X Low energy electron diffraction (LEED)

10-1 2-dimensional surface structures

Bulk: 14 Bravais lattices

Surface: 5 surface lattices

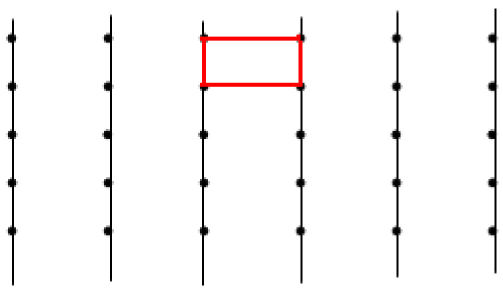
----- describe all possible periodic surface structures

----- Miller index

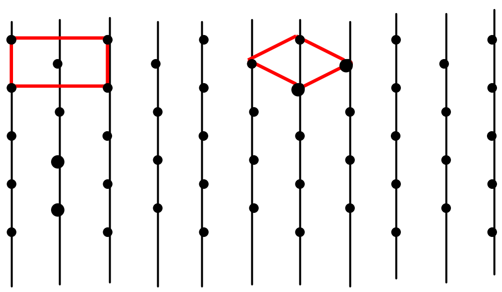
----- structure = lattice point + basis

----- derivation by symmetry

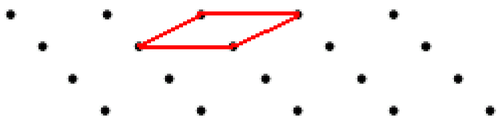
(a) Rectangular lattice ($a \neq b$, $\gamma = 90^o$)



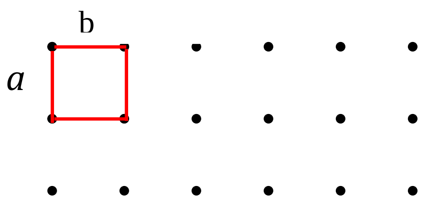
(b) Center Rectangular lattice ($a \neq b$, $\gamma = 90^o$)



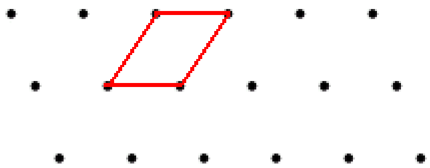
(c) Parallelogram lattice ($a \neq b$, $\gamma \neq 90^o$)



(d) square lattice ($a = b$, $\gamma = 90^o$)



(e) hexagonal lattice ($a = b$, $\gamma = 120^o$)



For example:

The ideal Si(111) surface is a hexagonal lattice.

The ideal Si(100) surface is a square lattice.

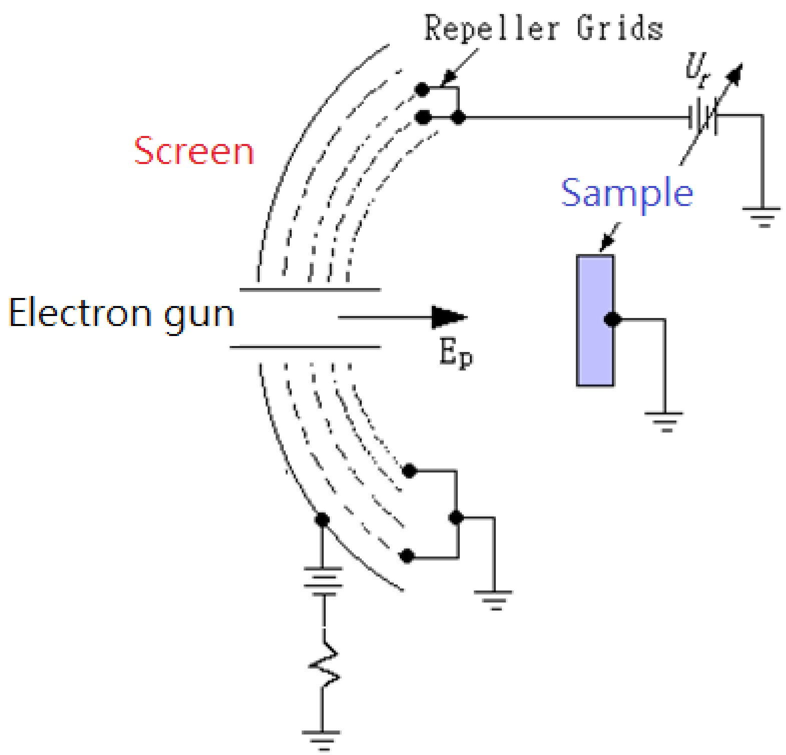
The (110) surface of Au is a rectangular lattice.

