「KEK低速陽電子実験施設における陽電子回折研究およびPsビーム研究の新展開」
2012年10月3日（水）～4日（木）
KEK研究本館小林ホール

陽電子回折への期待

Expectation for positron diffractions

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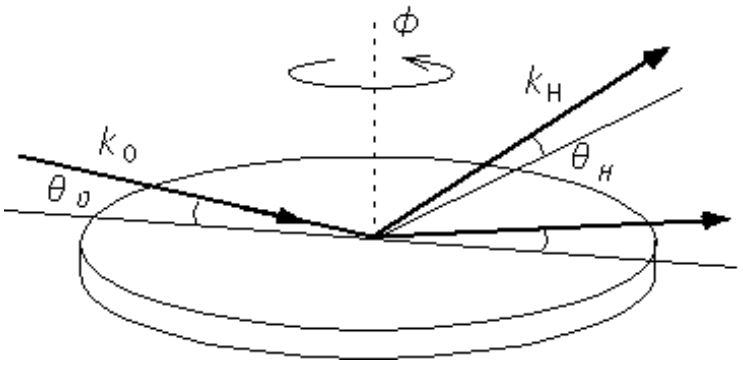
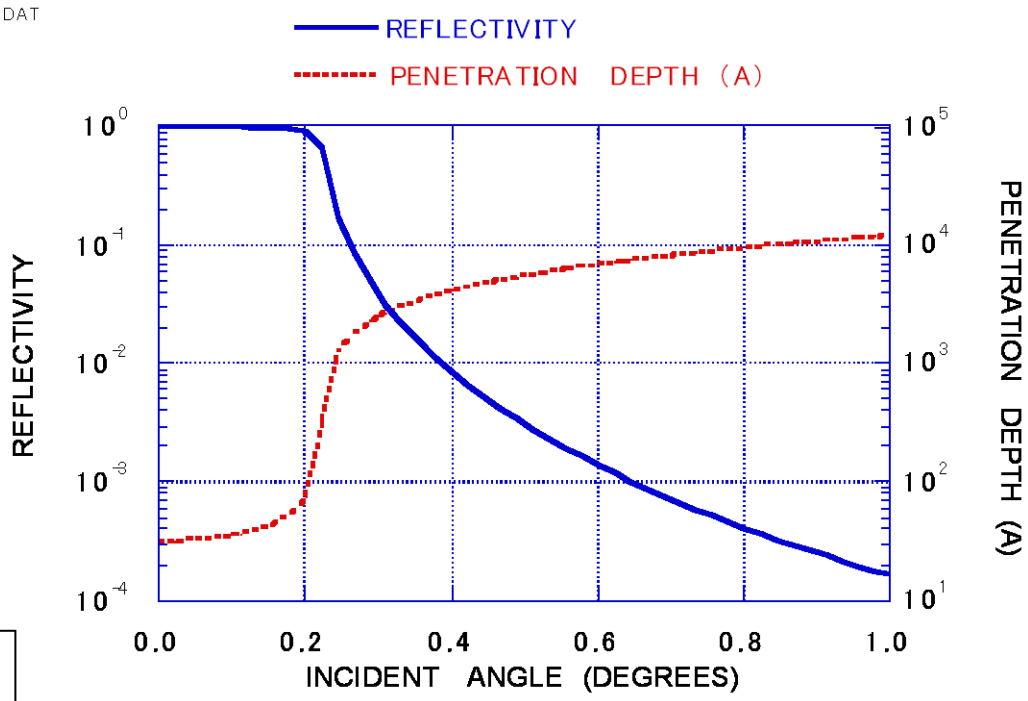
outline

1. Surface X-ray diffraction
2. Difficult cases for SXD
   - large unit cell
   - deeply reconstructed structures
   - substrate with complicated structures
3. Experimental geometry
4. Analysis
   - holography
   - an example of SXD

