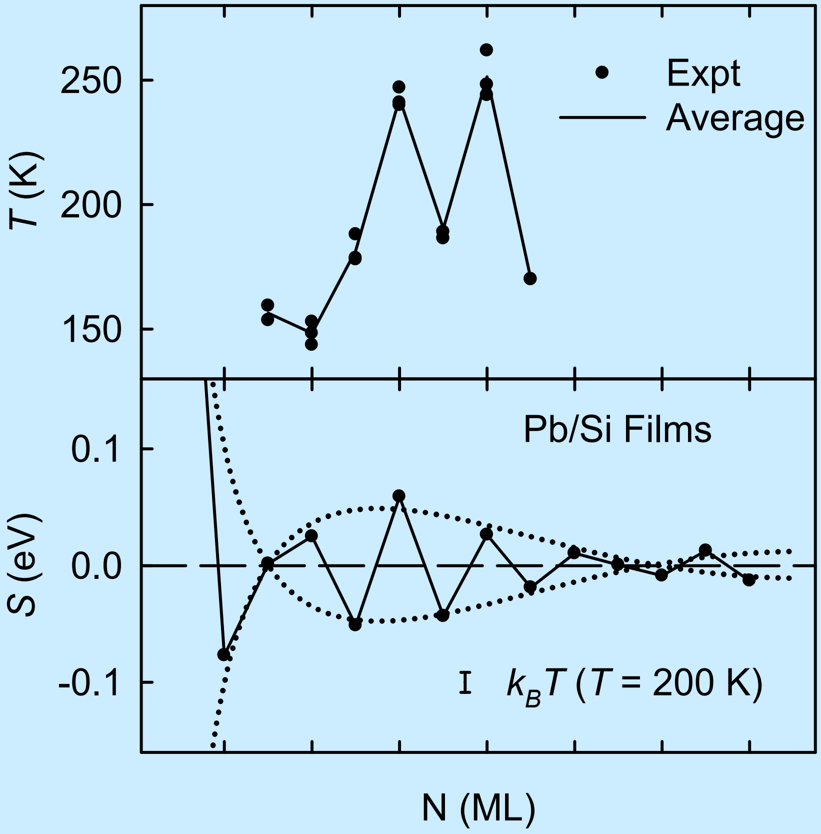
Dispersion Measurement – 6ML



Surface Energy

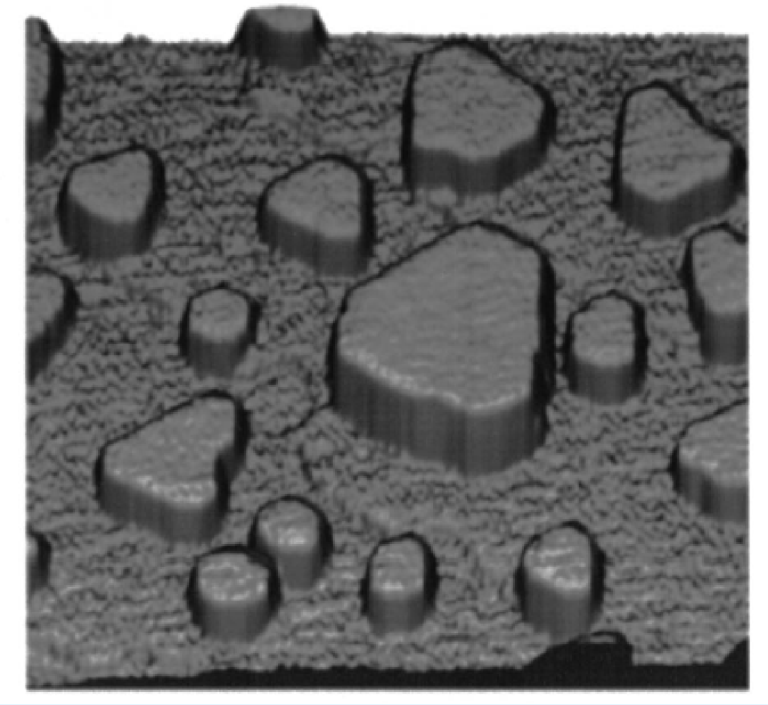
$$\underbrace{E_S(N)}_{\text{surface energy of N layer film}} = \tfrac{1}{2}(\underbrace{E(N)}_{\text{energy of N layer film}} - N\underbrace{E_B}_{\text{energy of bulk}})$$

