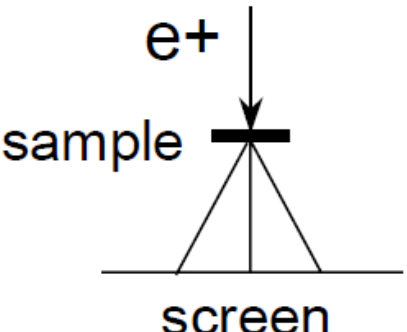# Positron diffraction

• **positron diffraction**

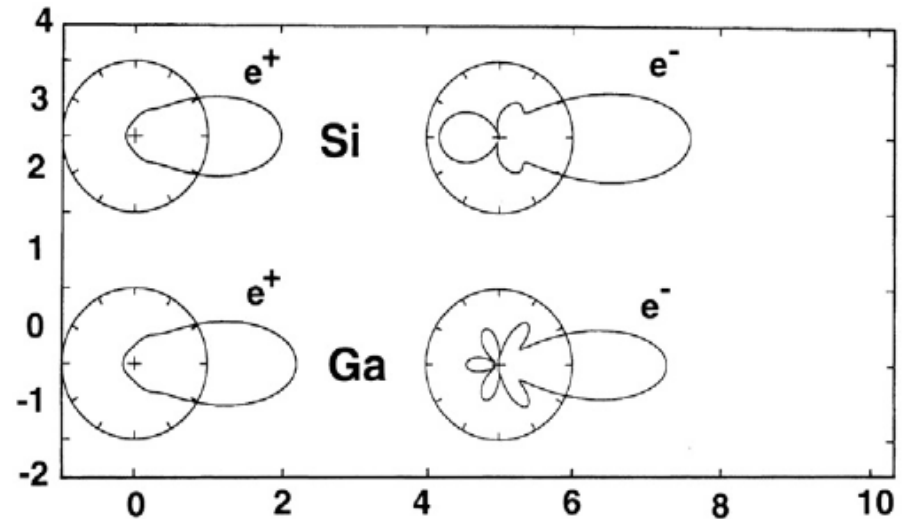|		
e+ ↓ sample screen	screen sample	e+ screen sample
TPD **Transmission** **Positron** **Diffraction**	**LEPD** **Low Energy** **Positron** **Diffraction**	**RHEPD** **Reflection High** **Energy Positron** **Diffraction**
100keV ▪ 1MeV	10 ▪ 500eV	10 ▪ 100keV
Bulk ▪ Study	▪ **Surface** ▪ **Study** ▪	

Positron diffraction

- **differential scattering factor**

- 100 eV e⁻ and e⁺

- Cu
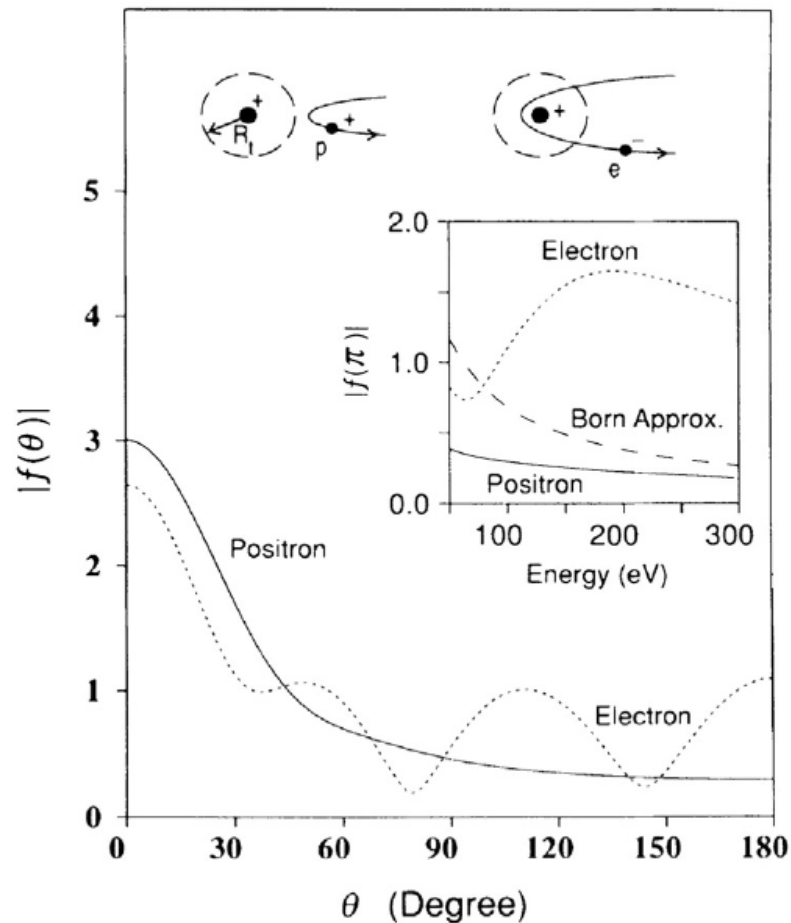
- **differential scattering factors**

- 100 eV e⁻ and e⁺
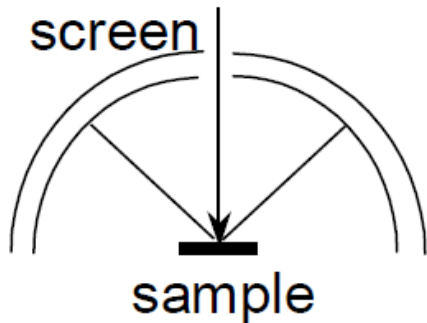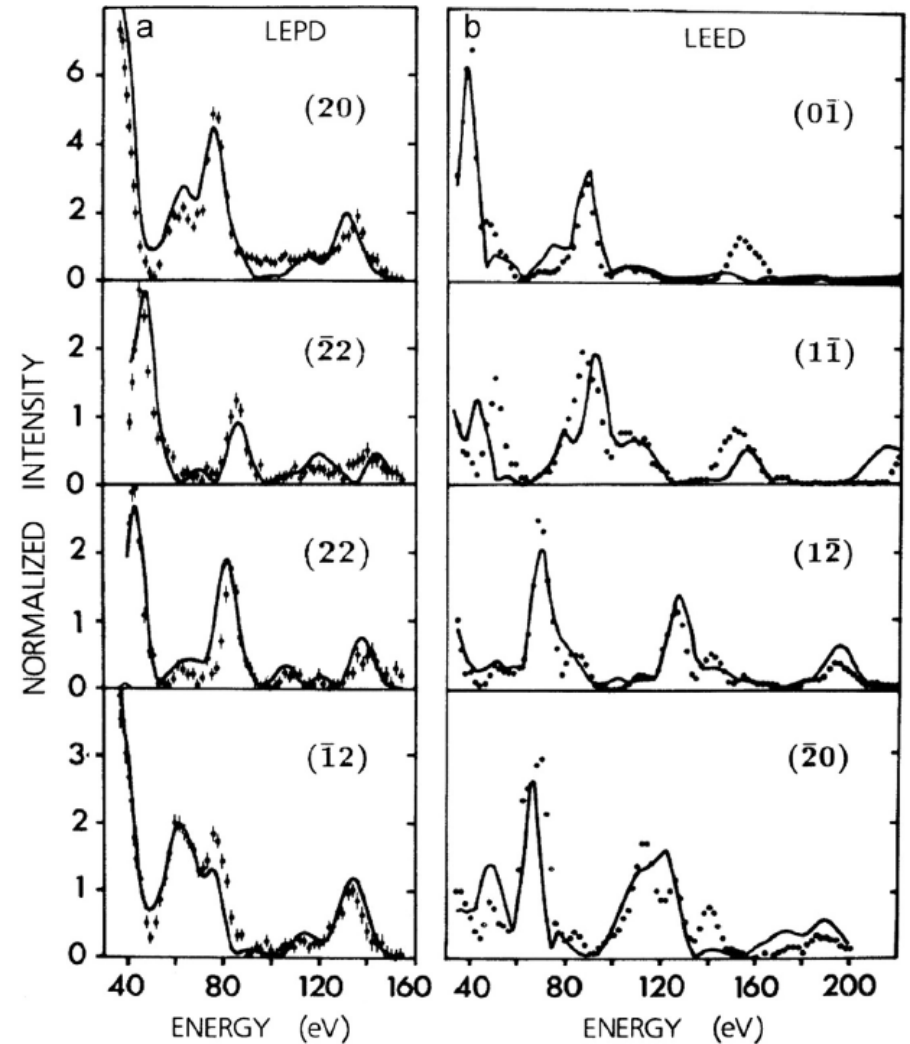
- Si, Ga