Grazing incidence in-plane X-ray diffraction
GIXD





全反射

X線の侵入深さ浅い

表面に敏感

散乱ベクトルが面内 :Qz(=L)= 0

表面投影2次元構造

penetration depth:

more than 100 Å

1000 Å to 1μm

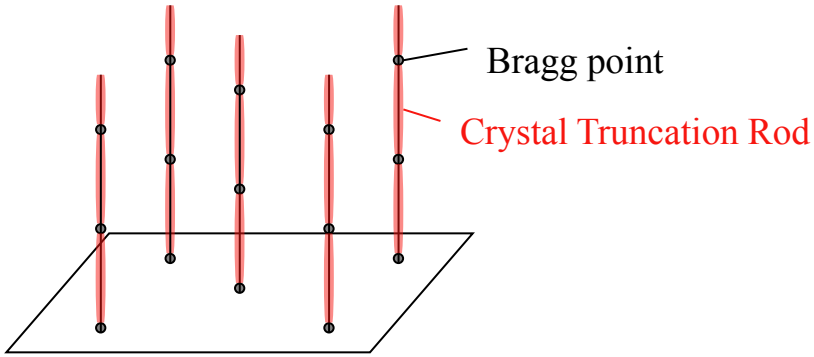
X-ray CTR scattering

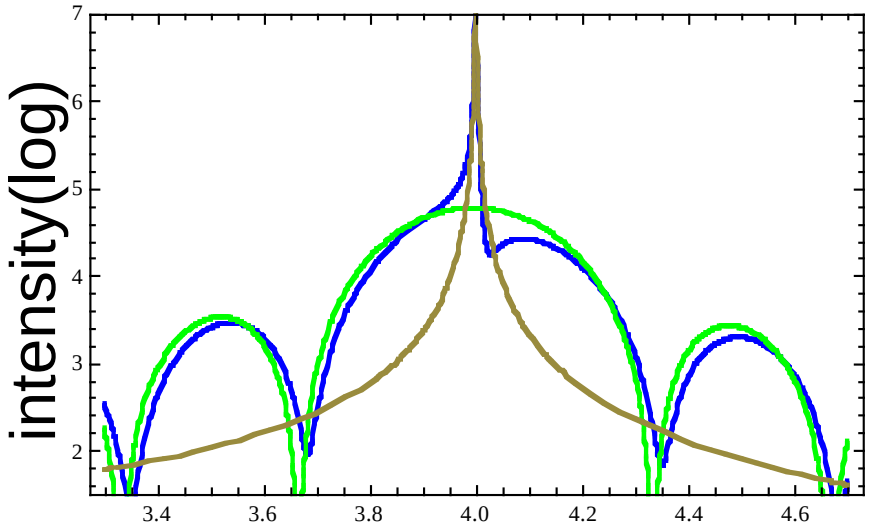
CTR (Crystal Truncation Rod) scattering

$$I(\mathbf{q}) \mu \left| F^{substrate}(\mathbf{q}) + \mathbf{e}^{i\mathbf{q}\times\mathbf{h}} F^{overlayer}(\mathbf{q}) \right|^2$$

干渉項

h: interfacial separation vector





原子レベルの表面・界面構造
薄膜内部構造

Surface Sensitivity in SXD

- Integral order rods
  - rod scan (CTR scattering, reflectivity)
  - in plane (GIXD)