- Surface energy = energy to create surface
- Local min (S>0) takes less energy ⇒ more stable film



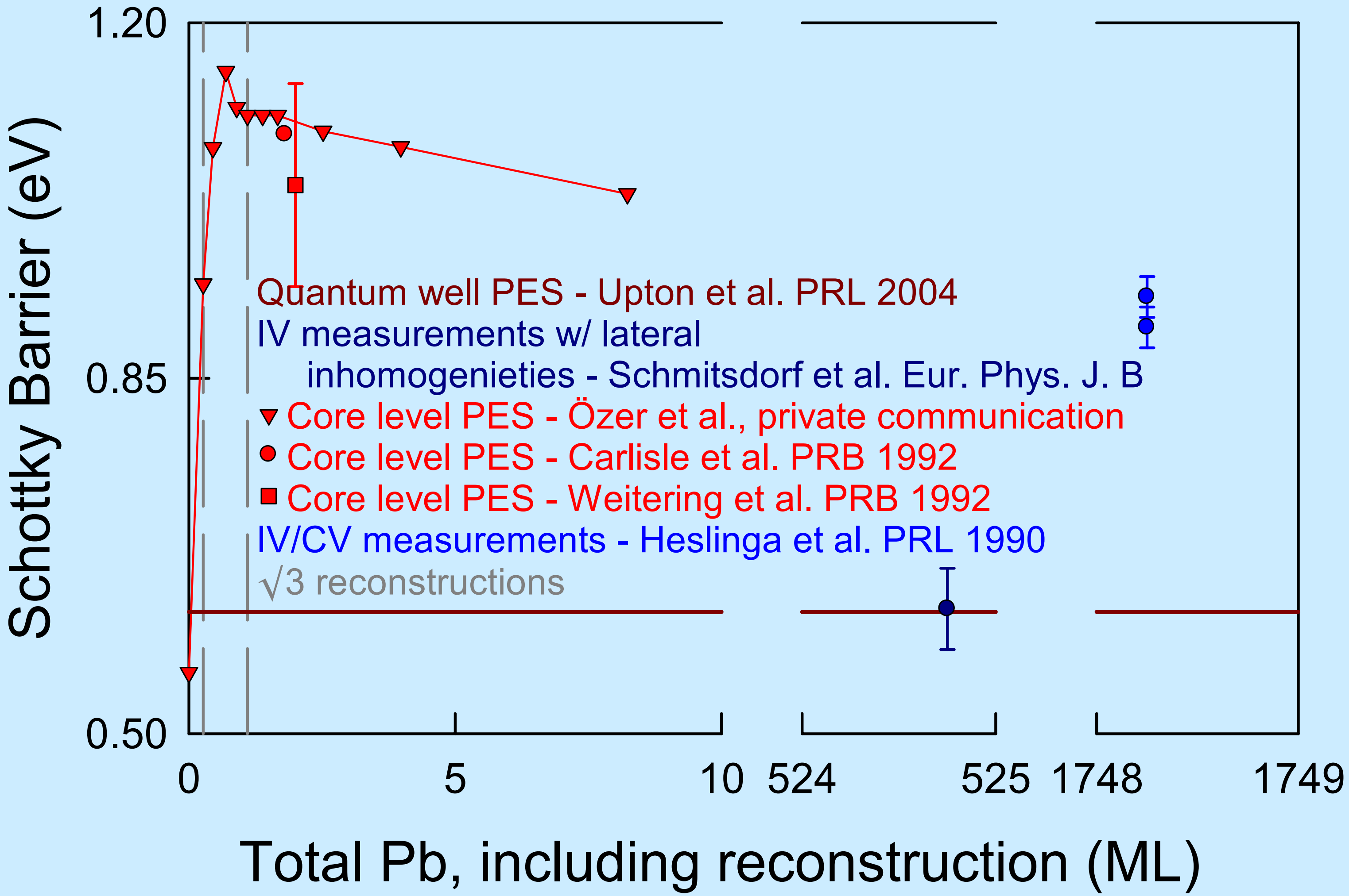
STM Results

- 200 K growth, 5-7-9 … ML grow sequentially on β phase *Hupalo, Yeh, Berbil-Bautista, Kremmer, Abram, and Tringides PRB 2001.*
- 77 K growth, flat topped islands observed at coverages 5-35 ML on annealed interface *Altfeder, Narayanamurti, and Chen PRL 2002.*



3 ML at 200 K on β phase *Hupalo et al.*

Schottky Barrier



What causes high m*?

- Proximity to Si VBM
