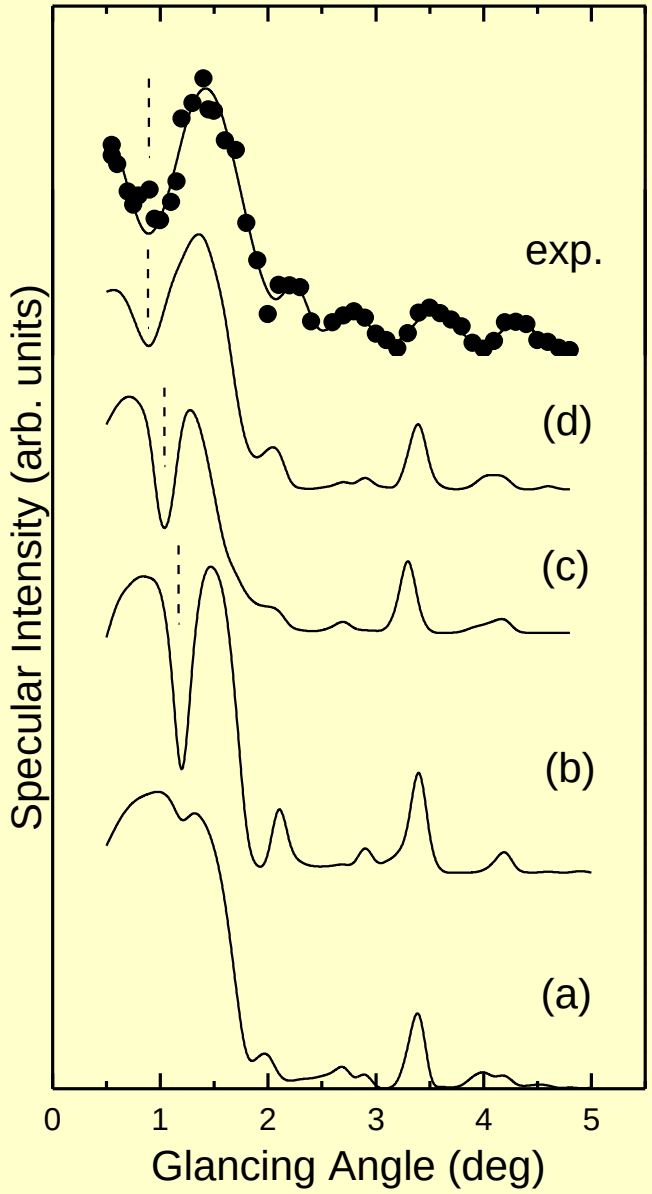
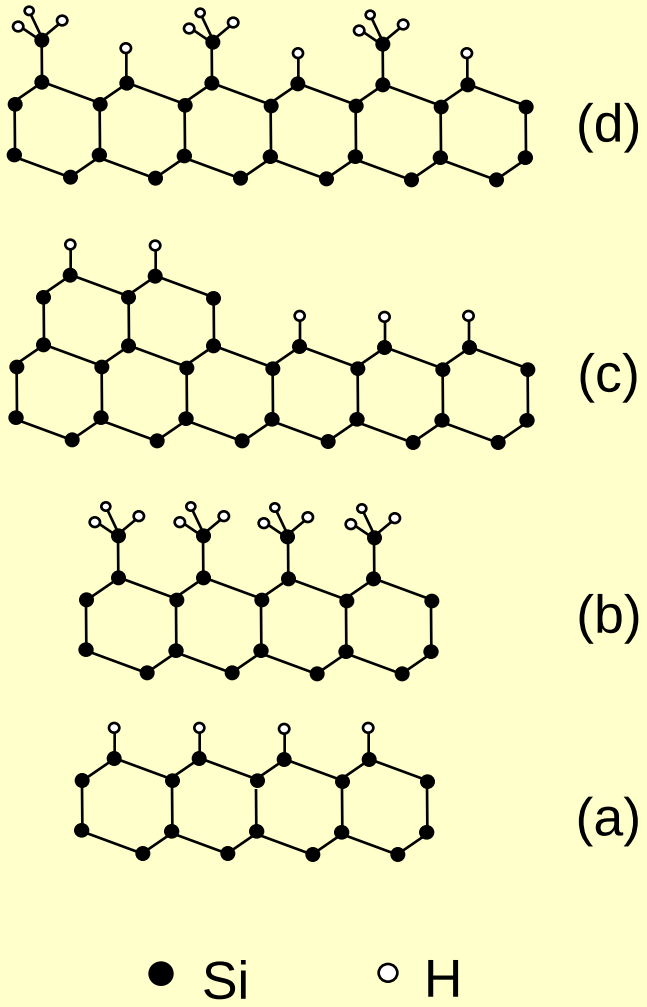
RHEPD intensity from Si(111)(1x1)-H surface for 15keV positrons.