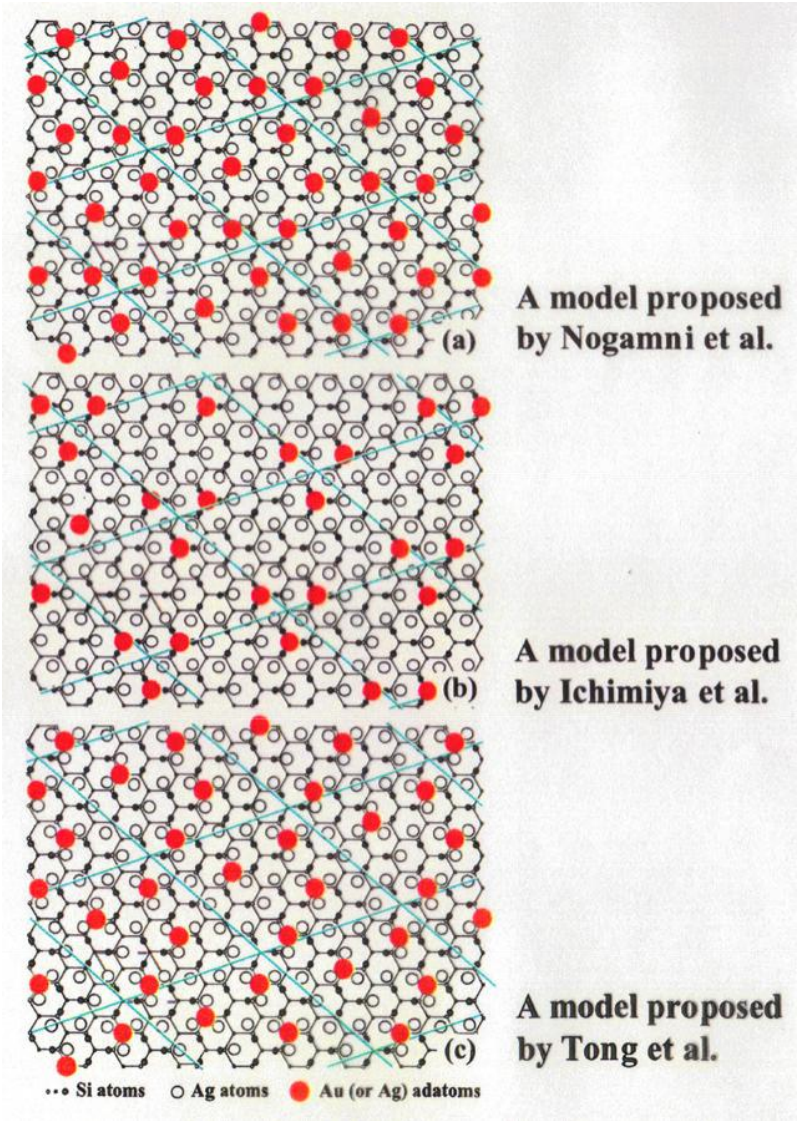
  100 Å to micron meter

- Fractional order rods:
  - rod scan
  - in plane (GIXD)

