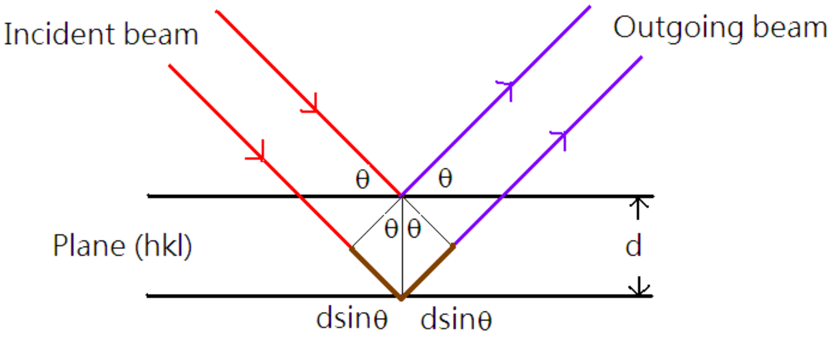
I Brief introduction

Several questions to ask in this course:

1) What is the objective of the course "introduction to crystal structure and diffraction theory"?
    - (a) Crystal structure
    - (b) Diffraction theory and techniques
2) What is the atomic arrangement in a crystal?
3) What is the crystal symmetry?
4) What is the basis of diffraction?
    - (a) The Bragg's law characterizing diffraction in the real space is expressed as $2d\sin\theta = n\lambda$ where n is the order of reflection.



When the total path difference $2d\sin\theta$ equals to $n\lambda$, diffraction occurs.

"d" in the Bragg's law is related to the arrangement of "object".

"λ" is related to the "wave"

(b) The diffraction theory in the reciprocal space will be emphasized in this course.

5) How many kinds of diffraction techniques useful for materials characterization?

XRD (X-ray diffraction; bulk)

--- used for bulk structure determination (in air)

LEED (low energy electron diffraction; surface)

--- used for surface structure determination in UHV (ultra-high vacuum)

RHEED (Reflection high energy electron diffraction; surface)

--- equipped in MBE (molecular beam epitaxy)

TEM (Transmission electron microscope; bulk)

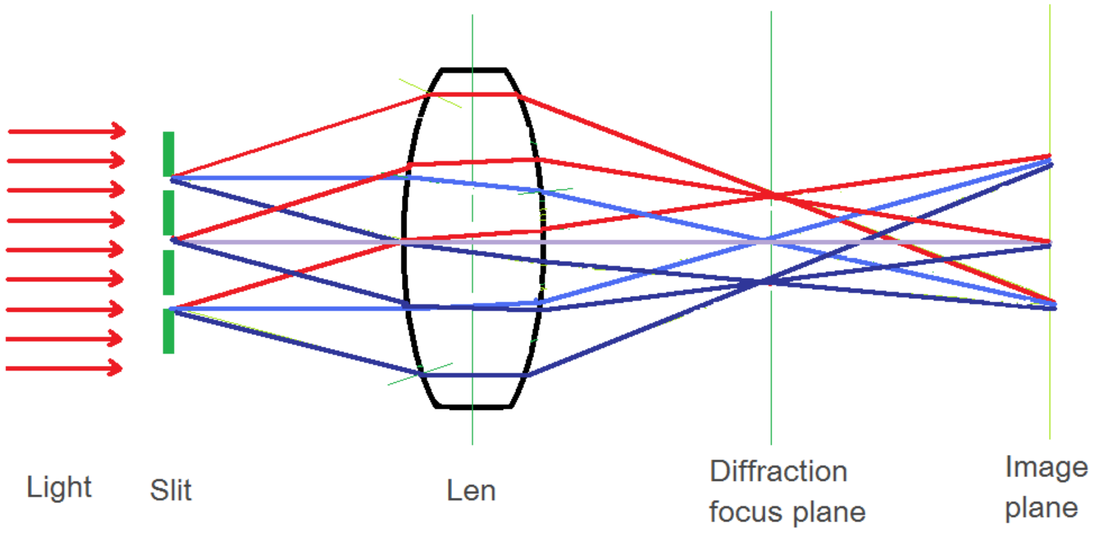
--- used for chemical and structure determination

6) What is the relationship between diffraction and

image formation?

