Structural Quantum Size Effects in Pb/Si(111)

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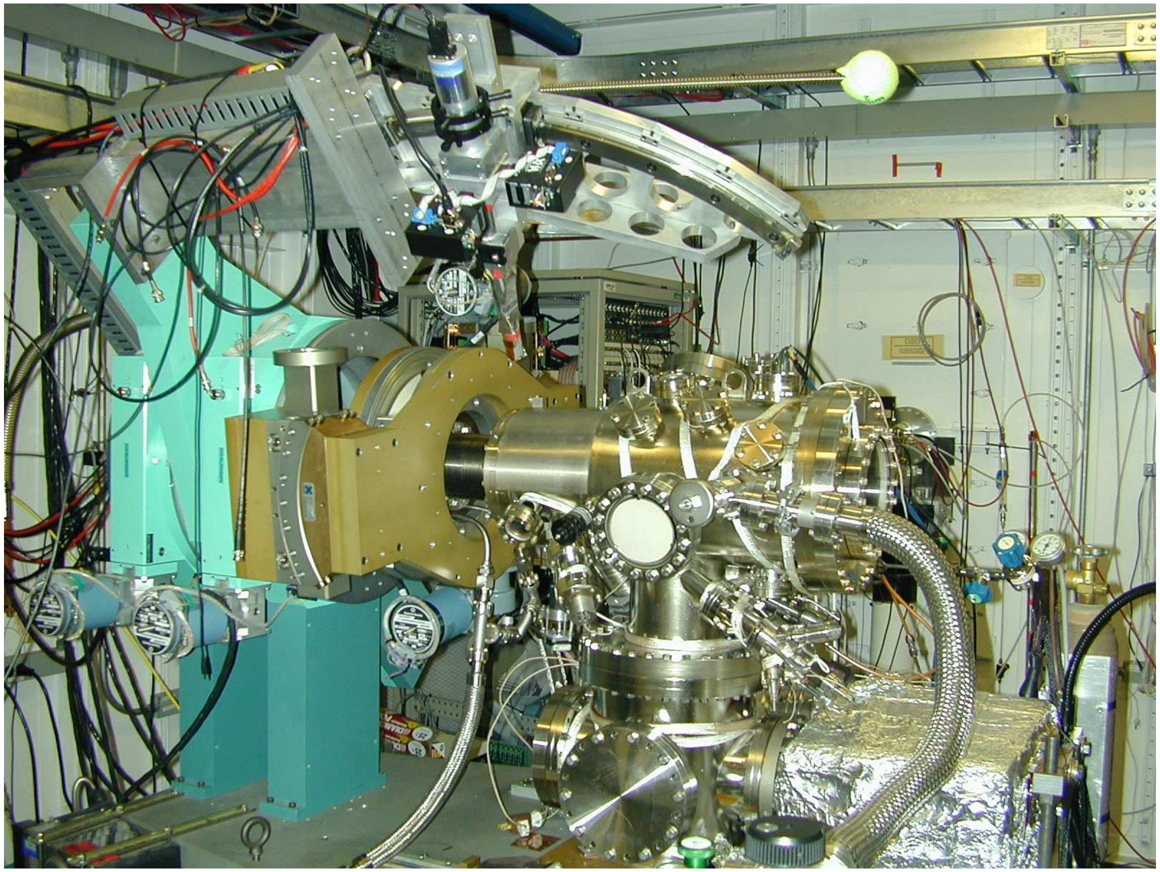
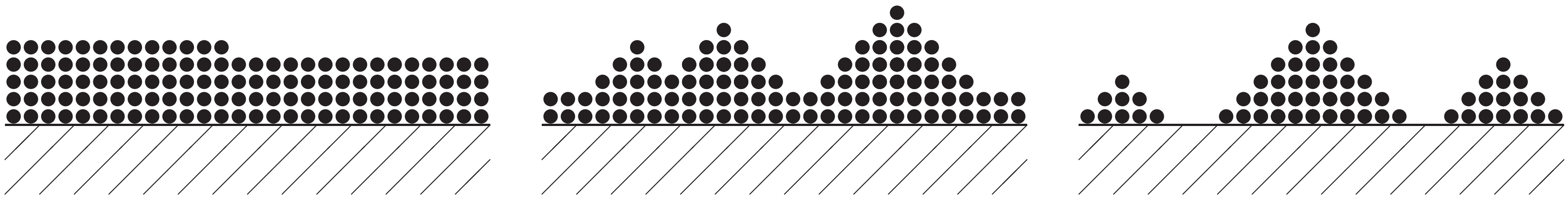
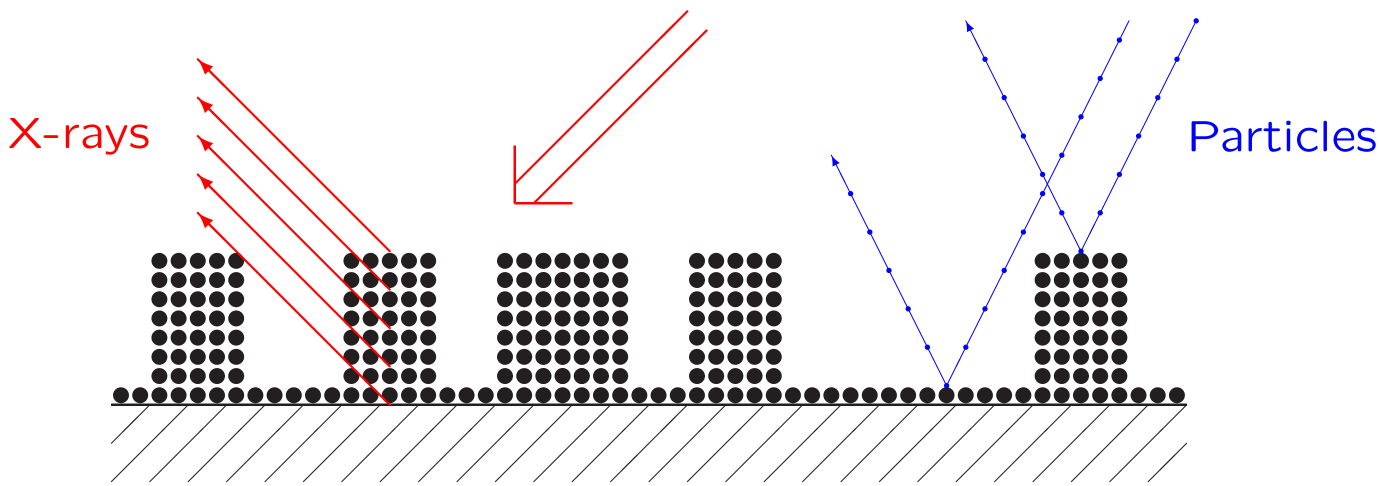