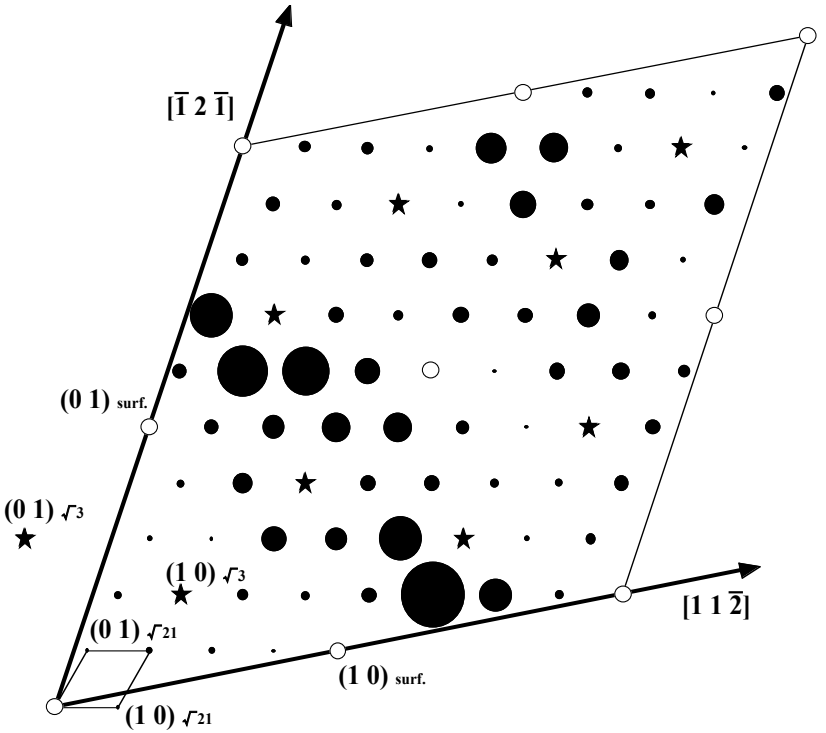
    all reconstructed layers

Si(111)-√21x√21-(Ag+Au)

Au/Si(111)-√3x√3-Ag



GIXD

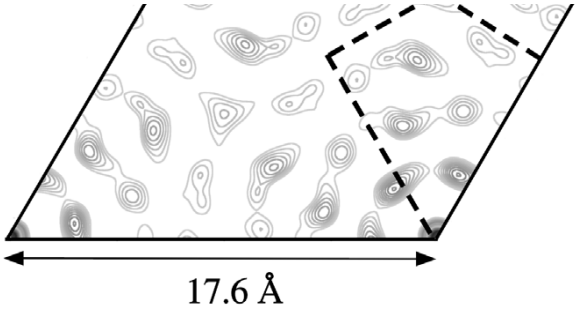


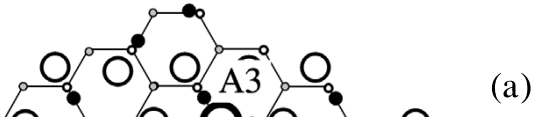
Inequivalentな72点の逆格子を測定

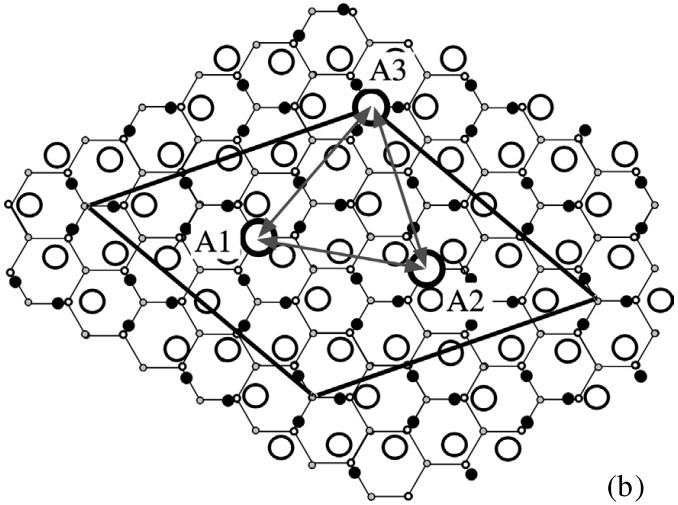
●：測定した逆格子点
（面積は積分強度に比例する）
○：表面1×1の逆格子
★：√3構造の逆格子