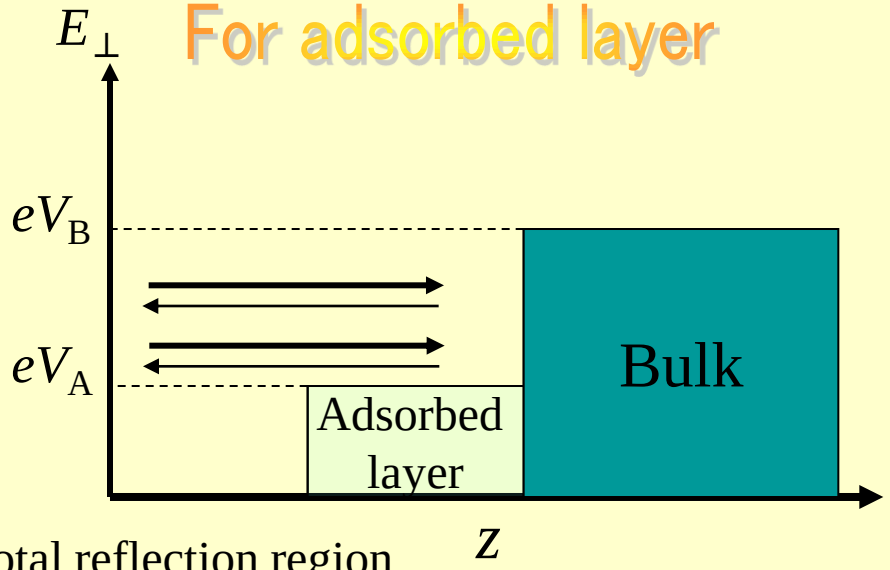


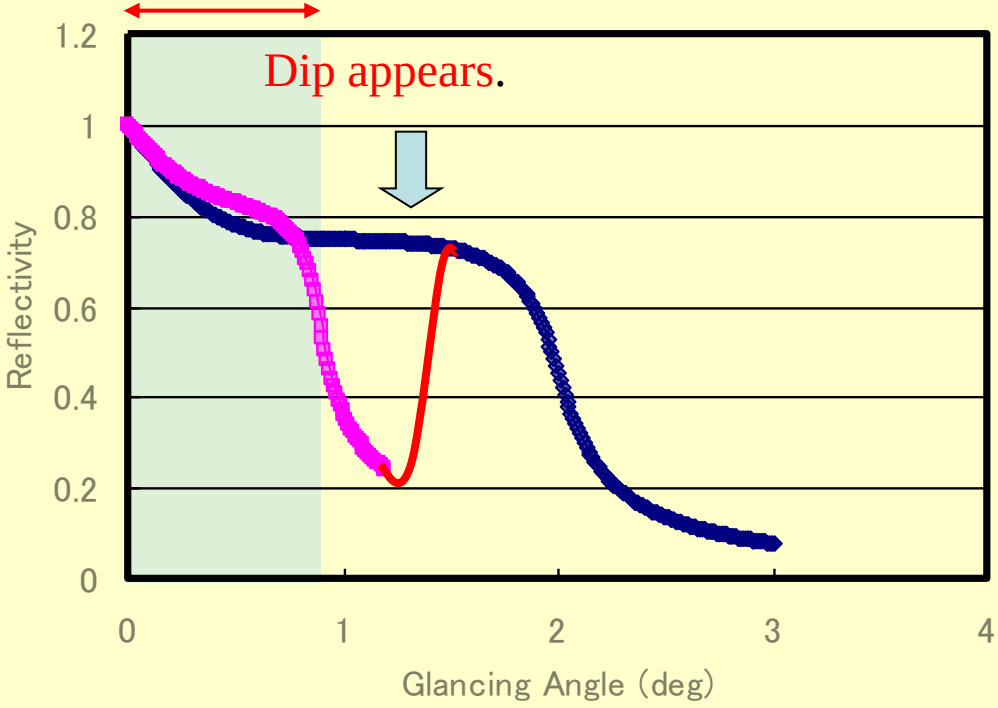

A. Kawasuso *et al.*

PRB61(2000)2102.

# For adsorbed layer



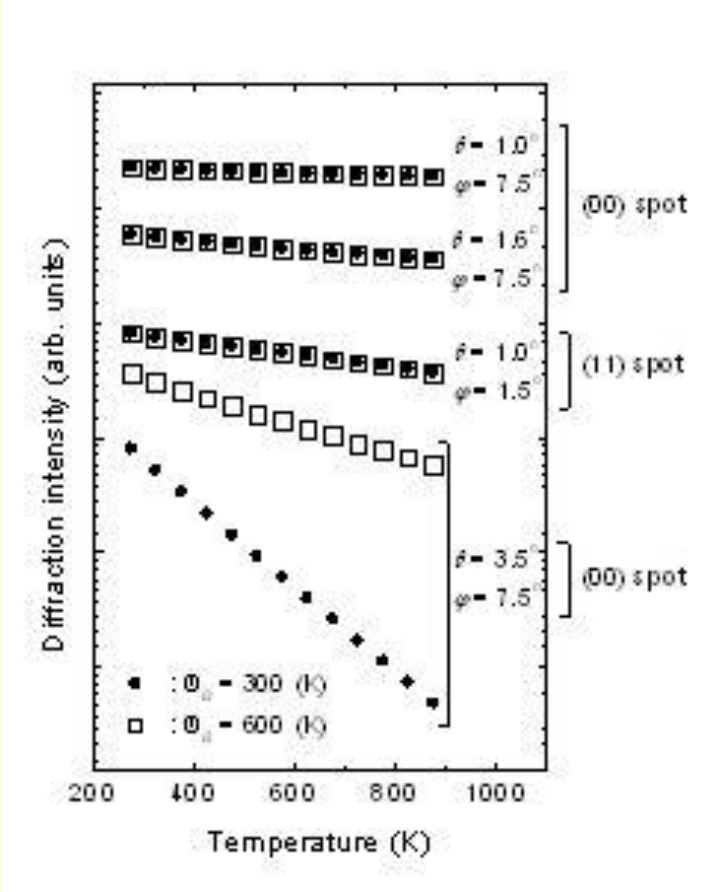

Total reflection region by adsorbed layer.




A dip appears at the total reflection region for bulk layers due to absorption effect in the adsorbed layer.