--- the image of the object is contained in each diffraction spot

--- diffraction focal plane and image plane

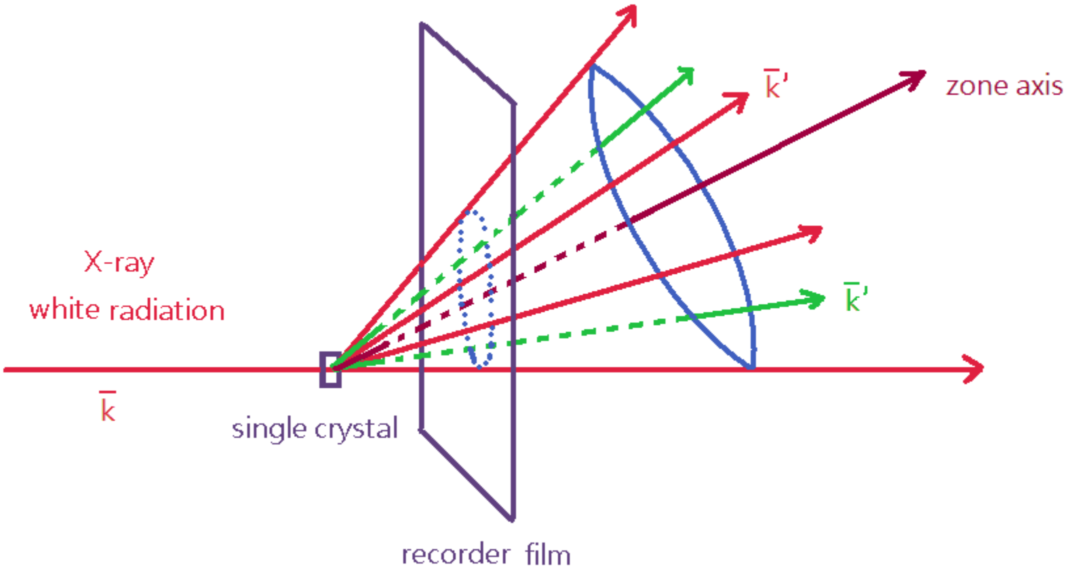


7) What are the diffraction techniques covered in the text?

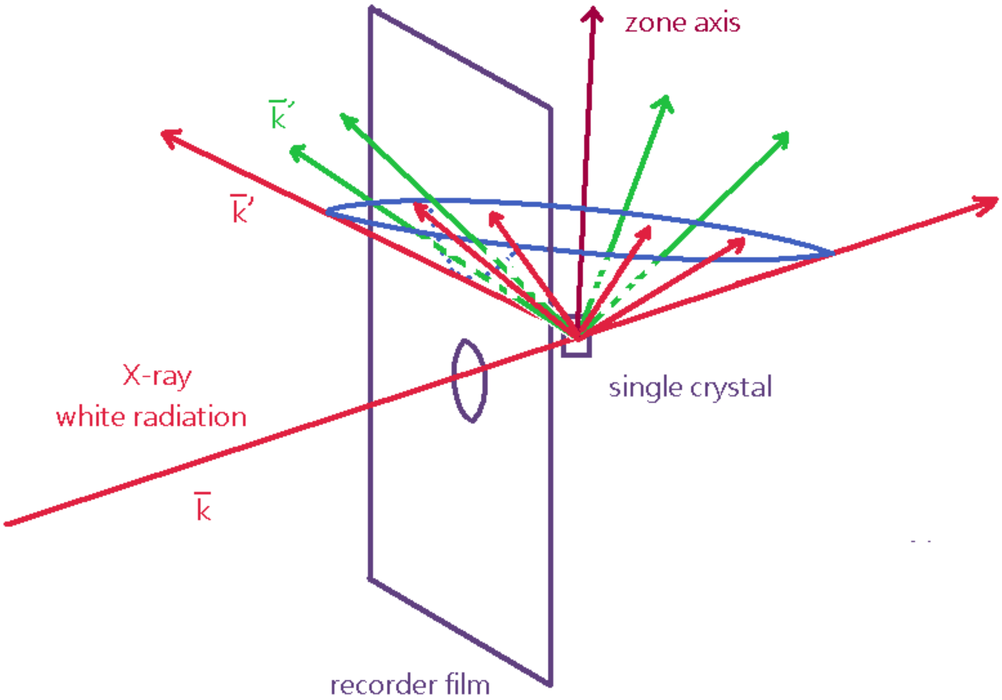
7-1 X-ray diffraction (XRD)