H.Tajiri et.al., Surf.Sci. 493(2001) 214

Patterson map





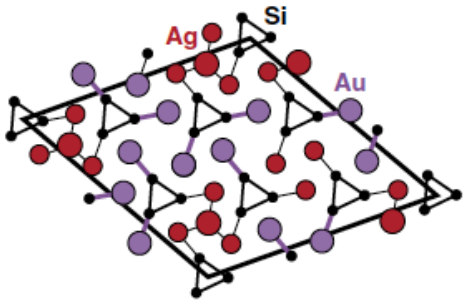


Ichimiya model
Tong model
peak A: cannot explain by Au-Au

Nogami model
peak Aは説明できるが合わない

新しいモデルを提案したが、不十分
未解決

- Ag, Au: mixing (alloy)
- √3x√3-Ag (Si) layer(s):
  √21x√21-periodicity



Ag/Si(111)-5x2-Au

H.Tajiri et.al., Surf.Sci. 493(2001) 214

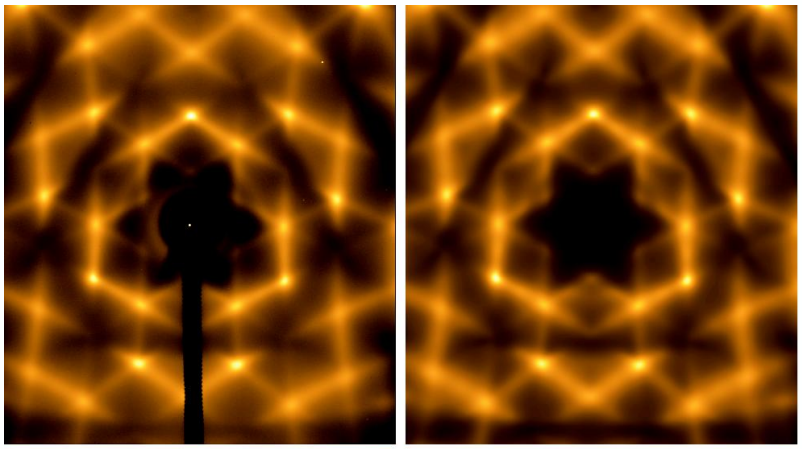
Y. Fukaya et. al., 606 919(2012)

Normal incidence geometry

- LEPD(LEED)
- Reflection geometry

symmetry:
plane group

- transmission X-ray diffraction
- TDS as a background
  - thin crystals



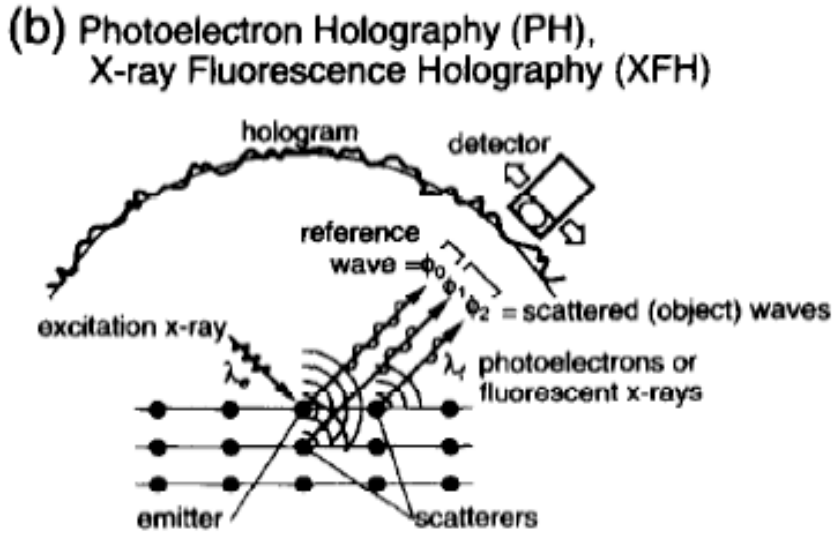
Si(111) observed calculated

phonon dispersion

M. Holt et al., Phys. Rev. Lett. 16 (1999) 3317.

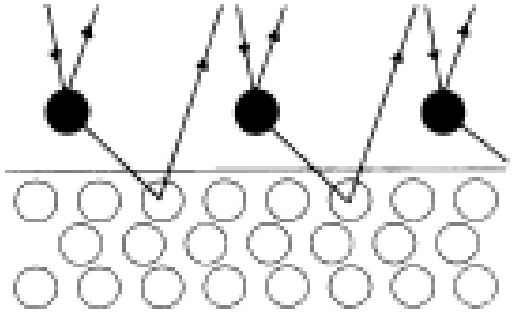
Holographic Methods

- Photoelectron holography
- X-ray fluorescence holography



C.S.Fadely et. al., PSS 54, 341(1997)