10-2 Techniques for surface structure determination

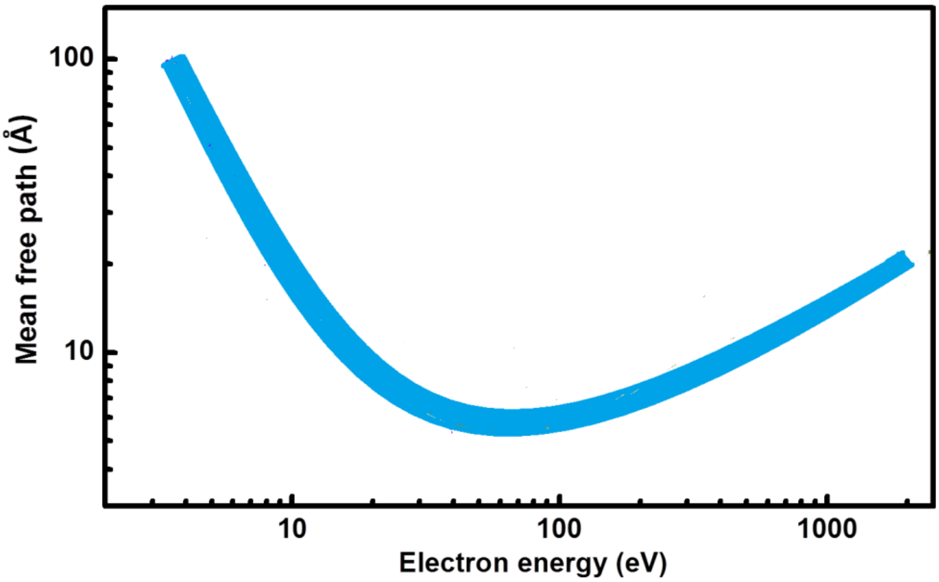
1. LEED (Low energy electron diffraction)
2. RHEED (Reflection high energy electron diffraction)
3. STM (Scanning tunneling microscope)
4. SEXAFS (Surface extended X-ray absorption fine structure)

In this course, LEED and RHEED will be covered.

10-3 LEED optics



Electron escape depth and surface sensitivity



Universal electron escape depth as a function of electron energy

The reciprocal lattice of the surface in LEED

Total scattering amplitude F for LEED is

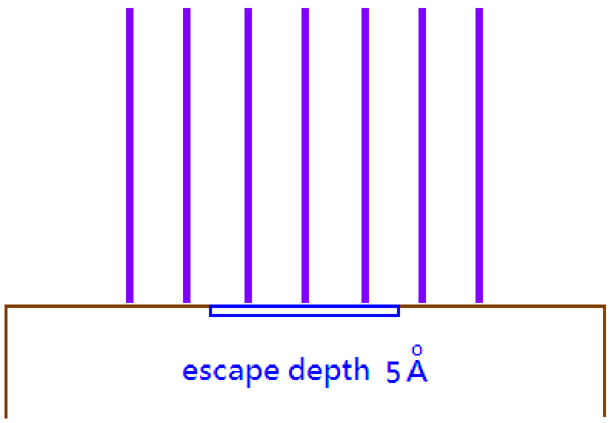
$$F = \int n(\vec{r}) e^{i(\vec{k}-\vec{k'})\cdot\vec{r}} d\vec{r}$$

where $n(\vec{r})$ is the volume that electrons are scattered and collected in the detector (screen).

In LEED, electrons are diffracted from volume within electron escape depth. If the electron beam size is 100 nm and the escape depth is 0.5 nm, the volume is in a disk shape.