# Temperature dependence of RHEPD intensities from the Si(111)7x7

Fukaya et al. PRB **70**, 245422 (2004)

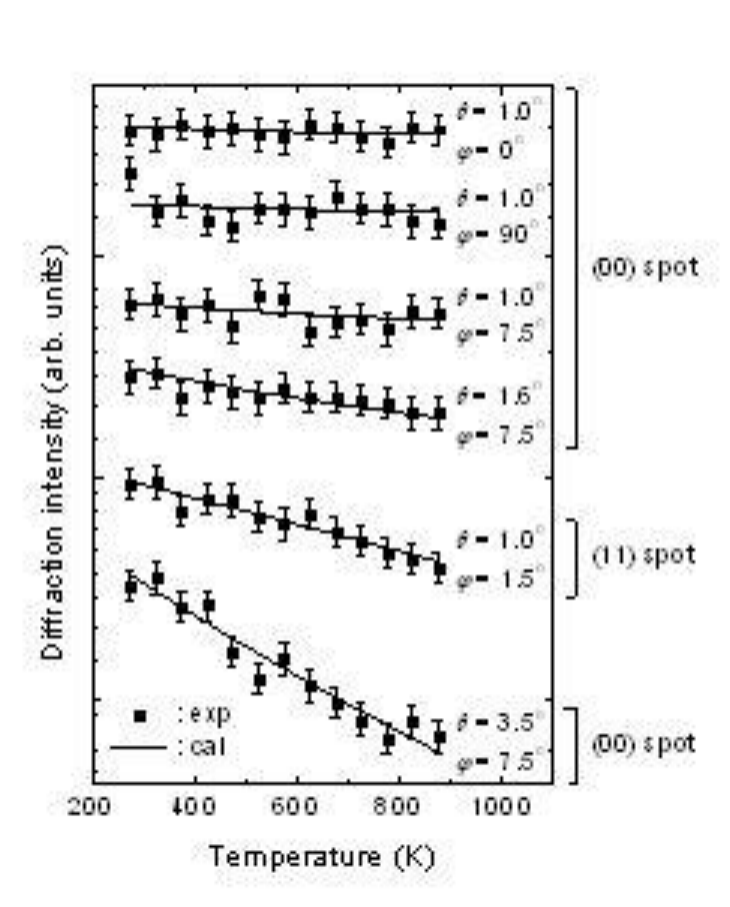



Calculated intensities for surface Debye temperature of 300K with bulk Debye temperatures of 300K (black circle) and 600K (white square).

At the total reflection condition, glancing angles θare 1.0° and 1.6°, intensities are mostly the same for different bulk Debye temperatures, but out of the region, θ= 3.5°, the intensities depend largely for the bulk Debye temperatures.

# Temperature dependence of RHEPD intensities from the Si(111)7x7

Fukaya et al. PRB **70**, 245422 (2004)




Experimental results

Surface Debye Temperature: 310 K

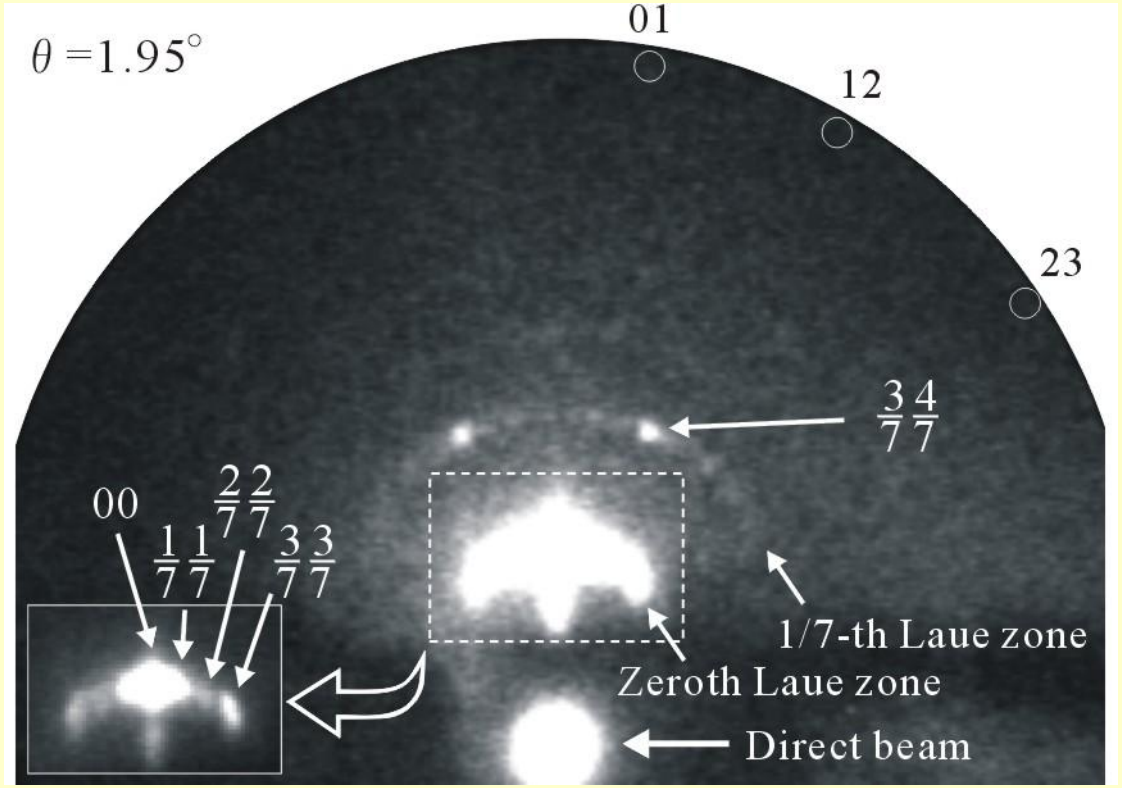
Root mean square of atomic vibration amplitude:
0.014 nm at room temperature.
0.025 nm at surface phase transition temperature of Si(111) at about 1000 K.