Thin Film Growth



Layer-by-Layer (van der Merwe) ⟶ Combination (Stranski-Krastanov) ⟵ 3-D island formation (Vollmer-Weber)



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Quantum confinement of electronic states

$\Downarrow$

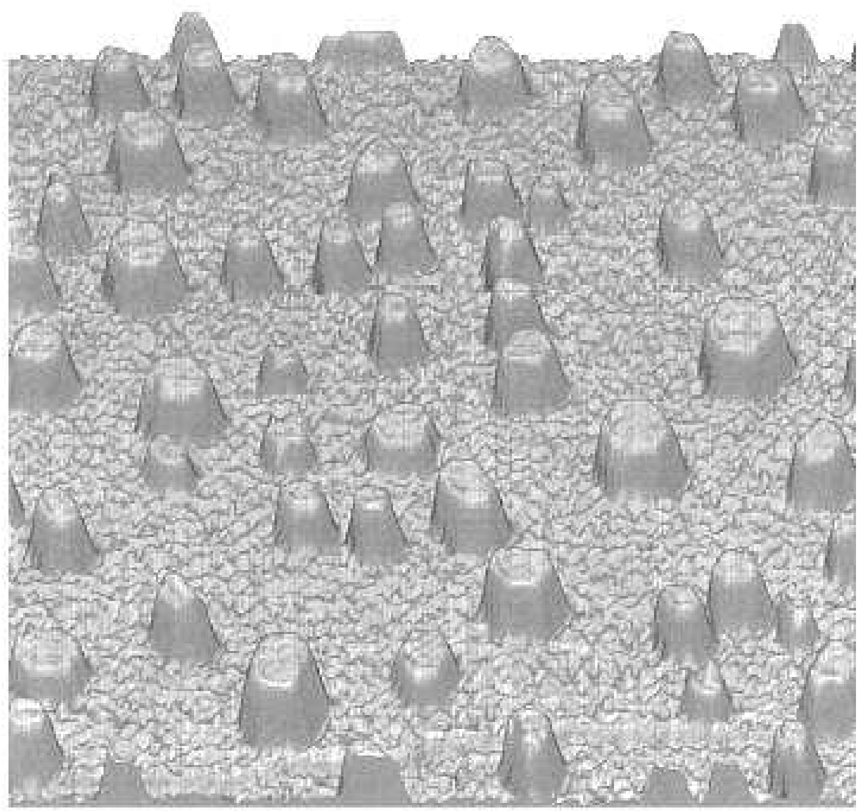
Preferred thicknesses

Quantum Size Effects in Pb/Si(111)

- Island heights appear to be highly uniform
  $\Rightarrow$ preferred thicknesses

- Self-organization attributed to QSE

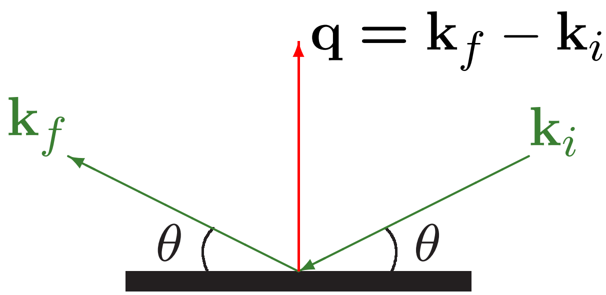
- Morphology depends on:
  $\longrightarrow$ Temperature
  $\longrightarrow$ Pb coverage
  $\longrightarrow$ Pb/Si interface
  $\longrightarrow$ Kinetic pathway



M. Hupalo, et. al., Surf. Sci. 493 (2001) 526

Surface X-ray Diffraction (SXRD)

Specular Reflectivity

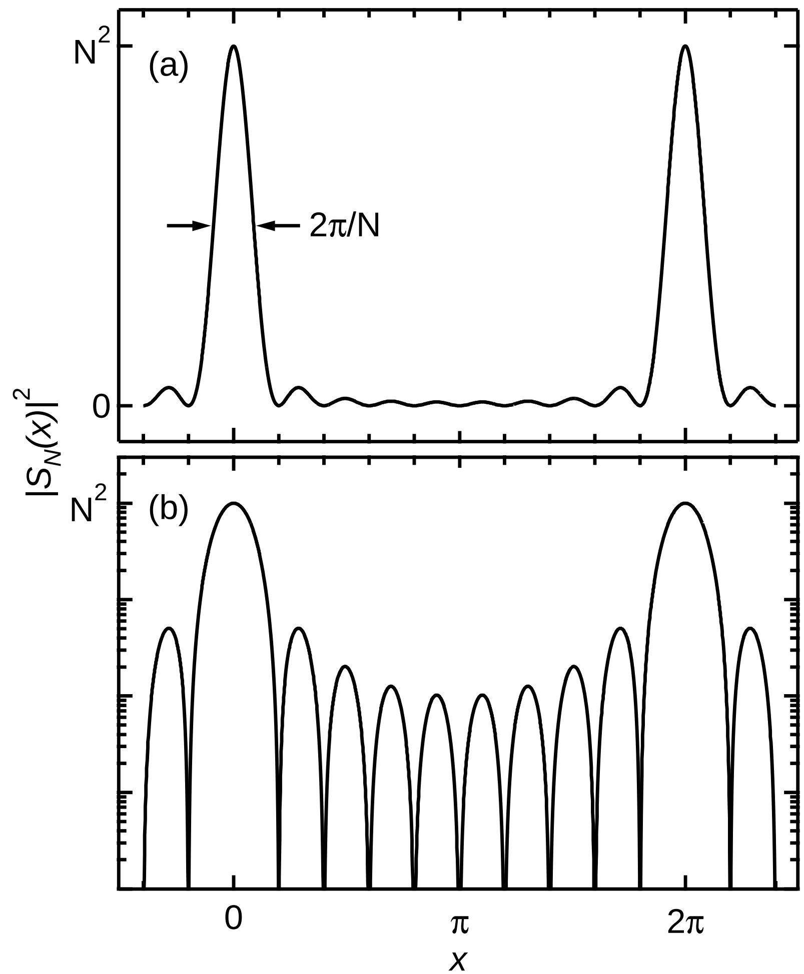


- Since $\mathbf{q} \cdot \mathbf{a}_1 = \mathbf{q} \cdot \mathbf{a}_2 = 0$, the specular rod is insensitive to in-plane order