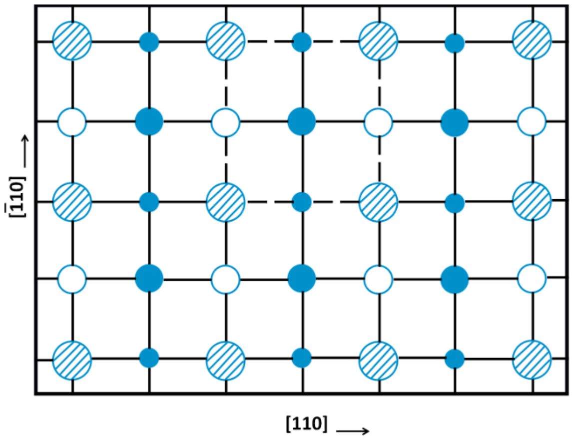
Then,

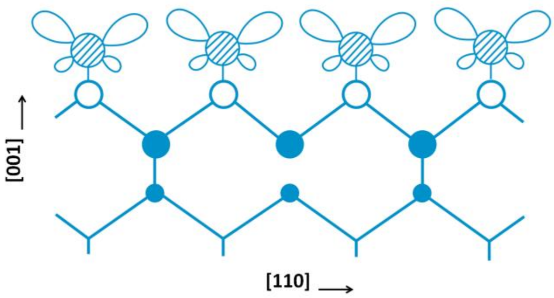
Reciprocal lattice is a forest of rods due to "shape effect".



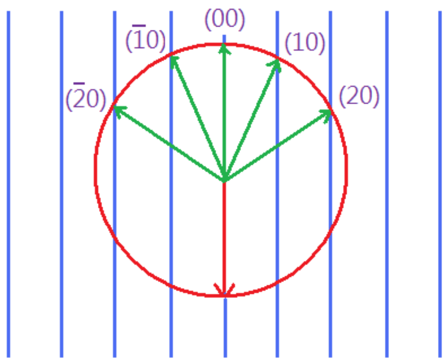
10-3 Ewald sphere construction the Si(100) ideal surface in LEED

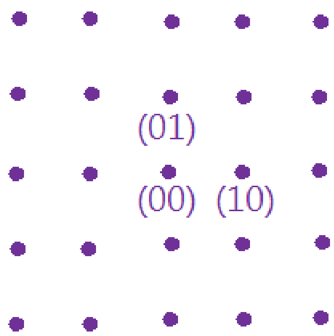
The atomic structure of the Si(100) ideal surface





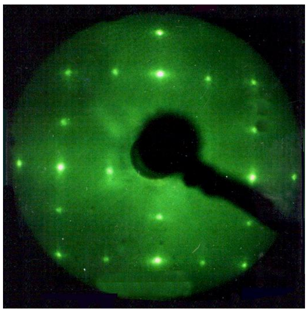
Ewald sphere construction and the expected LEED pattern





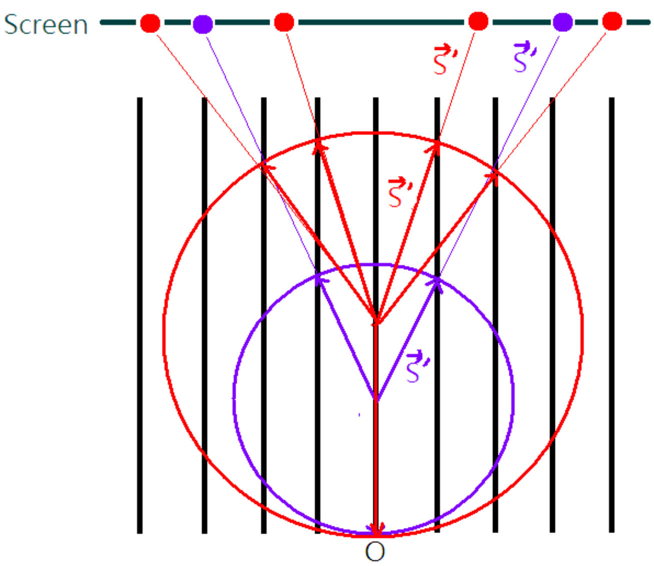
However, the LEED pattern of as-cleaned Si(100) is not a square lattice

The LEED pattern for the Si(100) surface cleaned at 950℃ is double domain Si(100)-2x1 shown below, rather than Si(100)1x1.



The symbol Si(100)2x1 is the Wood’ s notation for the reconstructed Si(100) surface.

> LEED using different electron kinetic energies



When the kinetic energy of electron increases, k increases such that more diffracted spots move inwards the screen.