Bulk Debye Temperature: 600 K

Root mean square of atomic vibration amplitude:
0.02 nm at boiling temperature of silicon.

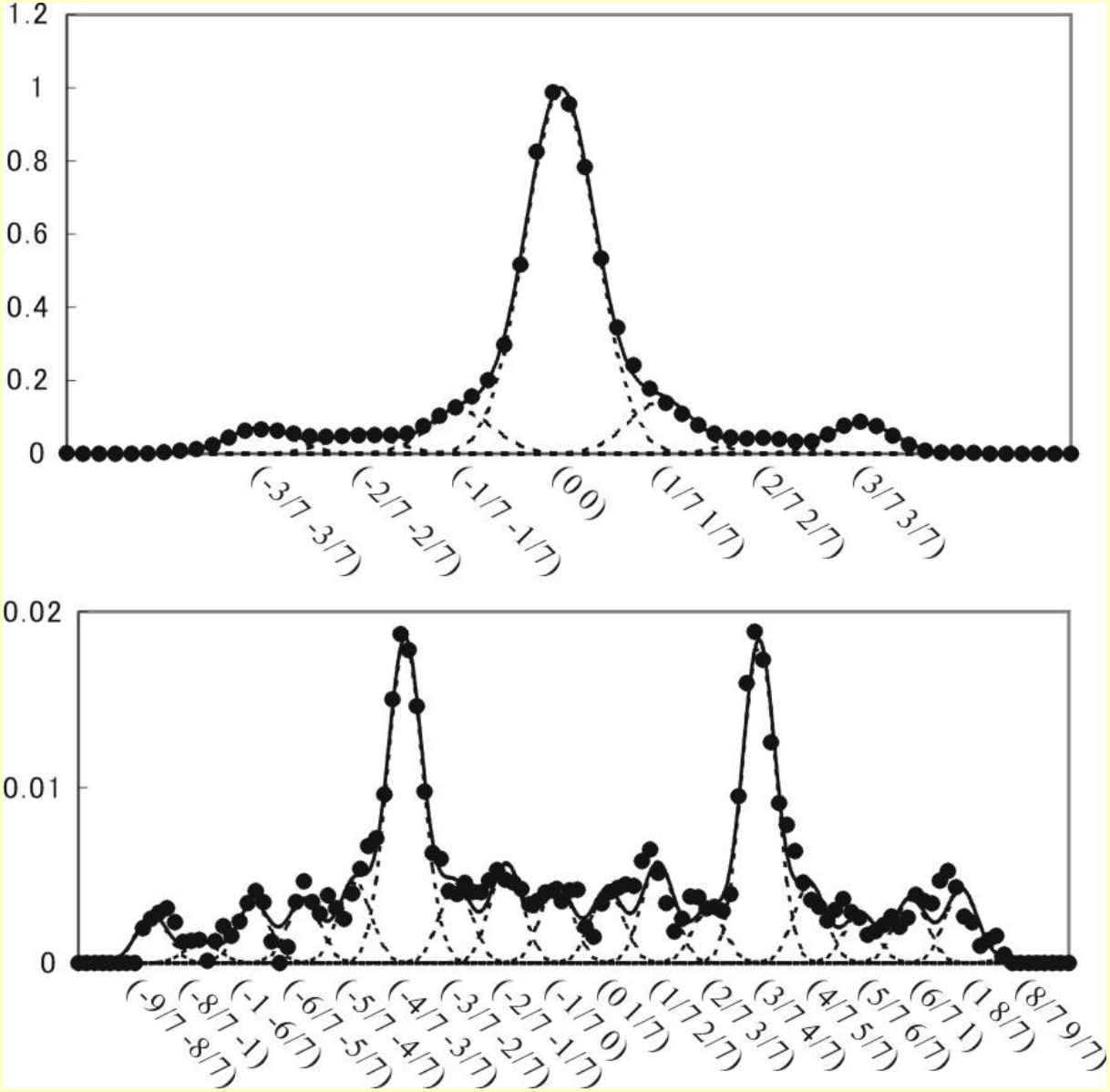
# Structural analysis of Si(111)7x7 surface by RHEPD pattern