- **positrons**

  - lower elemental sensitivity

  - lower penetration depth, turning point $R_t = \dfrac{Ze^2}{E_k}$

  - low anisotropy

LEPD = Low Energy Positron Diffraction

• *I-V* curves: intensity of fixed Bragg peak when kinetic energy of incident positrons is varied
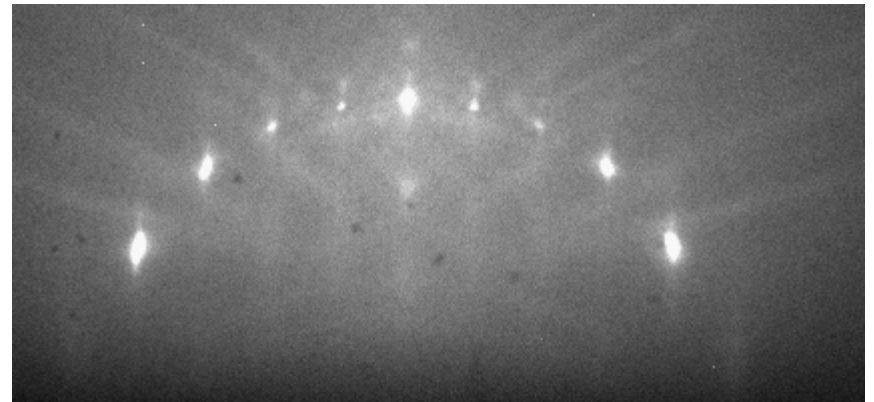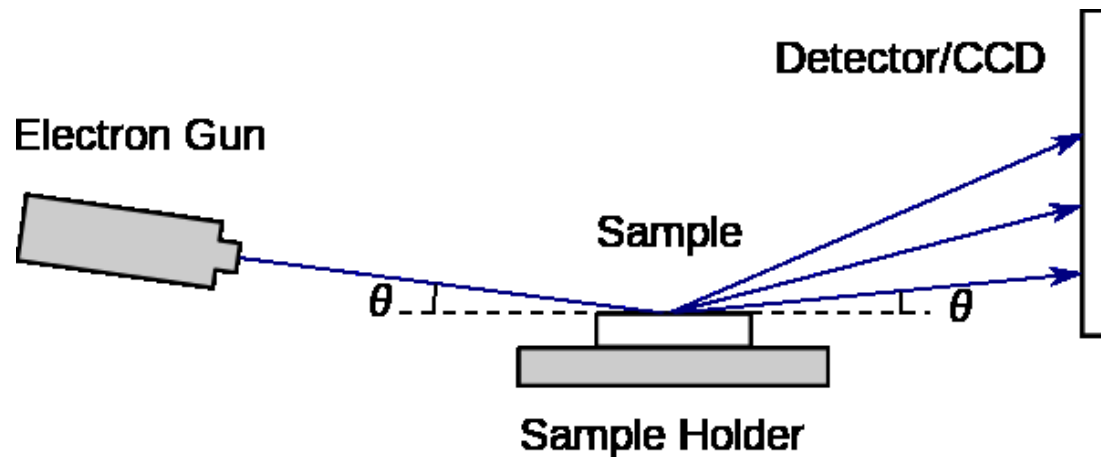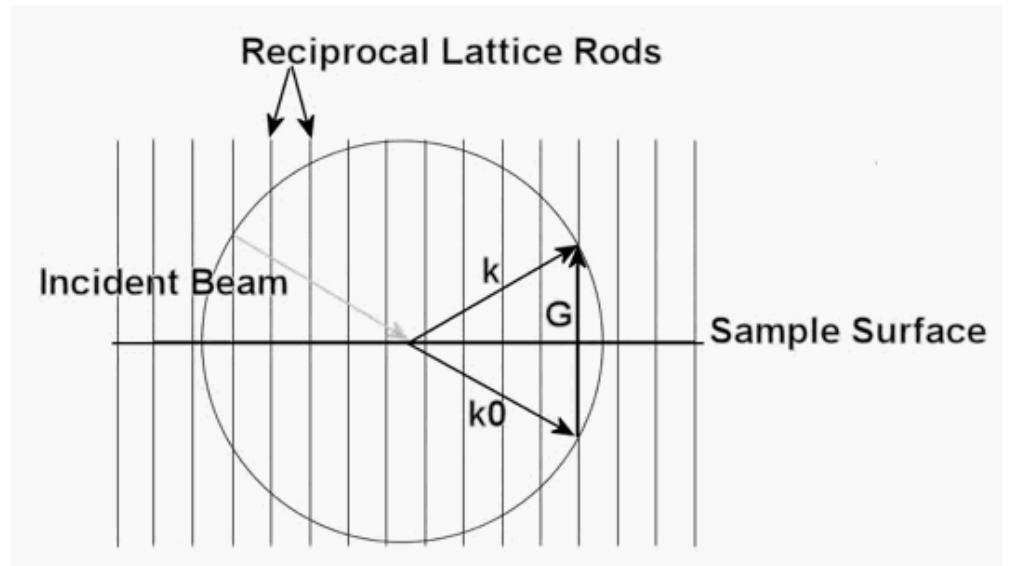
CdSe (11-20) surface

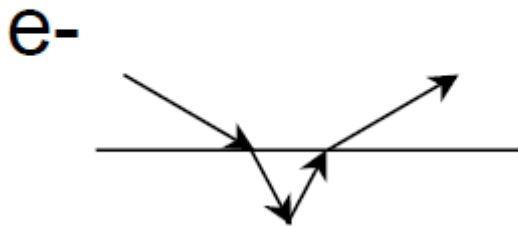# RHEPD = Reflection High-Energy Positron Diffraction

- **electron diffraction on surface**

- quality monitoring of thin films

- kinetic energy of incident particles 10-20 keV

Reciprocal Lattice Rods

Incident Beam

Sample Surface

k

G

k0

Electron Gun

Detector/CCD

Sample

θ

θ

Sample Holder

RHEPD = Reflection High-Energy Positron Diffraction

• electrons

• potential for electrons

• negative inner potential
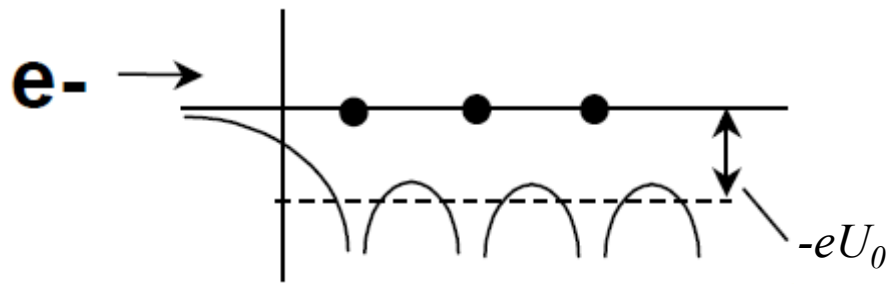
• positrons

• potential for positrons

• positive inner potential

RHEPD = Reflection High-Energy Positron Diffraction

- **RHEPD**

$$\left(-\frac{\hbar}{2m}\nabla^2 + eU_0\right)\psi = E\psi$$

- outside crystal $V = 0$
- inside crystal $V > 0$

RHEPD = Reflection High-Energy Positron Diffraction

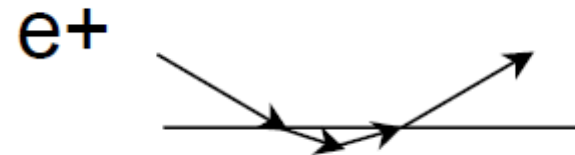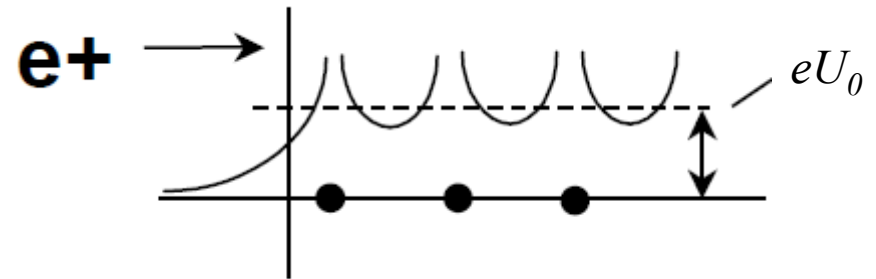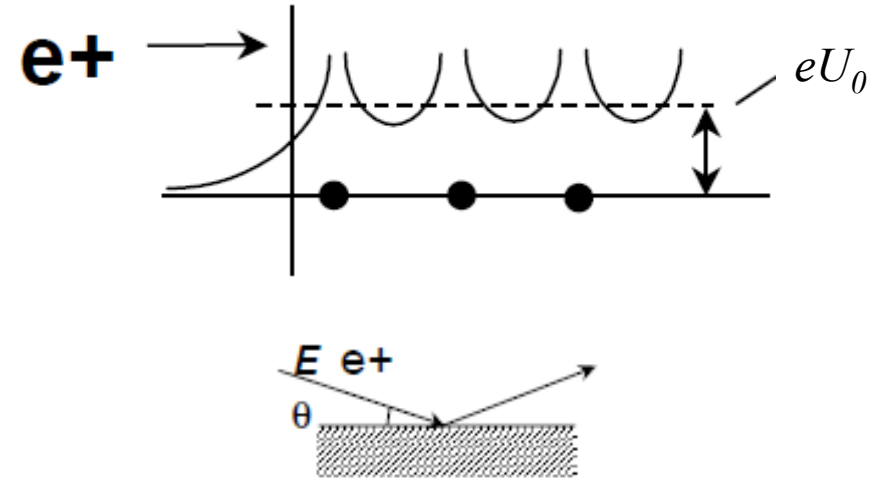- Snell law $\dfrac{\lambda}{\lambda_s} = \dfrac{\cos\theta}{\cos\theta_s}$

- de Broglie wavelength
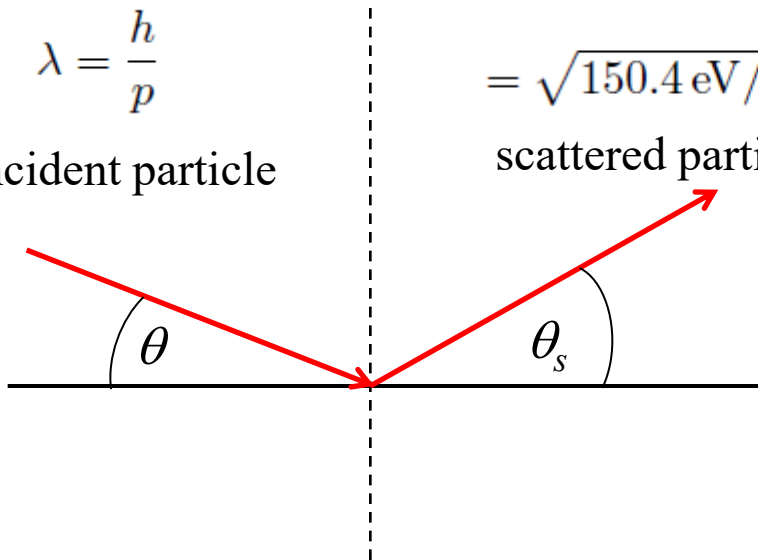
- Bragg condition $2d\sin\theta_s = k\lambda_s$