- LEED/LEPD holography

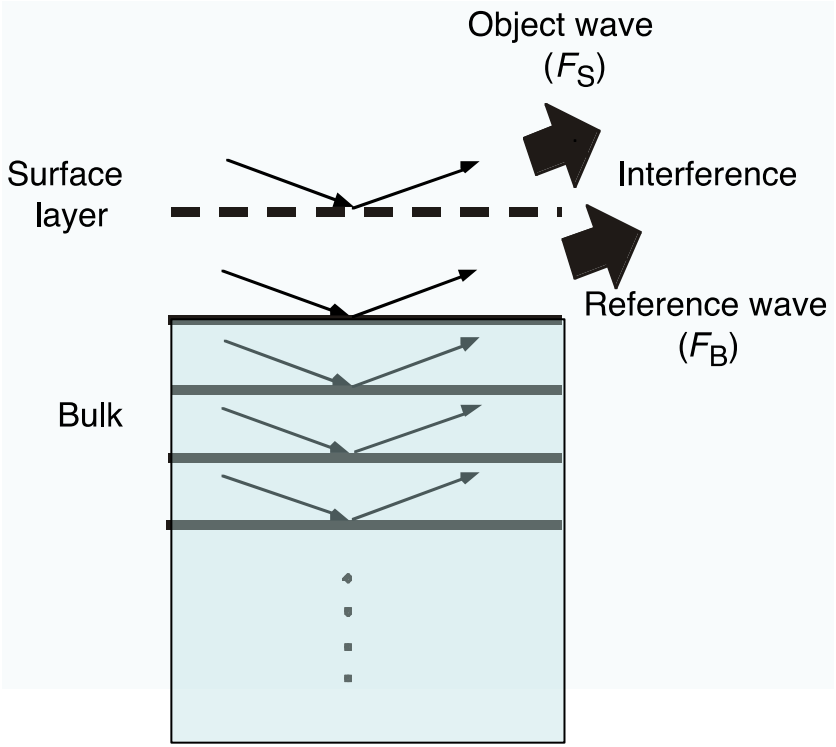


- CTR scattering holography

S.Y. Tong et. al., PRL 69, 3654(1991)

CTR scattering holography

CTR (Crystal truncation rod) scattering



表面構造／単結晶

$$I = |F_B + F_S|^2 = |R + O|^2$$

hologram

F_B : scatering amplitude by bulk

F_S : scatering amplitude by surface

$$F_B = \text{known(reference)}$$
$$F_S = \text{unknown(object)}$$

$$F_B = \sum_{n=1}^{\infty} F \exp(i2\pi n l) = \frac{F}{1 - \exp(-i2\pi l)}$$

$$\boldsymbol{k} = h\mathbf{a}^* + k\,\mathbf{b}^* + l\,\mathbf{c}^*$$

scattering vector

T. Takahashi, K. Sumitani, S. Kusano; Surf. Sci. 493, 36 (2001)

CTR Holographic Method

Hologram function in SXD

$$C(\boldsymbol{k}) = \frac{I - I_0}{F_B^{\,*}}$$

$$= \frac{F_B^{\,*} F_S + F_B F_S^{\,*} + |F_S|^2}{F_B^{\,*}}$$

$$= F_S + \frac{F_B}{F_B^{\,*}} F_S^{\,*} + \frac{|F_S|^2}{F_B^{\,*}}$$

$$= O + \frac{R}{R^*} O^* + \frac{|O|^2}{R^*}$$

F_S : electron density

Reconstruction of atoms

$$U(\boldsymbol{r}) = \int_{h,k,l} C(\boldsymbol{k}) \exp(-i\,2\pi \boldsymbol{k}\boldsymbol{r})\, d\boldsymbol{k}$$