- Thin film overlayers will contribute an amplitude similar to the N-slit interference function,

$$S_N(x) = \sum_{n=0}^{N-1} e^{i\,nx}$$

- $x = 0, 2\pi \rightarrow$ Bragg peaks



N-Slit Interference Function

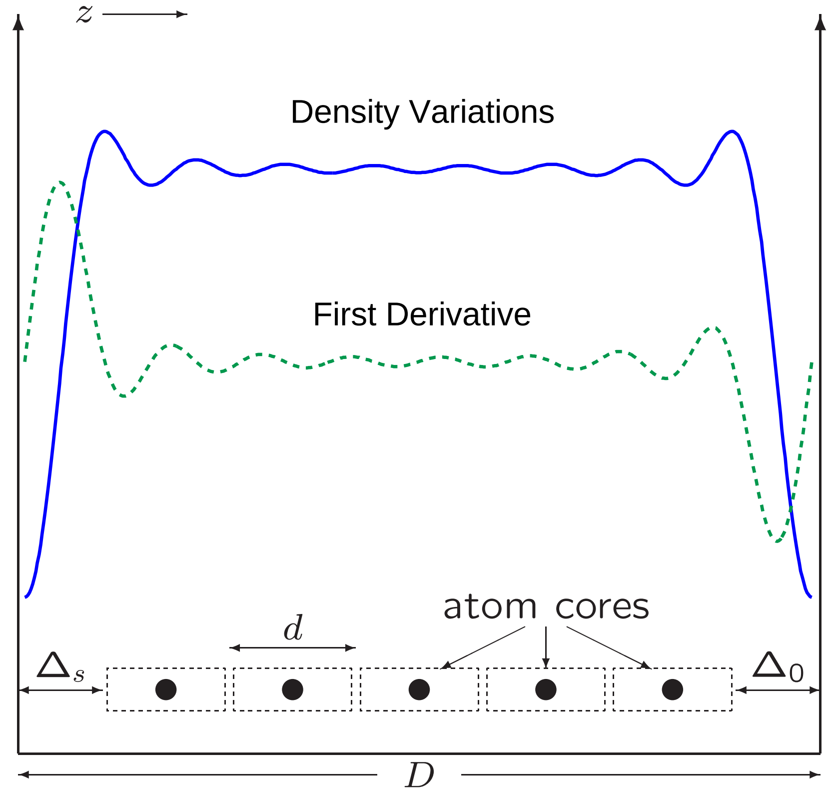
Electron Confinement and Quantum Size Effects (QSE)

- Conduction electrons in thin metal films take on particle-in-a-box-like states
- Free-electron charge density exhibits Friedel oscillations in z-direction
- Oscillations have a wavelength $\approx \pi/k_F = \lambda_F/2$