- inter-planar distance

$\lambda = \dfrac{h}{p}$

$\lambda_s = \dfrac{h}{p_s} = \dfrac{h}{\sqrt{2m(E_k - qU_0)}}$

$= \sqrt{150.4\,\text{eV}/(E_k - qU_0)}\,\text{Å}$

incident particle

scattered particle

- Bragg condition for e^+ or e^- scattering

$$E_k \sin^2\theta = \dfrac{k^2}{d^2} 37.5\,\text{Å}^2\,\text{eV} + qU_0$$

- example:

  Si: $qU_0 = \pm 12\,\text{eV},\ d = 3.14\,\text{Å}$

- electron scattering $qU_0 < 0$

$$E_k \sin^2\theta < 0$$

**first order Bragg peak ($k = 1$)
from surface parallel planes not visible**

RHEPD = Reflection High-Energy Positron Diffraction

• Snell law $\quad \dfrac{\lambda}{\lambda_s} = \dfrac{\cos\theta}{\cos\theta_s}$
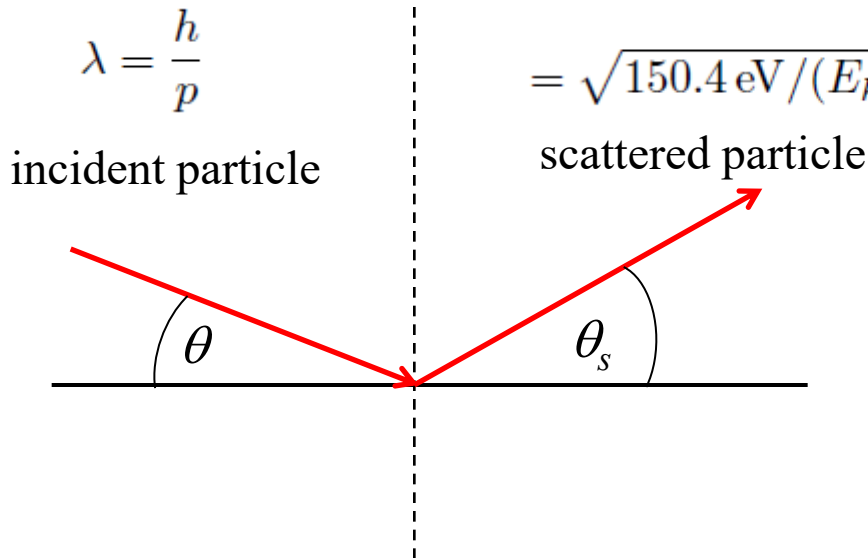
• de Broglie wavelength

• Bragg condition $\quad 2d\sin\theta_s = k\lambda_s$

• inter-planar distance

$$\lambda_s = \frac{h}{p_s} = \frac{h}{\sqrt{2m(E_k - qU_0)}}$$

$$= \sqrt{150.4\,\text{eV}/(E_k - qU_0)}\,\text{Å}$$

$$\lambda = \frac{h}{p}$$

incident particle

scattered particle

θ $\qquad$ θ_s

• Bragg condition for e$^+$ or e$^-$ scattering

$$E_k\sin^2\theta = \frac{k^2}{d^2} 37.5\,\text{Å}^2\,\text{eV} + qU_0$$

• example:

$\quad$ Si: $qU_0 = \pm 12\,\text{eV}, \ d = 3.14\,\text{Å}$

• positron scattering $qU_0 > 0$

$$E_k\sin^2\theta > 0$$

first order Bragg peak (k = 1) observable

• **total reflection critical angle**

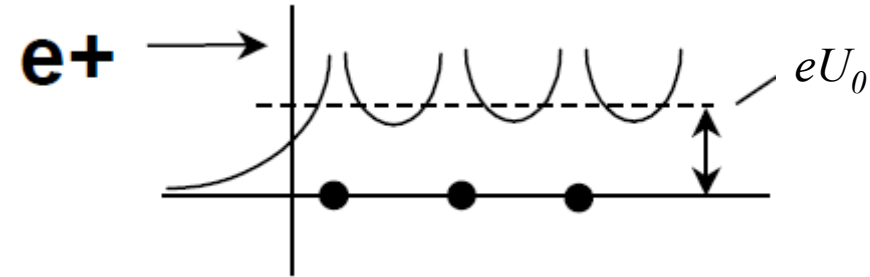$$\theta_C = \arcsin\left(\sqrt{eU_0/E_k}\right)$$

RHEPD = Reflection High-Energy Positron Diffraction

• **RHEPD**

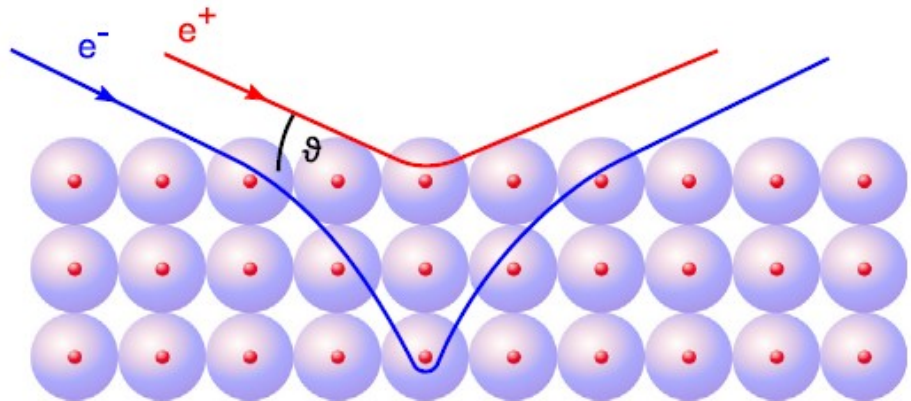$$\left(-\frac{\hbar}{2m}\nabla^2 + eU_0\right)\psi = E\psi$$

• outside crystal $V = 0$

• inside crystal $V > 0$

• **total positron reflection**

$$\theta_C = \arcsin\left(\sqrt{eU_0/E_k}\right)$$

• positron wave vector can be decomposed into longitudinal and transversal component

$$E_k = \frac{p^2}{2m} = \frac{h^2k^2}{2m} = \frac{h^2k_L^2}{2m} + \frac{h^2k_T^2}{2m} = E_{k,L} + E_{k,T}$$

$$E_{k,T} = E_k \sin^2\theta \longrightarrow \theta_C = \arcsin\left(\sqrt{eU_0/E_k}\right)$$

RHEPD = Reflection High-Energy Positron Diffraction

- **RHEPD**

$$\left(-\frac{\hbar}{2m}\nabla^2 + eU_0\right)\psi = E\psi$$

- outside crystal $V = 0$
- inside crystal $V > 0$

- **total positron reflection**
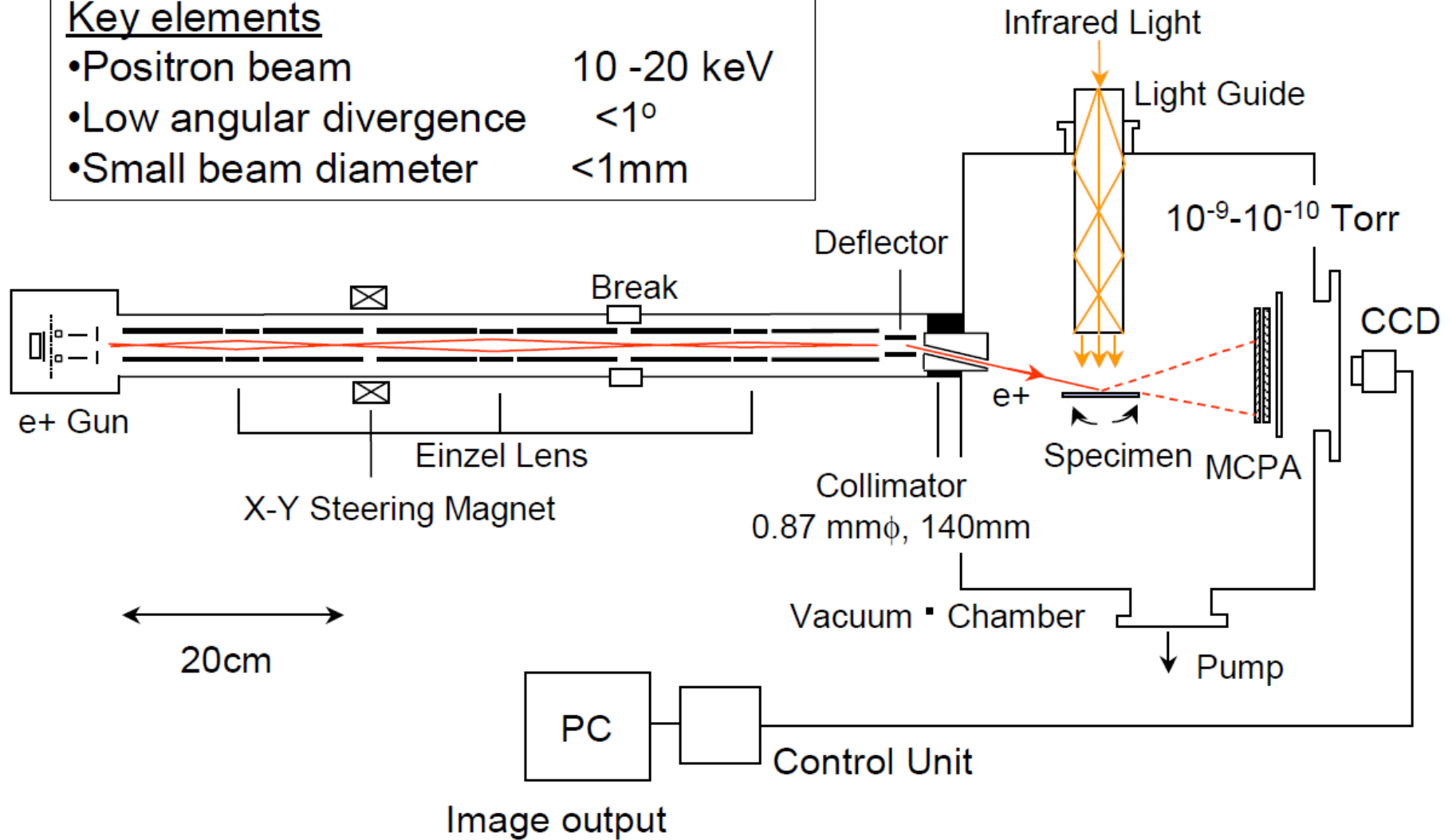
$$\theta_C = \arcsin\left(\sqrt{eU_0/E_k}\right)$$