K.Hayashi et al.
Surf. Sci. 600, 4426 (2006)




Total reflection positron diffraction pattern from Si(111)7x7 surface

Spot profiles of the TREPOD pattern.
Gaussian decomposition




Zero Laue zone

1/7 Laue zone

# Experimental Result and Dynamical Calculation Result
## 519-beam calculation

| Diffraction spots | Experimental intensities of diffraction spots | | | Calculation using bulk atomic potential R=7% | Calculation using modified potential R= 4.4% $A_{ad}$=1.2 $A_{rest}$=0.6. |
|---|---|---|---|---|---|
| 0,0 | 1.00 | | | 1 | 1 |
| 1/7,1/7 | 0.10 | ± | 0.01 | 0.05 | 0.09 |
| 2/7,2/7 | 0.03 | ± | 0.01 | 0.03 | 0.05 |
| 3/7,3/7 | 0.07 | ± | 0.01 | 0.11 | 0.08 |
| 0,1/7 | 0.004 | ± | 0.002 | 0.001 | 0.000 |
| 1/7,2/7 | 0.005 | ± | 0.002 | 0.003 | 0.002 |
| 2/7,3/7 | 0.003 | ± | 0.002 | 0.002 | 0.003 |
| 3/7,4/7 | 0.018 | ± | 0.002 | 0.017 | 0.016 |
| 4/7,5/7 | 0.004 | ± | 0.002 | 0.003 | 0.006 |
| 5/7,6/7 | 0.003 | ± | 0.002 | 0.002 | 0.002 |
| 6/7,1 | 0.003 | ± | 0.002 | 0.003 | 0.003 |
| 1,8/7 | 0.003 | ± | 0.002 | 0.008 | 0.006 |
| 8/7,9/7 | 0.001 | ± | 0.002 | 0.002 | 0.002 |

Good agreement

Good agreement

Modified potential: Electron distributions of adatoms are expanded and those of rest atoms are compressed.

Electron distributions of adatoms and rest atoms on the Si(111)7×7 surface are determined by the intensity analysis of the RHEPD pattern using the modified potential.

Compressed electron distribution (roughly 20%)
or a little more electrons (a little ionized).

Expanded electron distribution
(roughly 10%)