- Hybridization with Si band
- Lateral strain
- Small in-plan coherence length

Anticrossing

- Example: Si band gap.
- Electrons below Si VBM have different wave functions that those above Si VBM, => as they approach they have different energies and the band splits.

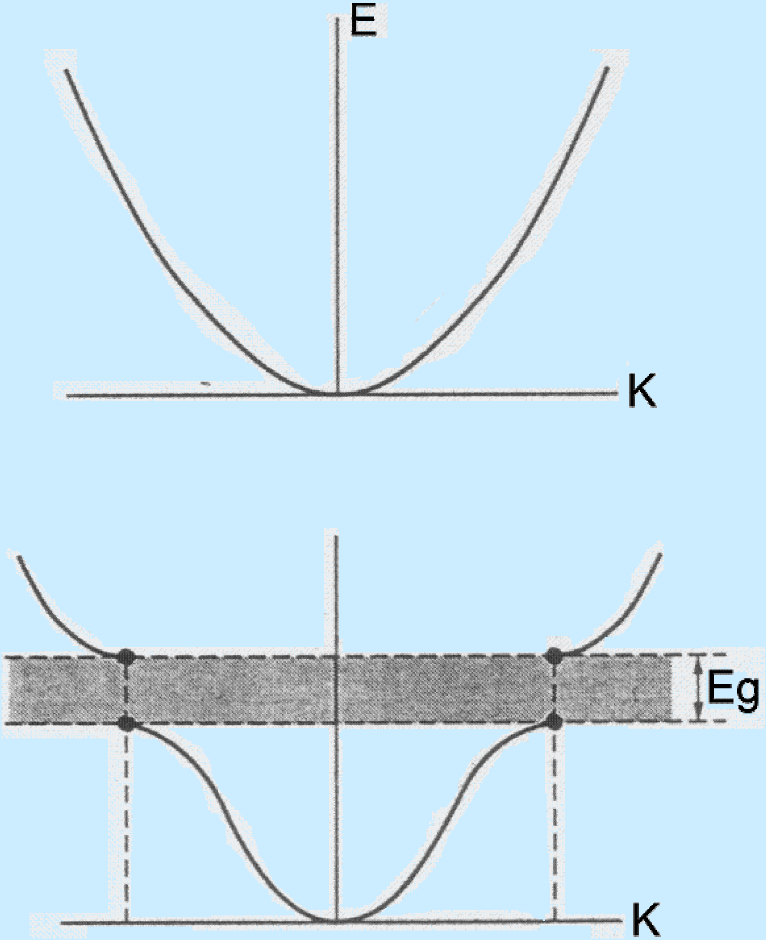


Figure from Kittel, 1996

Experiment

1. Grow Pb on 100 K Si(111)- ($\sqrt{3}$x $\sqrt{3}$) – Pb α (4/3 ML) or β (1/3 ML) reconstruction with Molecular Beam Epitaxy (MBE).
2. Study sample with photoemission (photons in, electrons out)