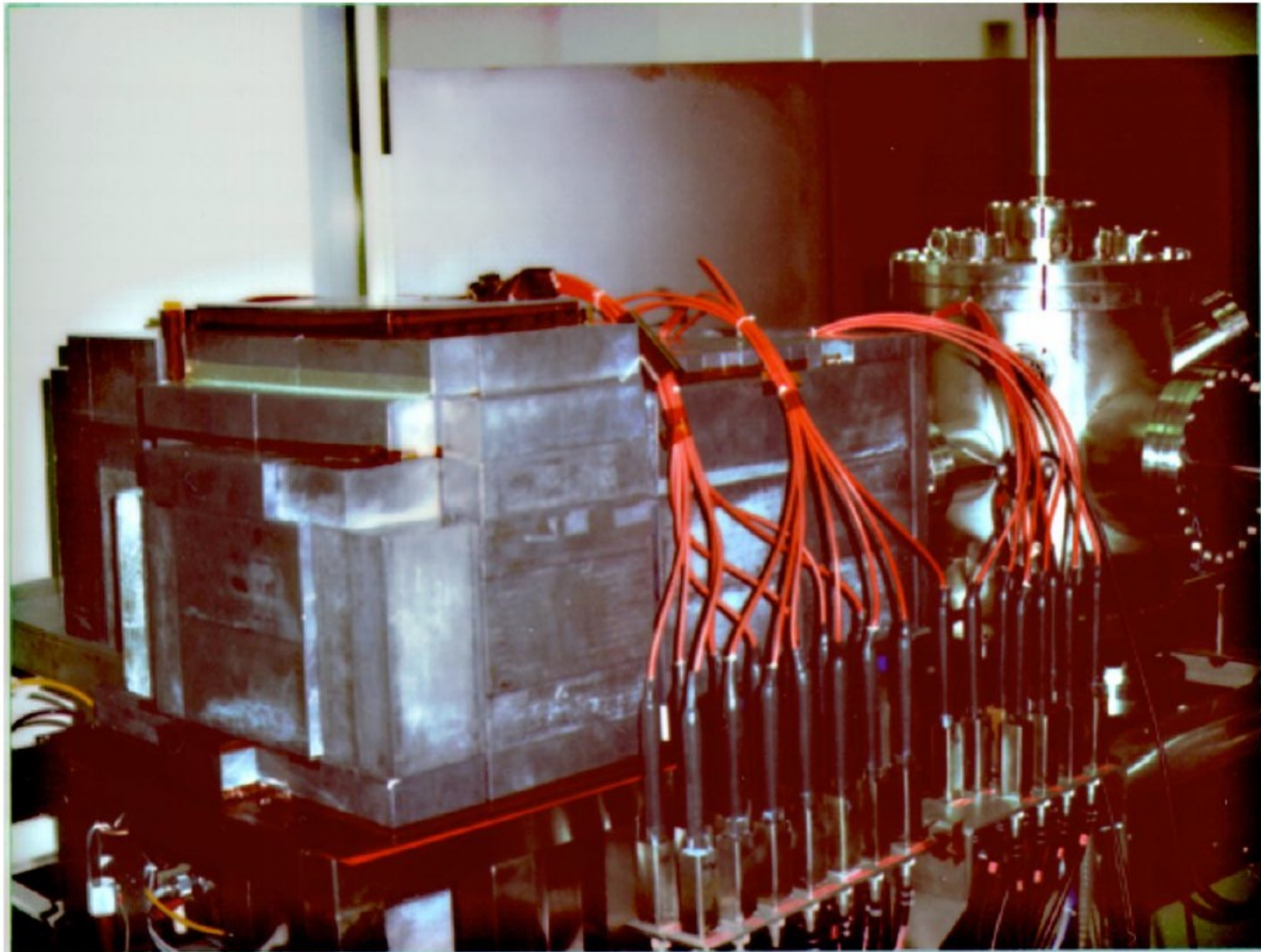- example Si: $\theta_C = 2^\circ$ for 10 keV positrons
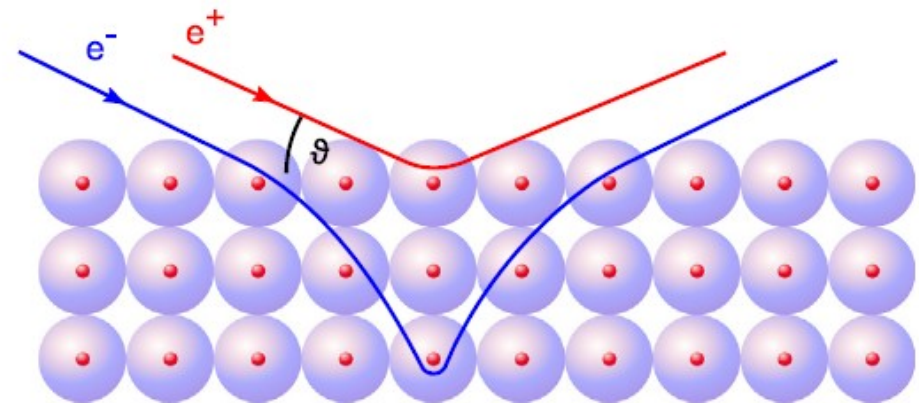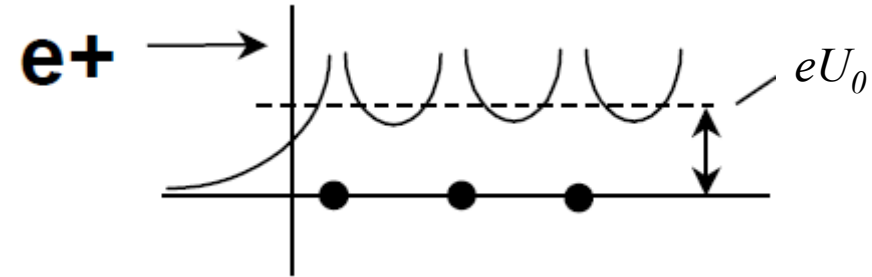
RHEPD = Reflection High-Energy Positron Diffraction

Key elements
- Positron beam   10 -20 keV
- Low angular divergence   <1°
- Small beam diameter   <1mm

Infrared Light
Light Guide
10^{-9}-10^{-10} Torr
Deflector
Break
CCD
e+ Gun
e+
Einzel Lens
Specimen MCPA
X-Y Steering Magnet
Collimator
0.87 mmφ, 140mm
20cm
Vacuum · Chamber
Pump
PC
Control Unit
Image output

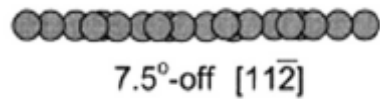# RHEPD = Reflection High-Energy Positron Diffraction