$$O = F_S$$

O : atom image

electron density $\rho(\boldsymbol{r})$

O^* : twin atom

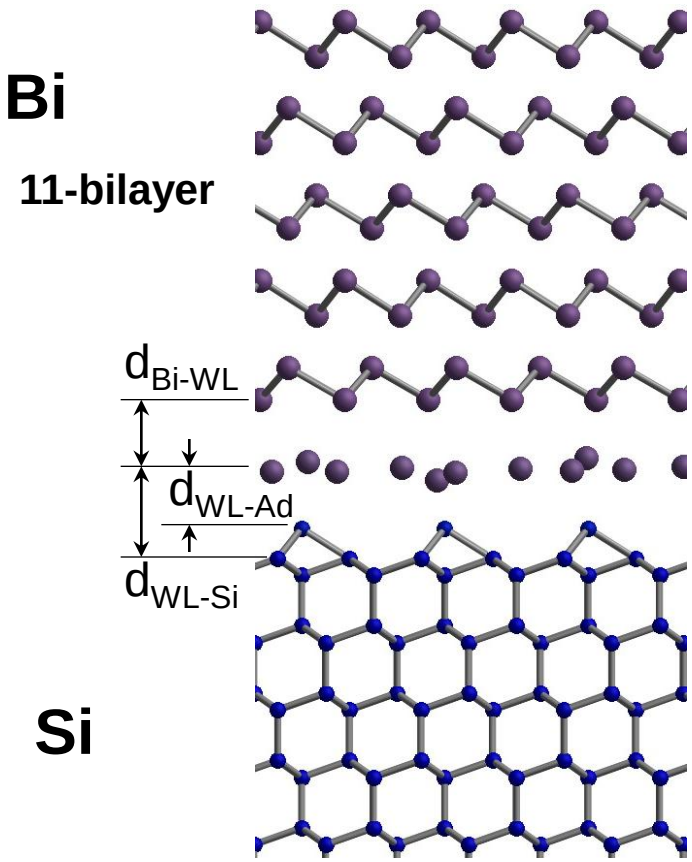
$$\mathrm{Re}\,(U(\boldsymbol{r})) \rightarrow \rho(\boldsymbol{r})$$

$$I = |F_B + F_S|^2 : \text{observed}$$

$$I_0 = |F_B|^2 : \text{calculated}$$

T. Takahashi, K. Sumitani, S. Kusano; Surf. Sci. 493, 36 (2001)

相互作用
Bi(001)-Wetting layer
Wetting layer-substrate



side view

Bi(001)/Si(111)-7x7

d_{Bi-WL} = 3.23 Å
Inter bilayer距離 2.38 Å
→ Bi(001)膜はfree standing
表面と界面層の構造もほぼ同じ
→ QWSのスピン縮退を説明

$d_{WL-Adatp,}$ = 2.7 Å
共有結合半径和 = 2.59 Å
Dalton Trans. 2832 (2008)

d_{WL-Si} = 4.12 Å
Van der Waals半径和 = 4.17 Å
(J. Phys. Chem. A , 5806 (2009))