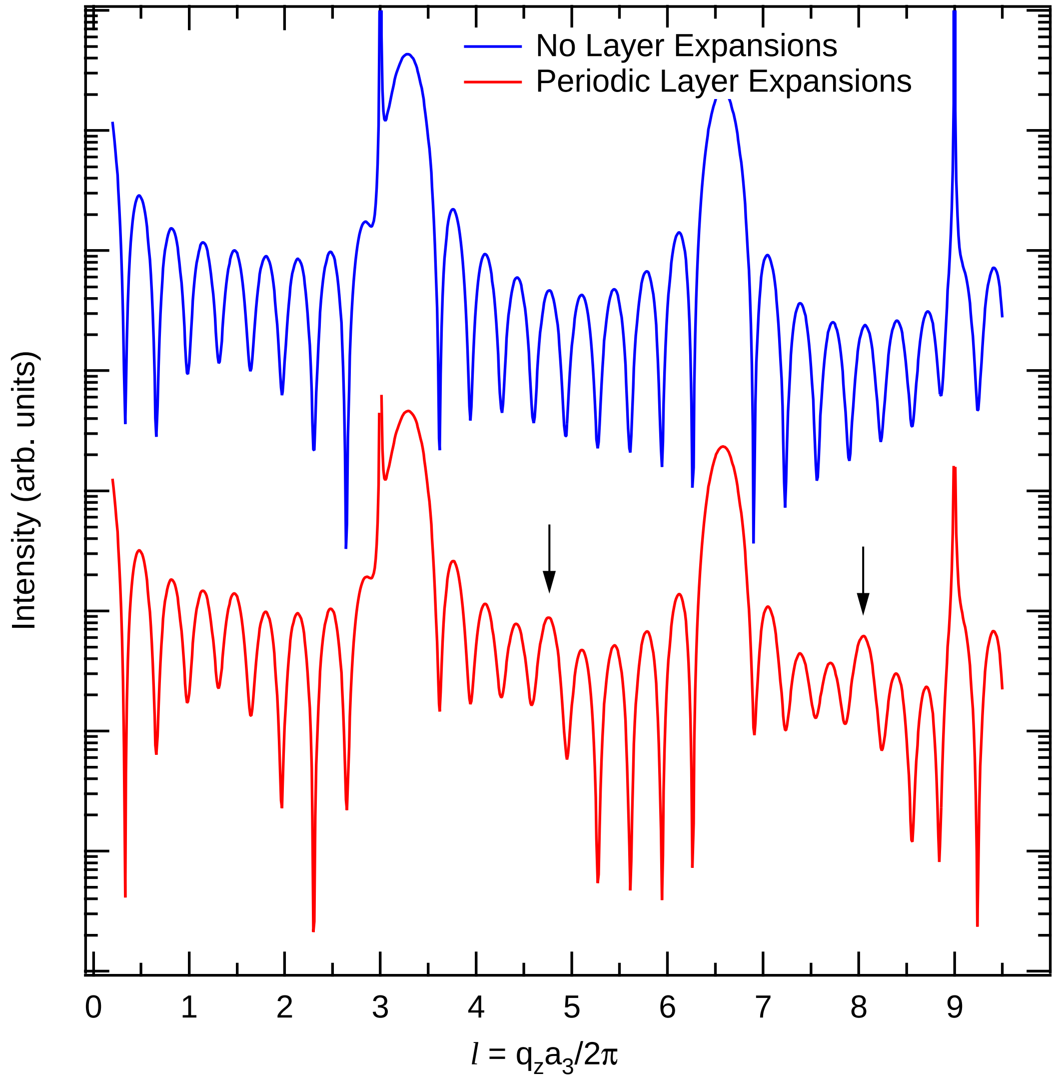
$$\delta\rho(z) = -\frac{1}{C_D}\left(k_F^2 + \frac{1}{4}\frac{\partial^2}{\partial z^2}\right) S_D$$

$$\Delta s(z) = A\,\frac{\partial}{\partial z}\delta\rho(z)$$

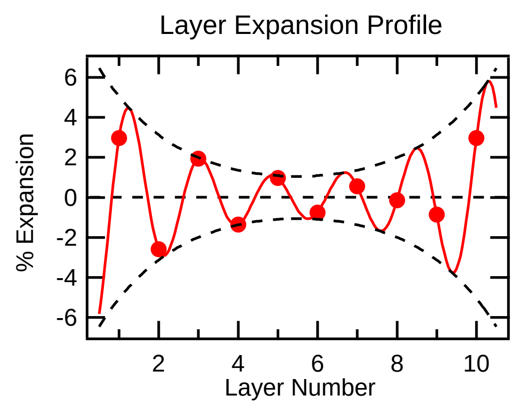
$$S_D = \frac{1}{2}\sin 2k_F z \cot\frac{\pi z}{D} - \sin^2 k_F z$$



SXRD Reflectivity Simulations



- Simulations are for 10 ML Pb on Si(111)-7x7
- For Pb(111), $\lambda_F/2 \approx 1.8d$
- Used simplistic sinusoidal model for z_j
- Half-order features appear with expansions