RHEPD = Reflection High-Energy Positron Diffraction

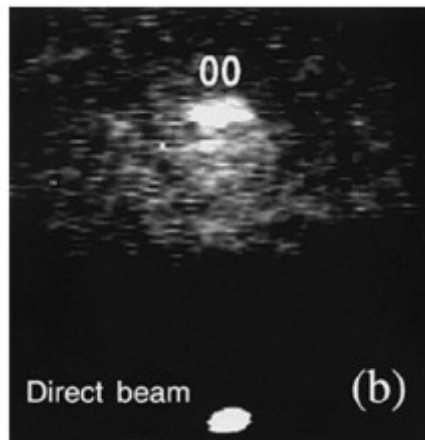• **electrostaticaly guided beam**
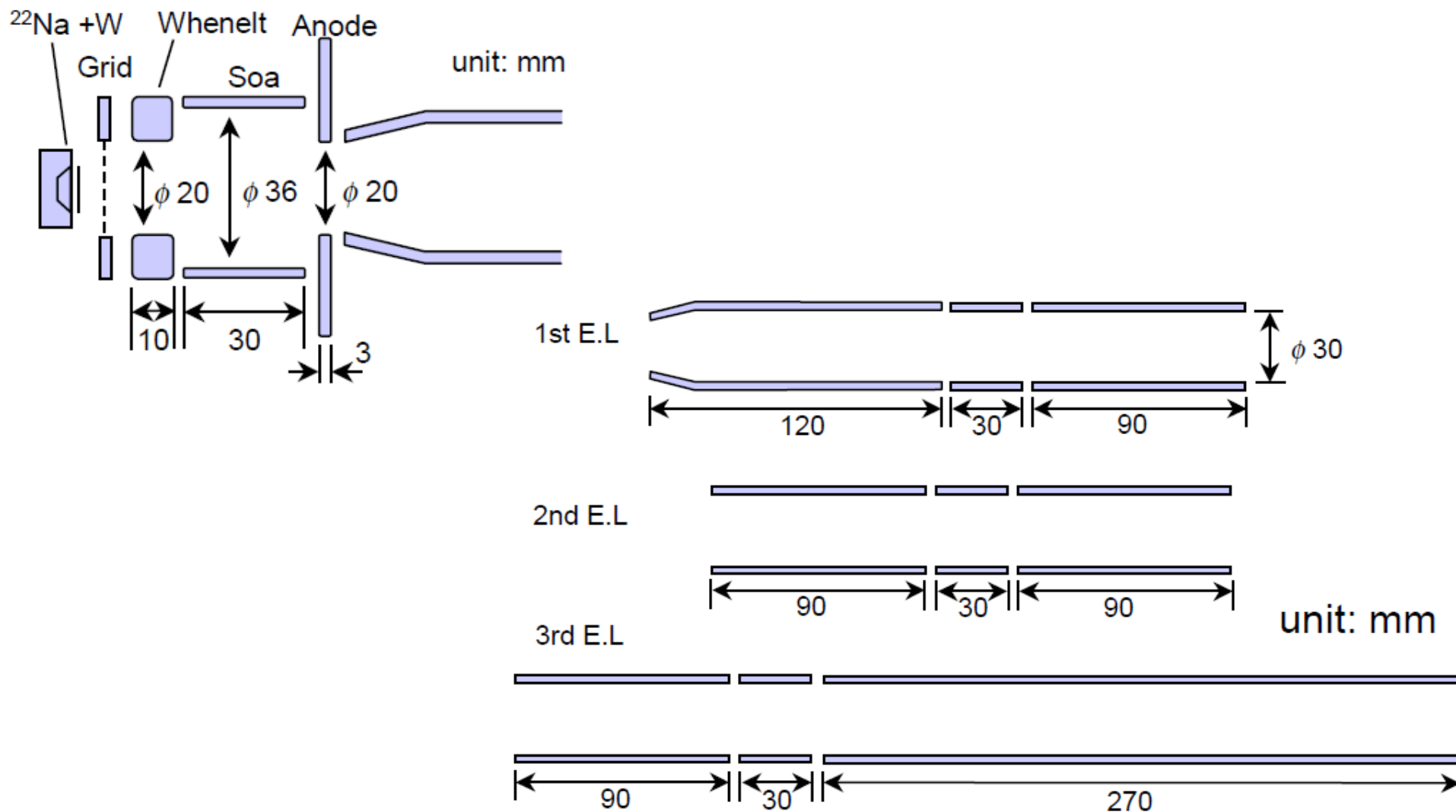
RHEPD = Reflection High-Energy Positron Diffraction
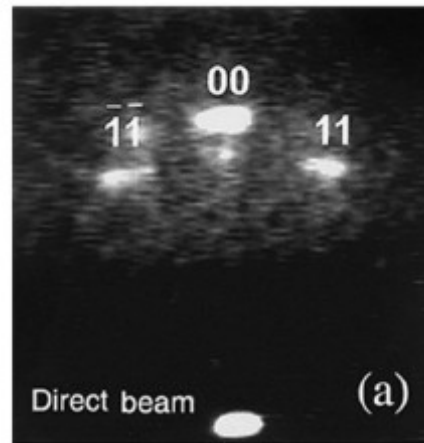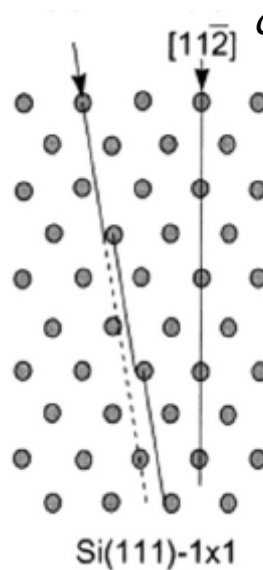
• **electrostaticaly guided beam**
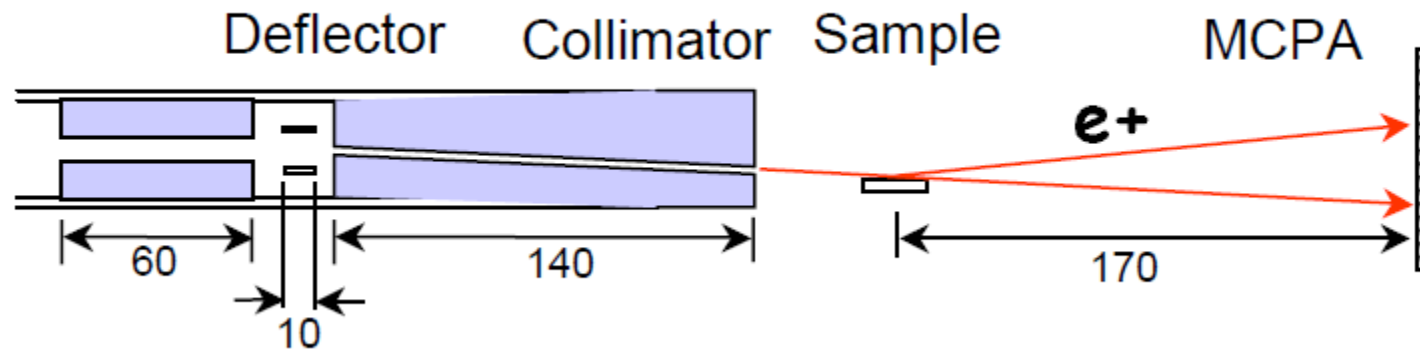
RHEPD = Reflection High-Energy Positron Diffraction

• **Si (111)** *unreconstructed surface*

Direct beam (b)

7.5°-off [11$\bar{2}$]

7.5° off [11-2] direction
one beam condition

Direct beam (a)

[11$\bar{2}$]

many beam condition

[11$\bar{2}$]

Si(111)-1x1

RHEPD = Reflection High-Energy Positron Diffraction
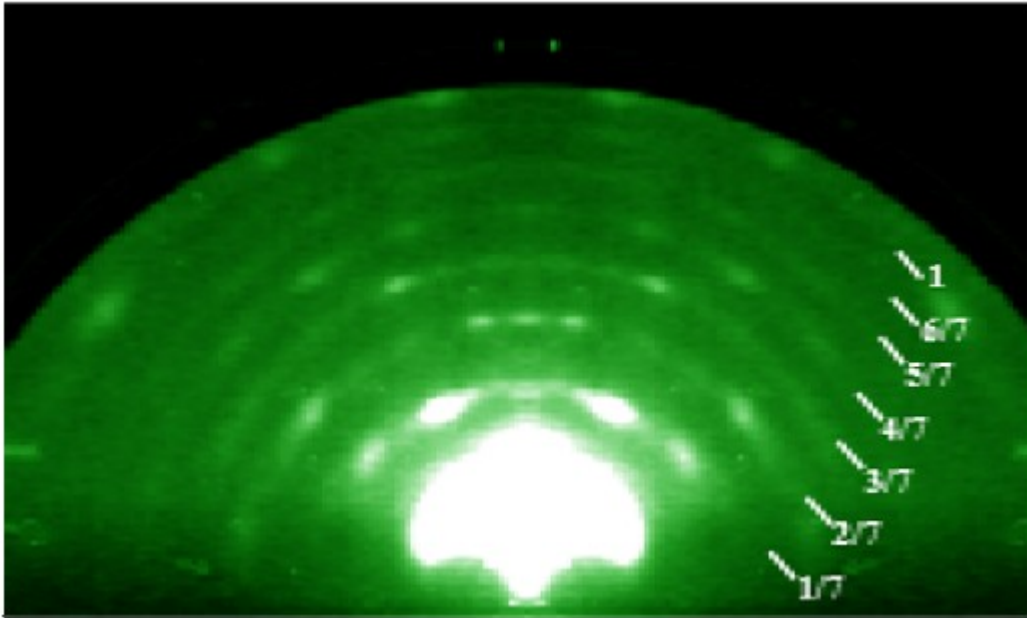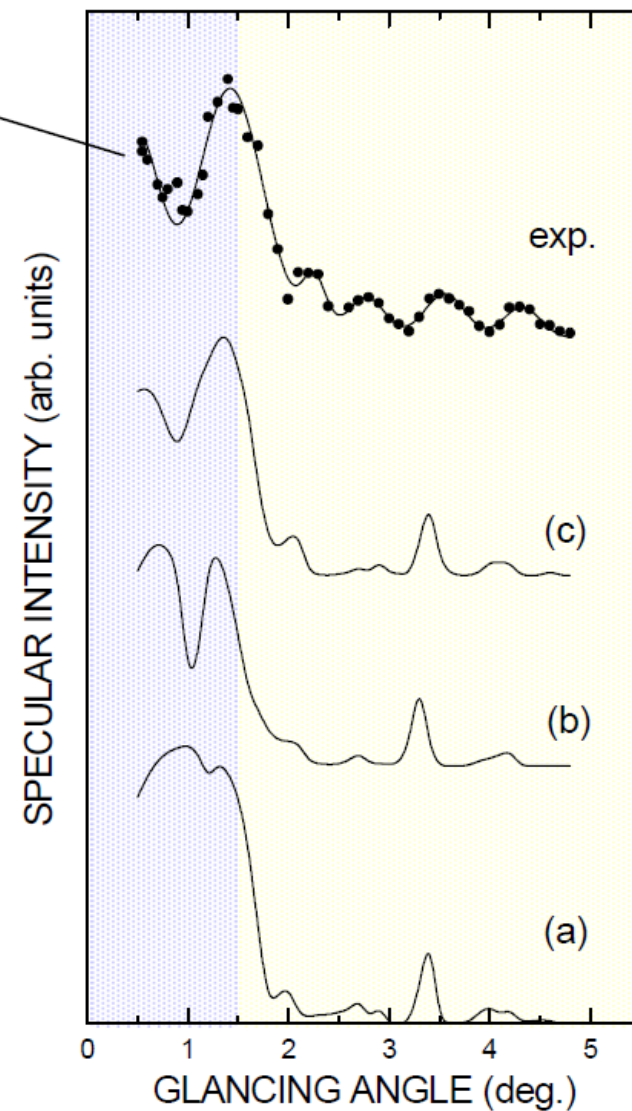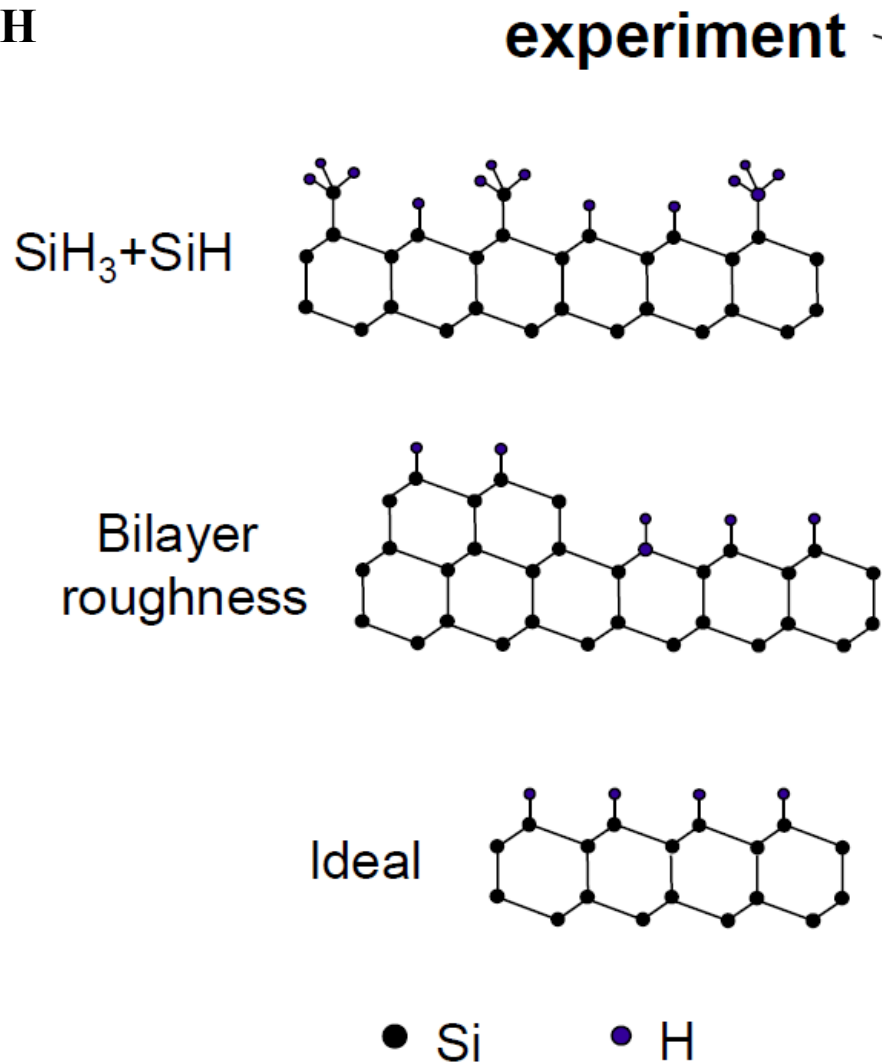
- **Si (111) H**