BiはSi adatomとのみ相互作用
STM観察結果と一致

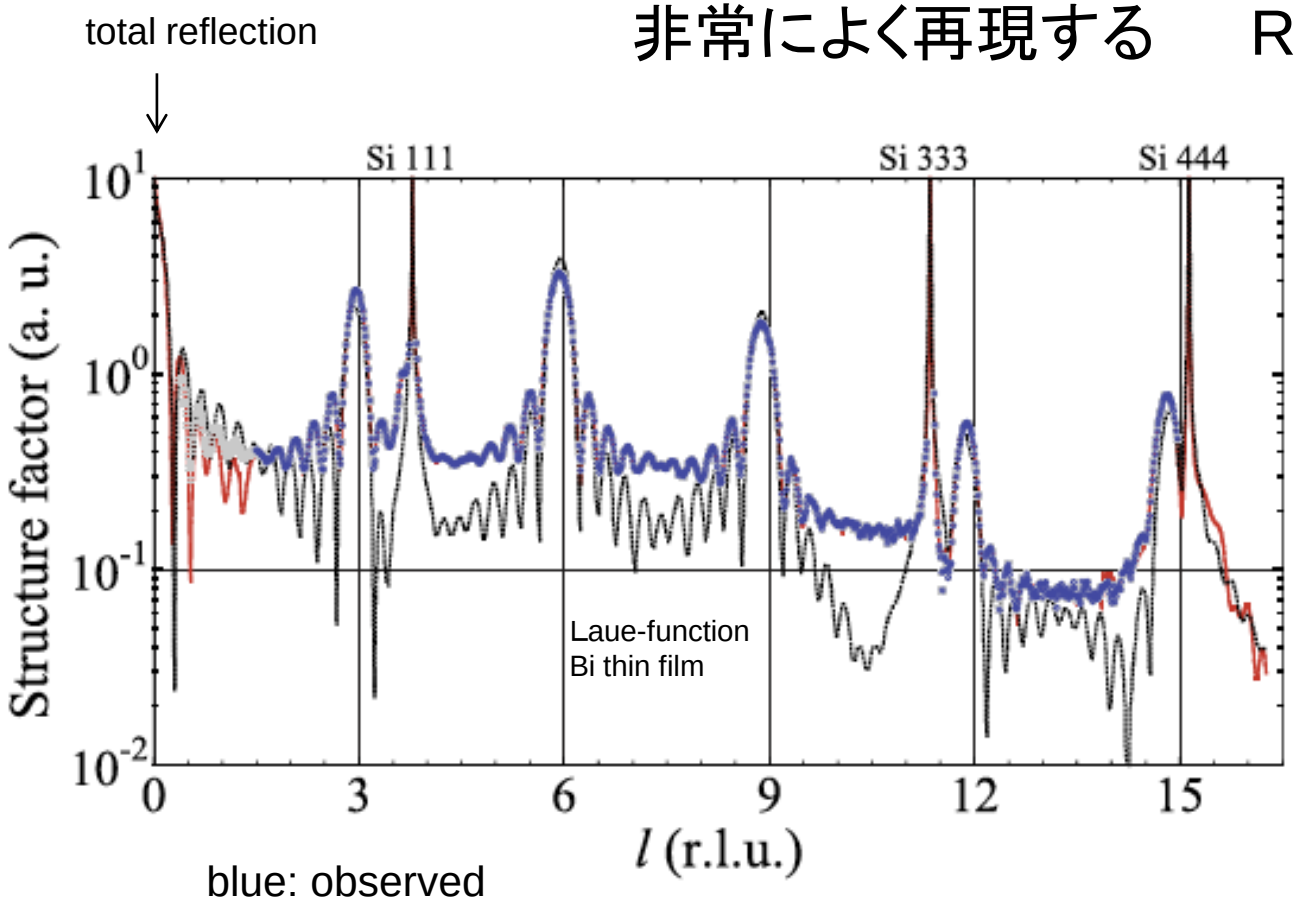
*Jour. Appl. Phys. 99, 014904 (2006).

T.Shirasawa et. al, PRB 84. 0754111(2100)

電子密度分布から計算した構造因子

Holography + iterative phase retrieval method

非常によく再現する　R = 0.025



blue: observed
red: calculated

T.Shirasawa et. al, PRB 84. 0754111(2100)

Summary

Expectation for positron diffractions

1) Surface sensitivity

determination of topmost layer(s)

- Large unit cell
- deeply distorted structures
- substrate with complicated structure

2) Normal incidence condition

symmetry of surface structures

3) Development of analyses

depending on the degree of multiple scattering

- holographic method
- Patterson map
- iterative phase retrieval method(?)

Thank you!