III Surface reconstruction (defined in the real space)

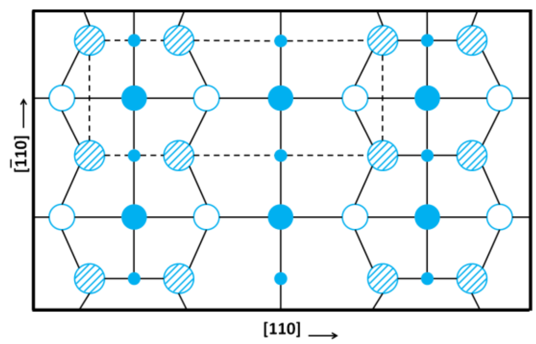
Wood' s notation

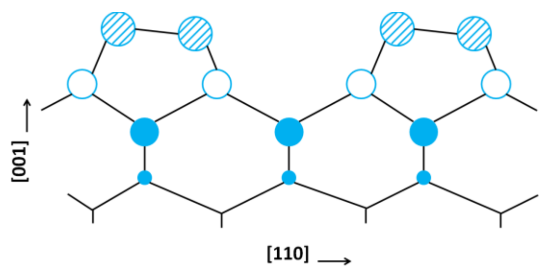
(a) For a reconstructed surface

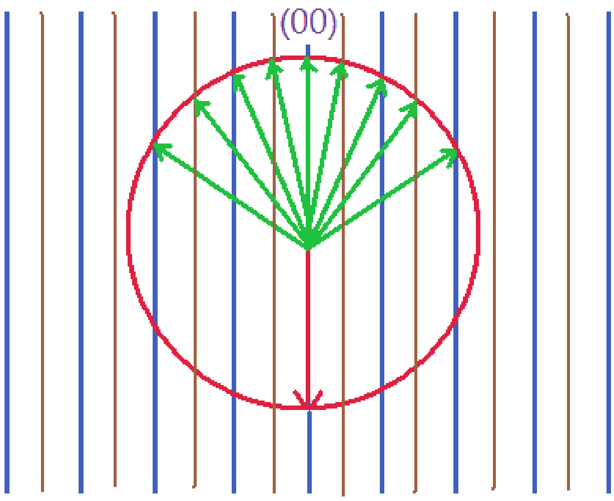
$$M(hkl)\frac{\vec{a}_s}{\vec{a}_b}\times\frac{\vec{b}_s}{\vec{b}_b}R\theta$$

Where M is the chemical element, (hkl) is the plane, R is the roation angle between the axes of surface and bulk.

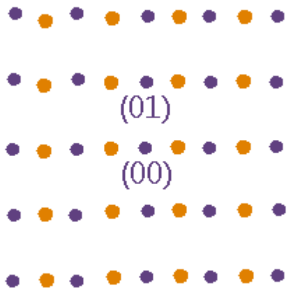
For example: Si(100)2x1



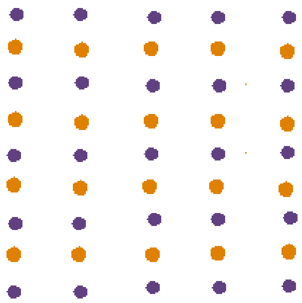




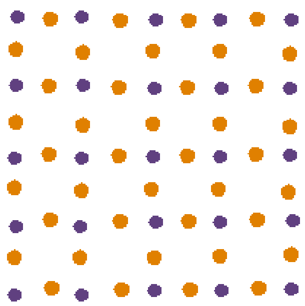
LEED pattern of single domain Si(100)2x1