RHEPD
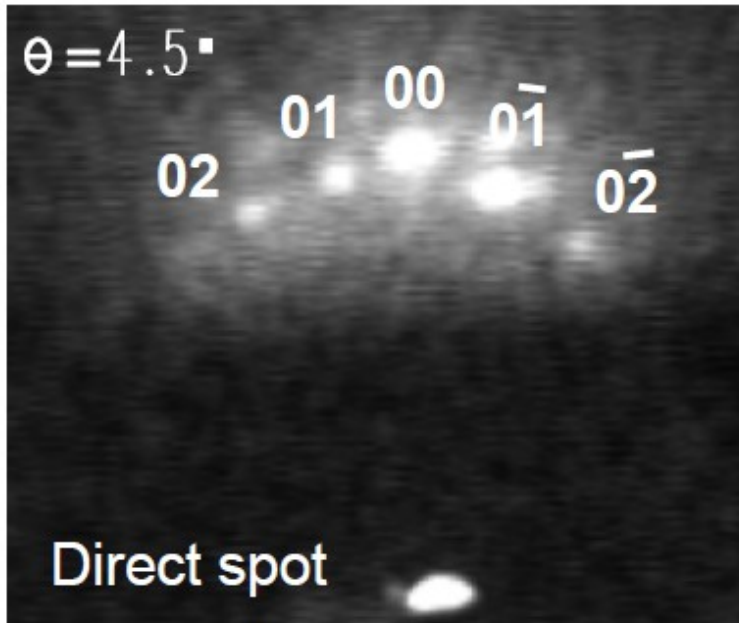
RHEED

RHEPD = Reflection High-Energy Positron Diffraction

- **Rocking curve**
- **Si (111) H**

RHEPD = Reflection High-Energy Positron Diffraction

- **Rocking curve**
- **Si (111) H**

SiH$_3$+SiH

Bilayer roughness

Ideal

experiment

exp.

(c)

(b)

(a)

SPECULAR INTENSITY (arb. units)
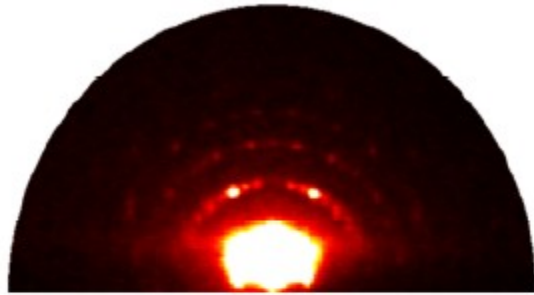
GLANCING ANGLE (deg.)

● Si ● H

TRHEPD = Total Reflection High-Energy Positron Diffraction
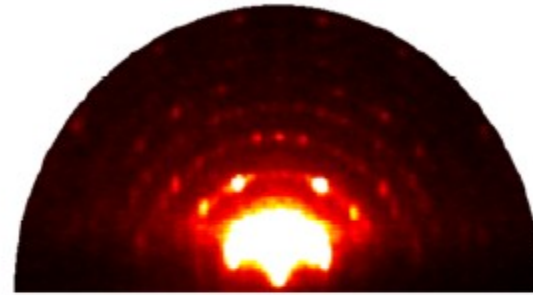
• **Si (111) 7 x 7 reconstructed surface**

TRHEPD
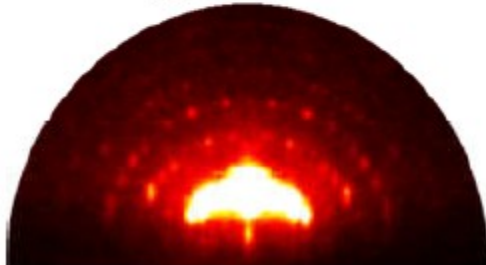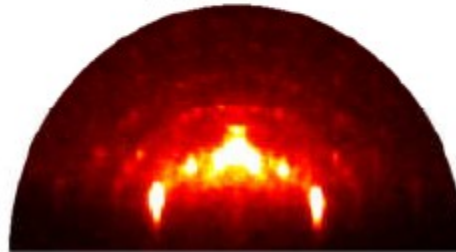
(1) $\theta = 1.3°$ (total reflection)

RHEPD

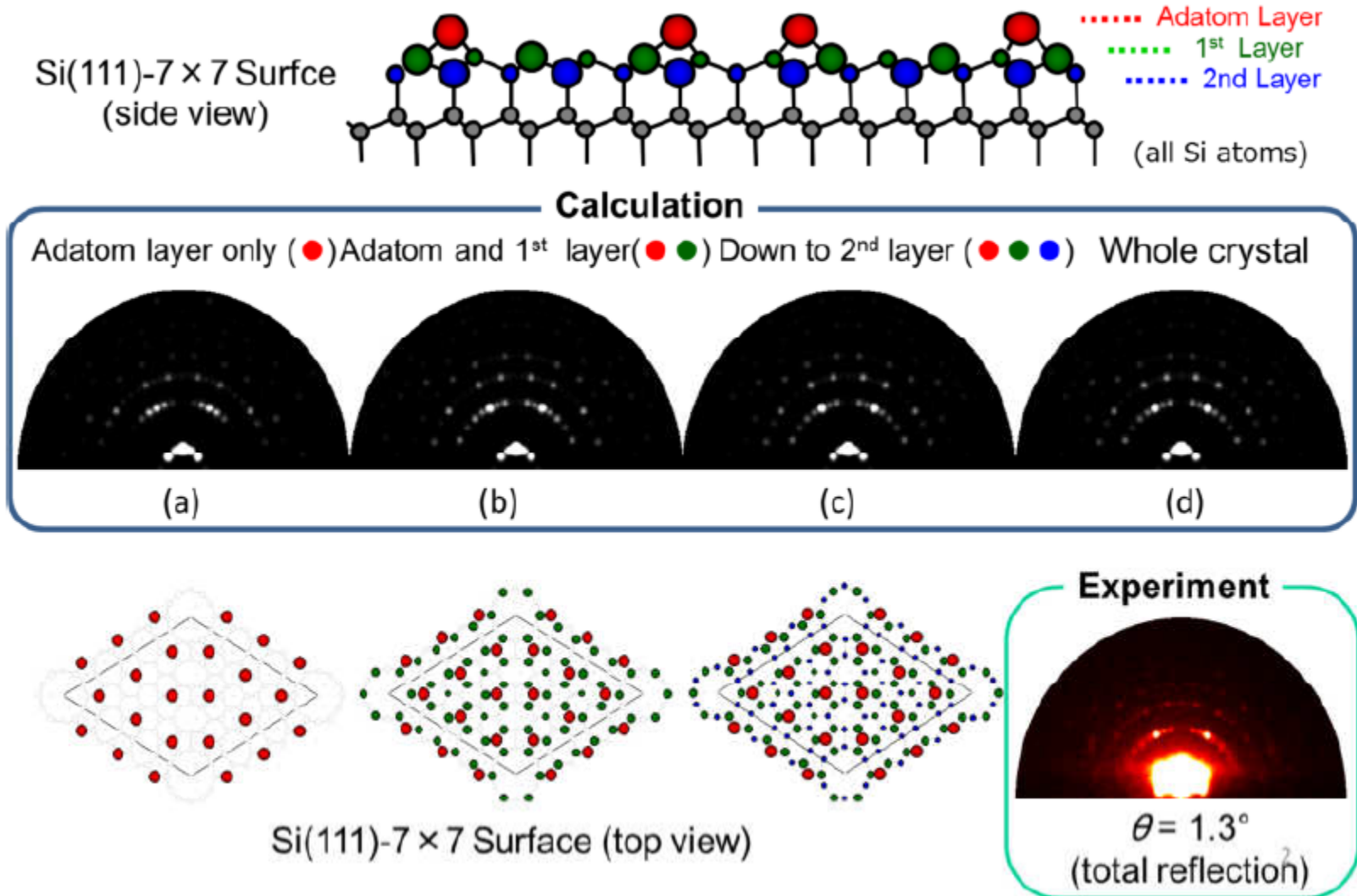(2) $\theta = 2.1°$

(3) $\theta = 2.9°$

(4) $\theta = 3.9°$

(5) $\theta = 4.9°$

TRHEPD = Total Reflection High-Energy Positron Diffraction

- **Si (111) 7 x 7 reconstructured surface**   **TRHEPD**

Si(111)-7 × 7 Surfce (side view)