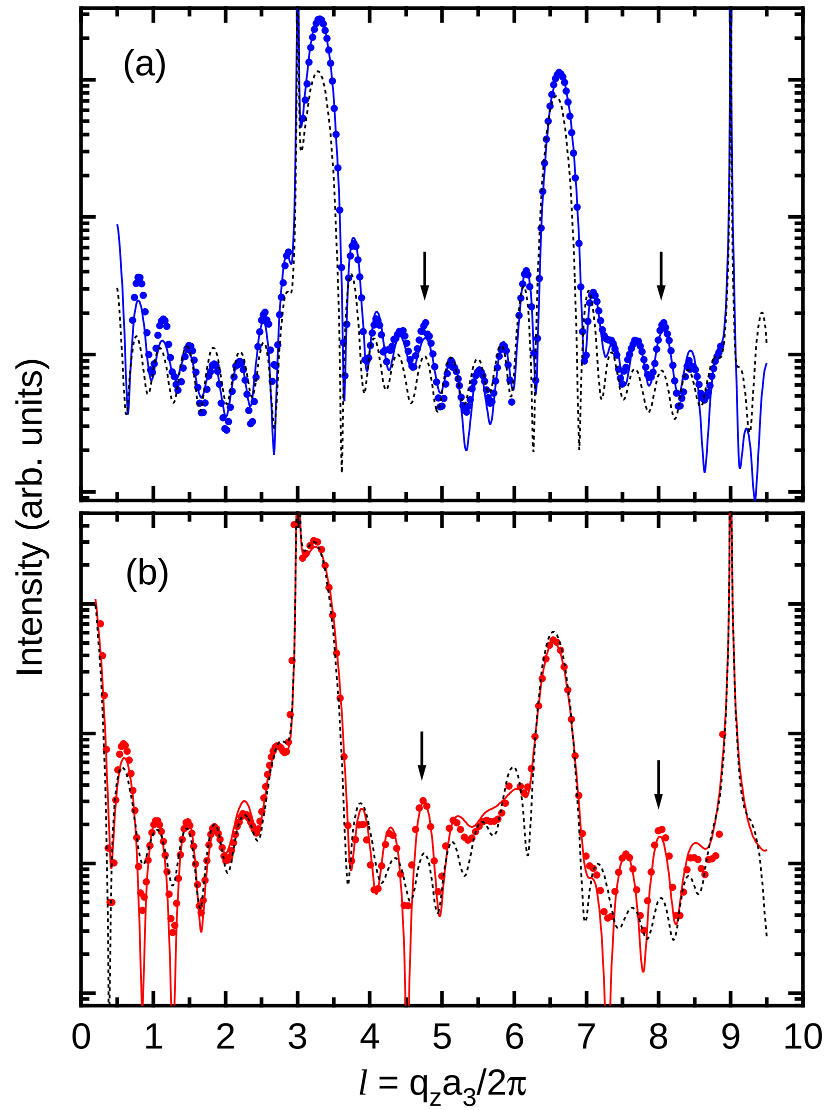


Layer Relaxations in Pb/Si(111)

- Pb was deposited on both the 7×7 and $\sqrt{3}\times\sqrt{3}$-β interfaces
- Profiles were fit with a range of island heights to allow for a non-uniform distribution
- Profiles were fit with and without ($A = 0$) layer relaxations $\Rightarrow$ half-order features not reproduced without layer relaxations