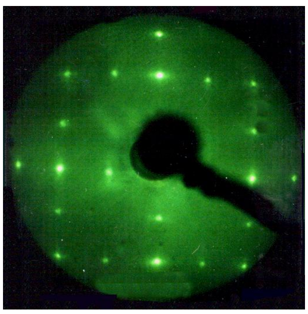


Another domain of Si(100)2x1



Supposition of two domain → double domain of Si(100)2x1



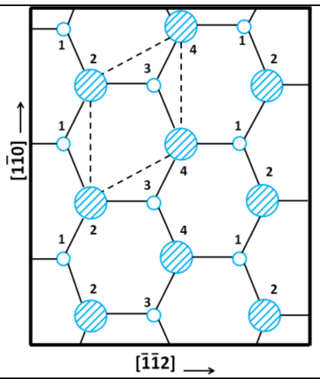
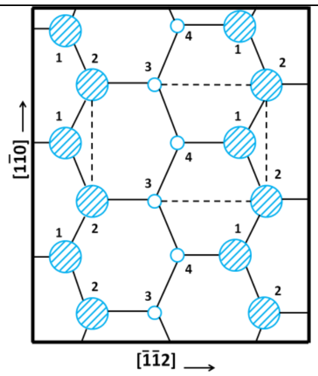
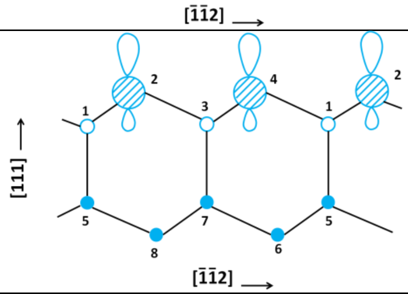
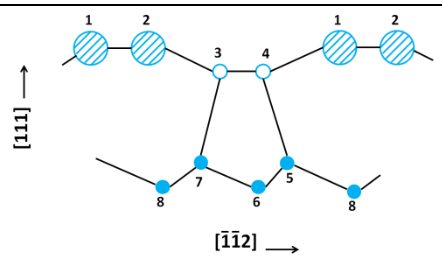
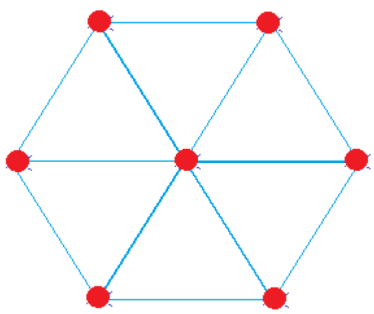
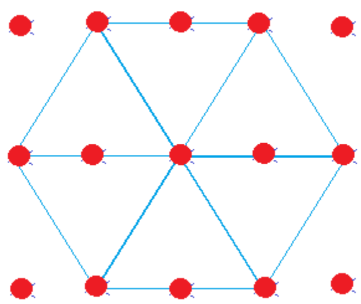


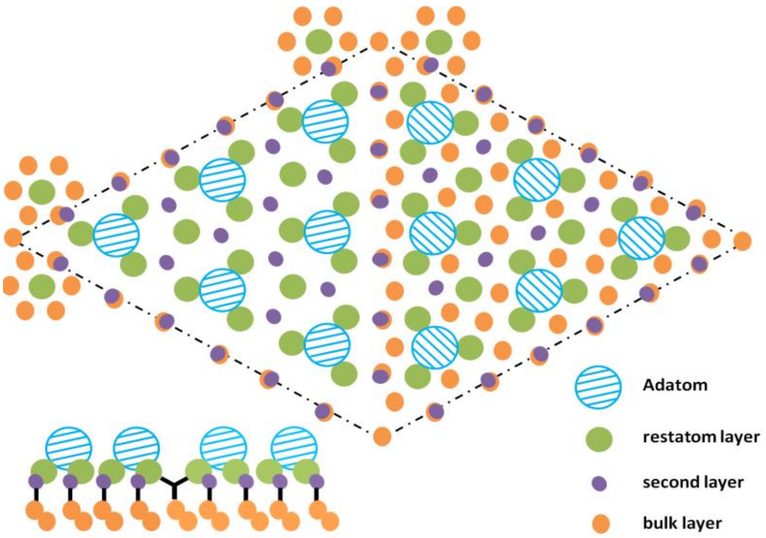
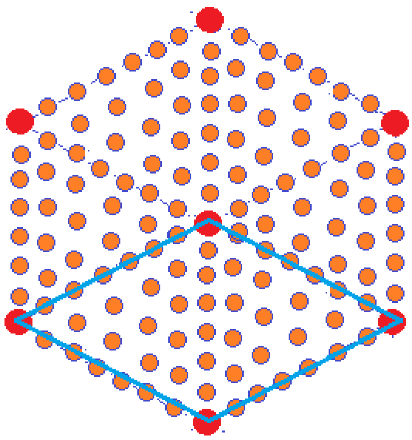
Discussion:

Si(111) surface reconstructions and their LEED patterns

Questions to ask:

1. What are the reciprocal lattices of the Si(111)1x1, Si(111)2x1, and Si(111)7x7 surfaces?
2. What are the LEED patterns of the Si(111)1x1, Si(111)2x1, and Si(111)7x7 surfaces?

Si(111)1x1	Si(111)2x1
Ideal surface	Π-Chain model
	
	
	

Si (111)
The DAS model: atomic structure of Si(111)7x7 (Dimer_Adatom_Stacking fault)



Please visit the webpage below to see the Si(111)7x7 LEED pattern

http://www.desy.de/~hasunihh/poster/beug/beug.html

10-5 Adsorbate surface structure

For an adsorbate surface

$$M(hkl)\frac{\vec{a}_s}{\vec{a}_b}\times\frac{\vec{b}_s}{\vec{b}_b}R\theta-A$$

Where M is the chemical element, (hkl) is the plane, R is the rotation angle between the axes of surface and bulk, and A is the adsorbate.

Example #1 Ni(110)-C2x2-O