⋯⋯ Adatom Layer
⋯⋯ 1st Layer
⋯⋯ 2nd Layer

(all Si atoms)

Calculation

Adatom layer only (●) Adatom and 1st layer (● ●) Down to 2nd layer (● ● ●) Whole crystal

(a)   (b)   (c)   (d)

Si(111)-7 × 7 Surface (top view)

Experiment

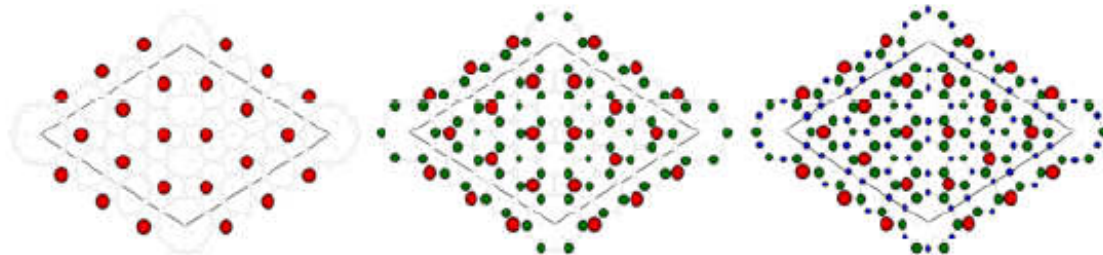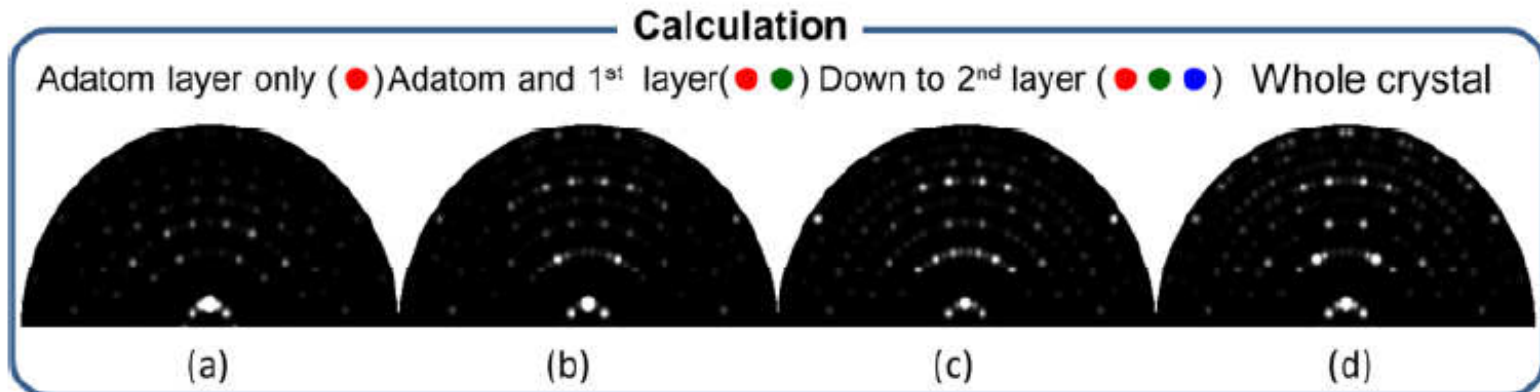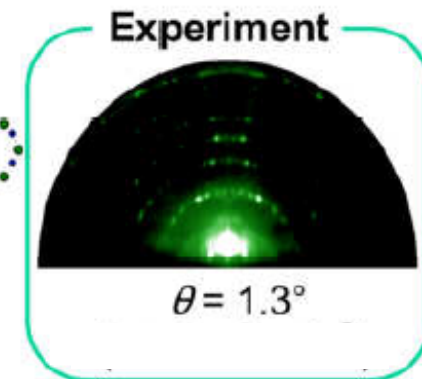$\theta = 1.3°$
(total reflection)

RHEED = Reflection High-Energy Electron Diffraction

• **Si (111) 7 x 7 reconstructured surface   RHEED**

RHEED = Reflection High-Energy Electron Diffraction
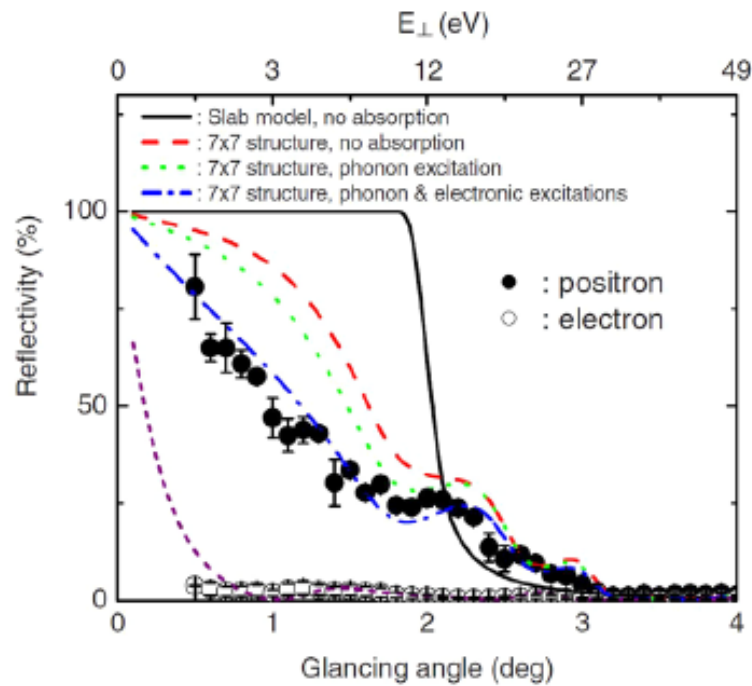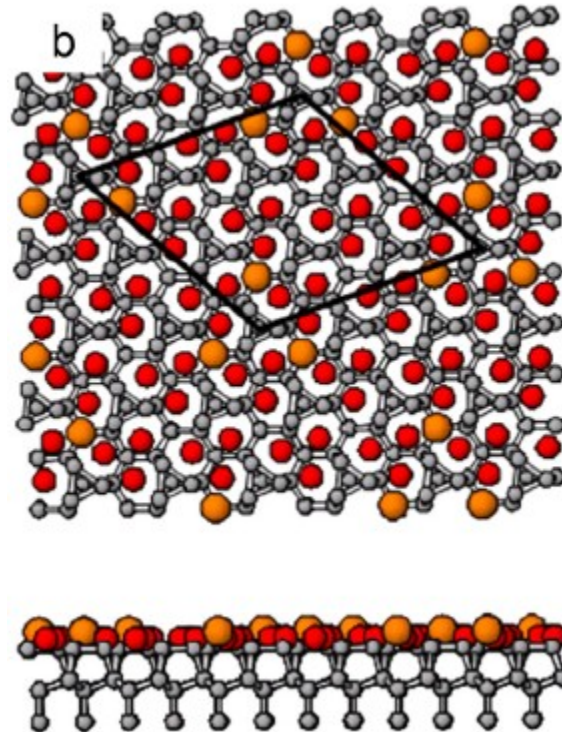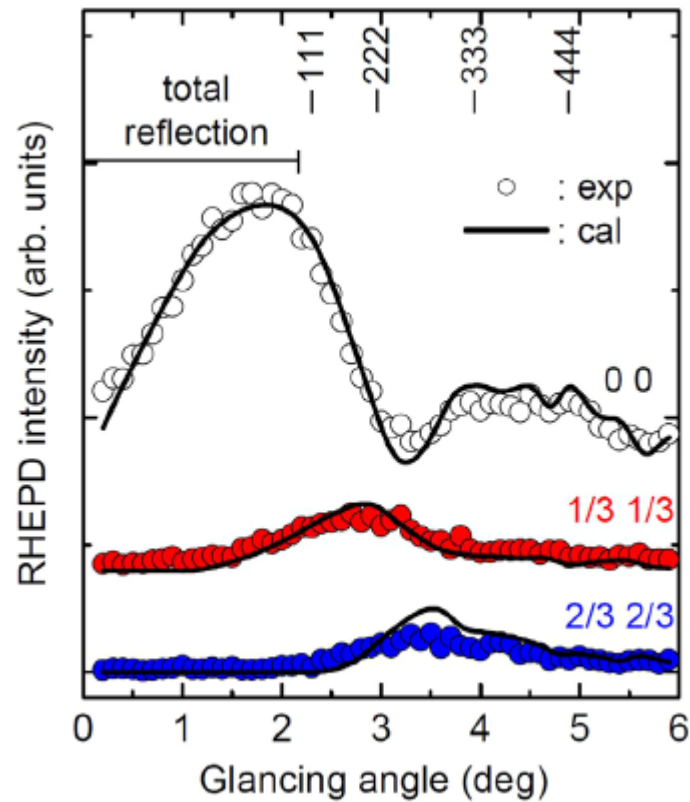
• **Si (111) 7 x 7 reconstructured surface**