(a) 8.5 ML Pb on Si(111)-7×7
Deposited at 185 K
$N = 10$ islands

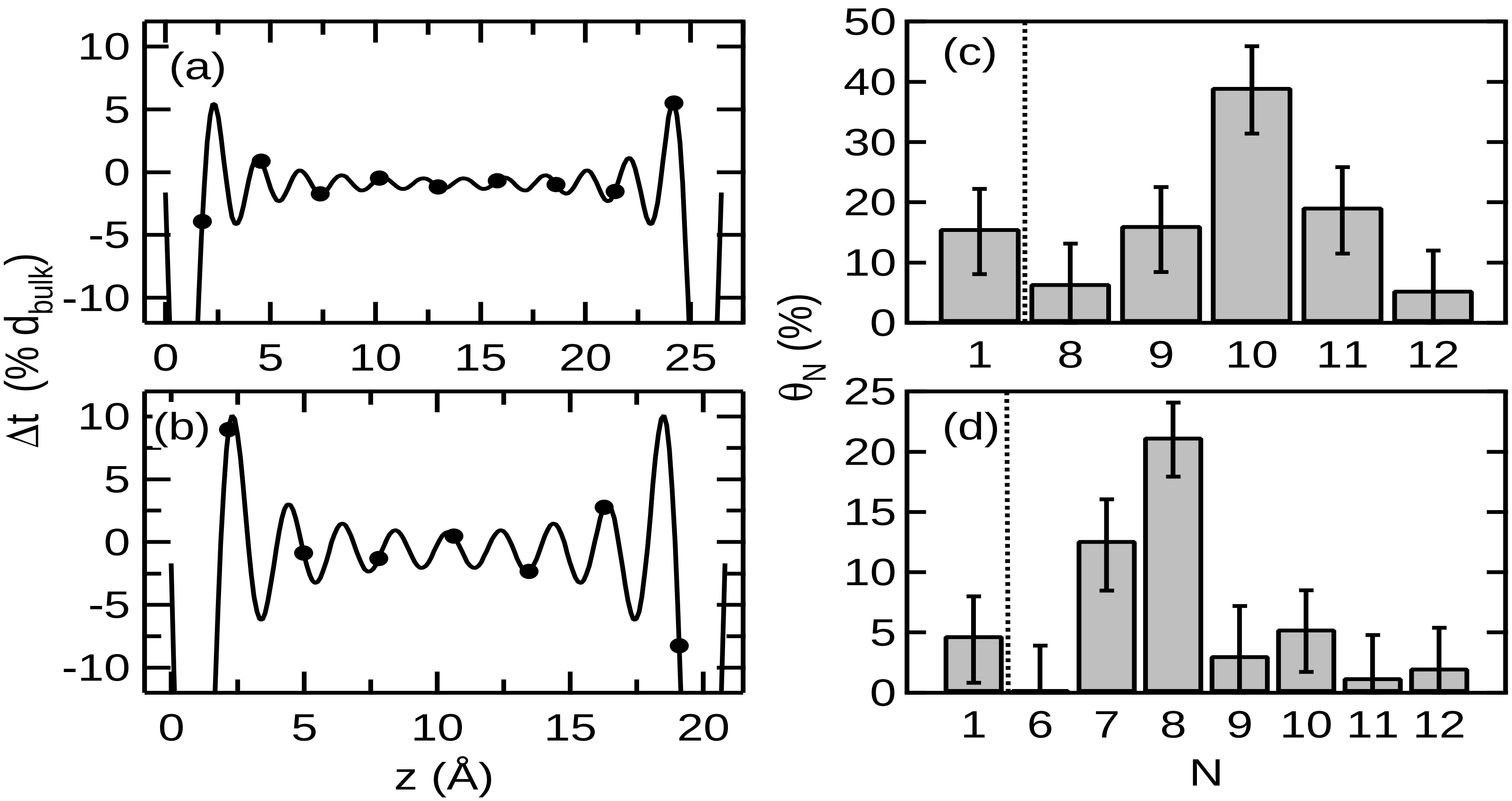
(b) 4.5 ML Pb on
Pb/Si(111)-$\sqrt{3}\times\sqrt{3}$-β
Deposited at 115 K
Annealed to 180 K
$N = 8$ islands



Layer Relaxation Results

Parameter	7×7 N=10	$\sqrt{3} \times \sqrt{3}$-β N=8
A (Å^2)	86±35	135±35
Δ_s (Å)	0.36±0.05	0.76±0.25
Δ_0 (Å)	0.90±0.40	0.31±0.08
δd (%)	-0.90±0.31	-0.77±0.65

- More data needed for trends
- Oscillatory relaxations apparent



Summary

- QSE can be an important factor in the behavior of thin film growth
- Quantum confinement can have sizable structural consequences in thin metal films
- These effects can be understood in Pb/Si(111) in terms of Friedel oscillations in the electronic charge density
- Emphasizes the importance of considering quantum effects in the engineering of nanostructures