absolute reflectivness
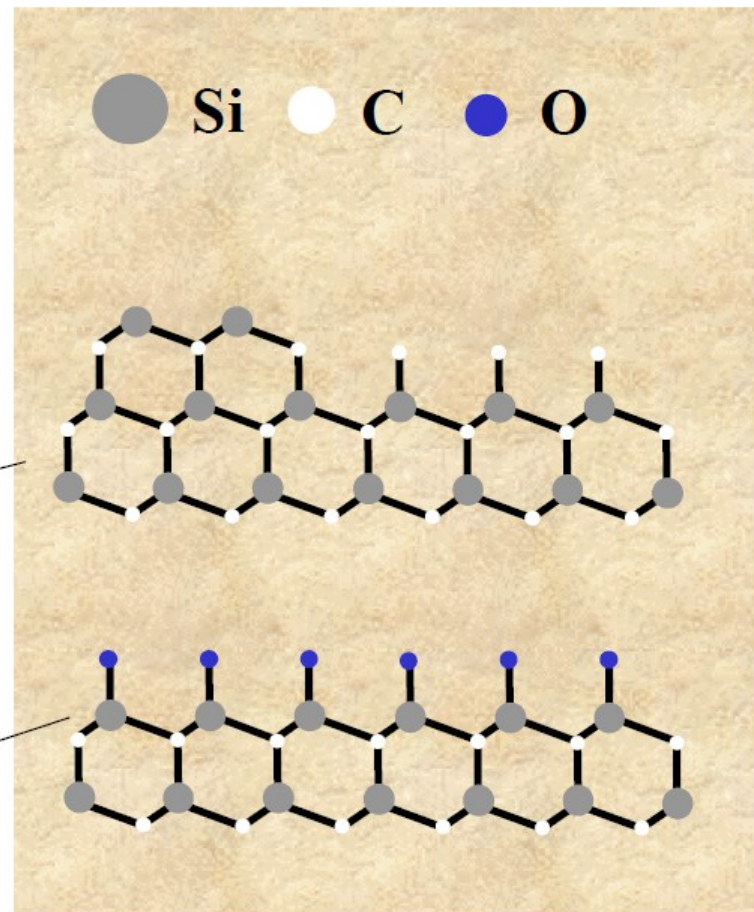
RHEED = Reflection High-Energy Electron Diffraction
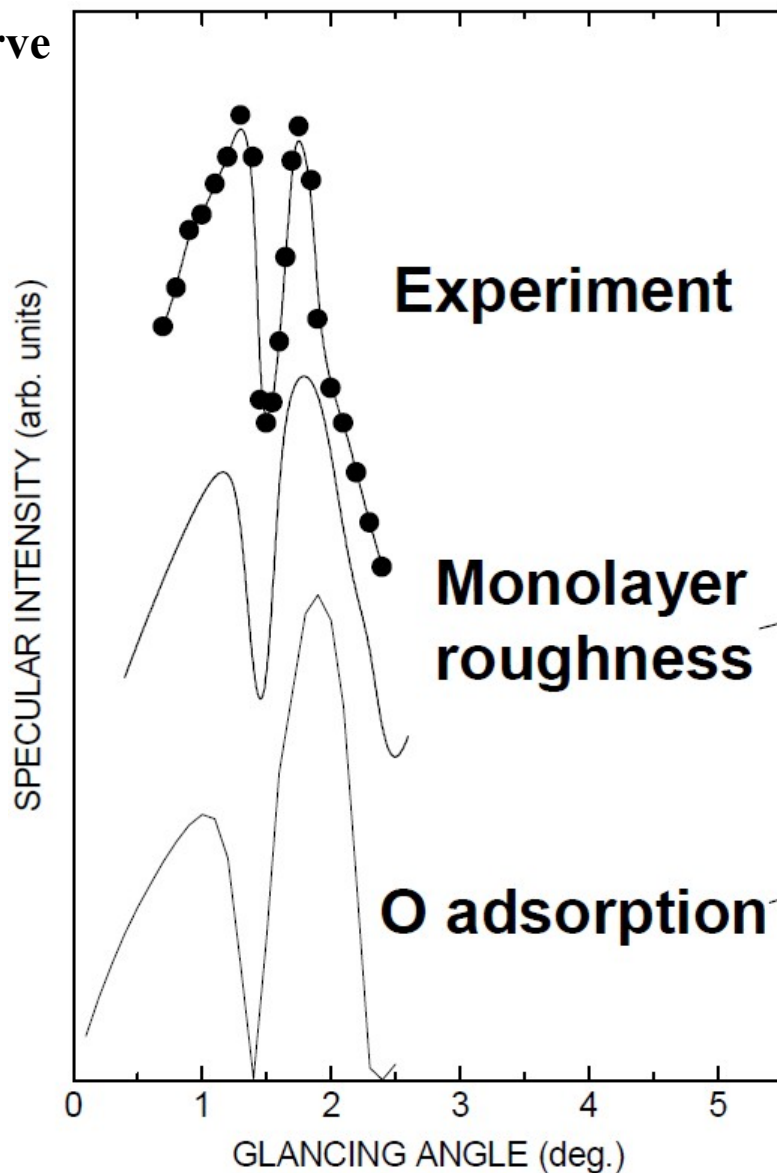
$$Si(111) - \sqrt{21} \times \sqrt{21} - Ag$$
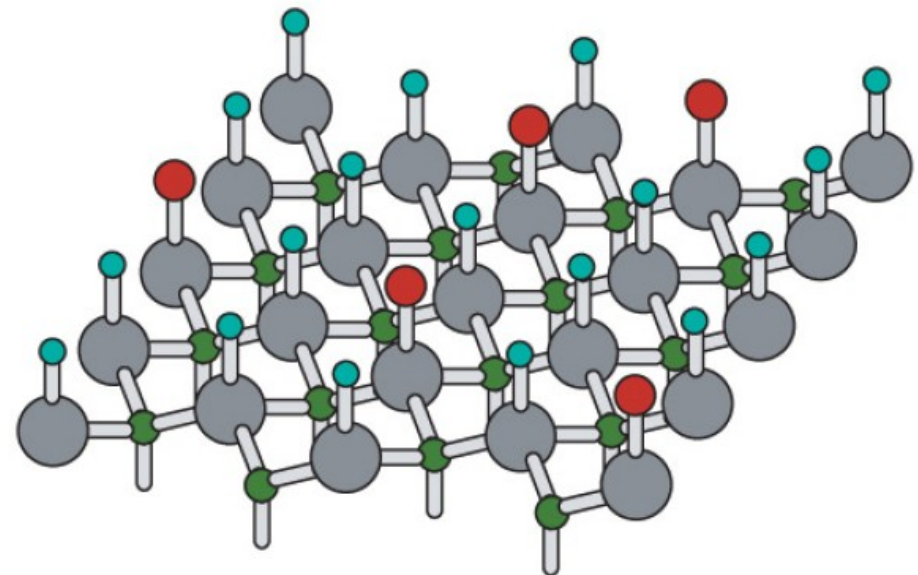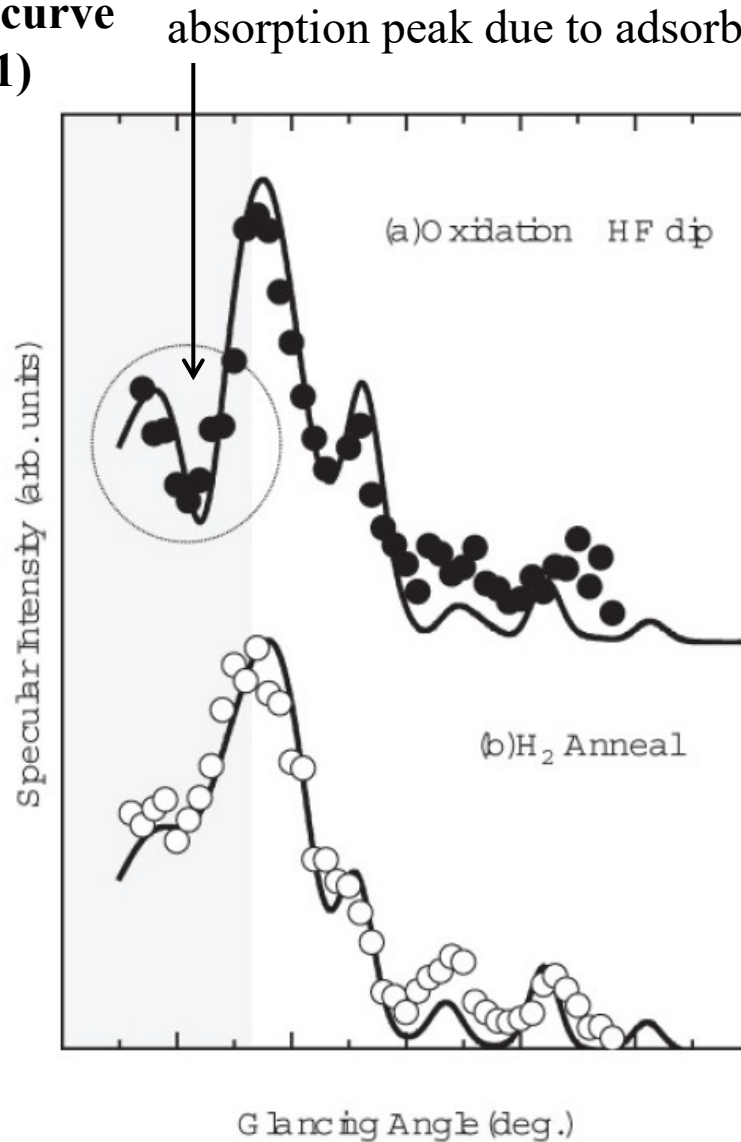

• many beam condition

RHEPD = Reflection High-Energy Positron Diffraction

- **Rocking curve**
- **SiC (0001)**

RHEPD = Reflection High-Energy Positron Diffraction

- **Rocking curve**
- **SiC (0001)**

absorption peak due to adsorbed oxygen

RHEPD = Reflection High-Energy Positron Diffraction

- **Rocking curve** Flashing by infra red lamp at 1020ºC in UHV → full covering by graphite monolayer
- **SiC (0001)**

1020 x10m in anneal

Specular intensity (arb. units)

Glancing angle (deg.)

○ Si ● C ⬡○ Graphite