7-1-a X-ray Laue method

--- orientation determination



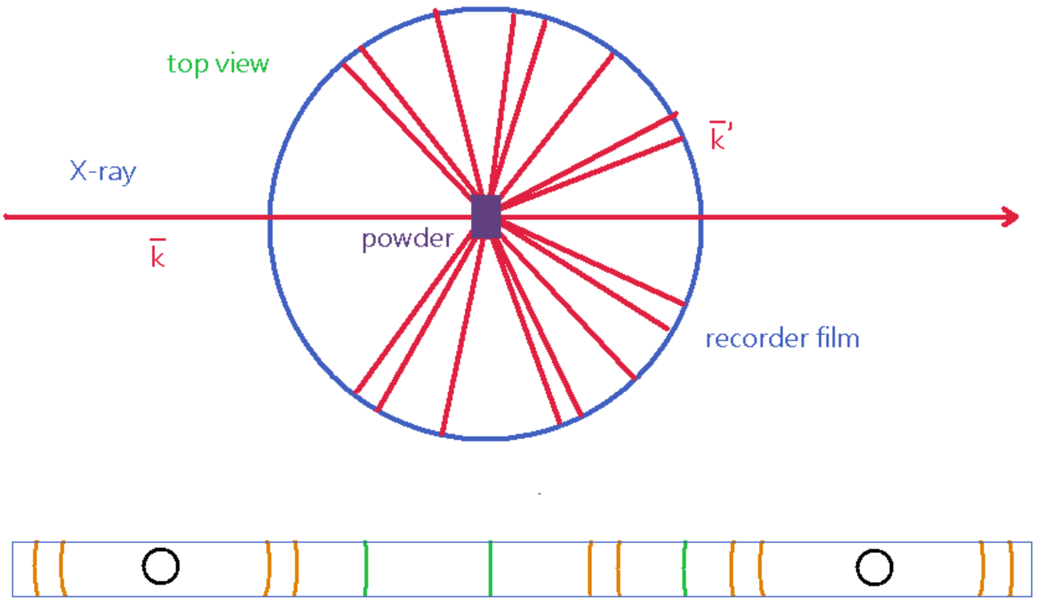
Laue spots on an ellipse



Laue spots on a hyperbola

7-1-b X-ray powder method (Debye-Scherrer)

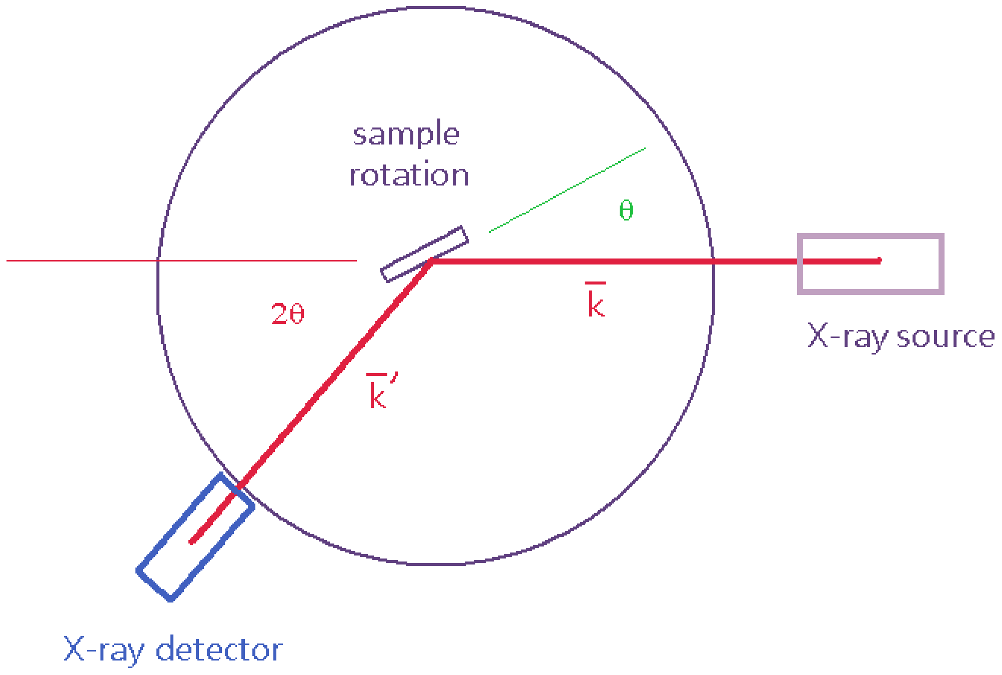
--- crystal structure characterization



Debye- Scherrer powder pattern

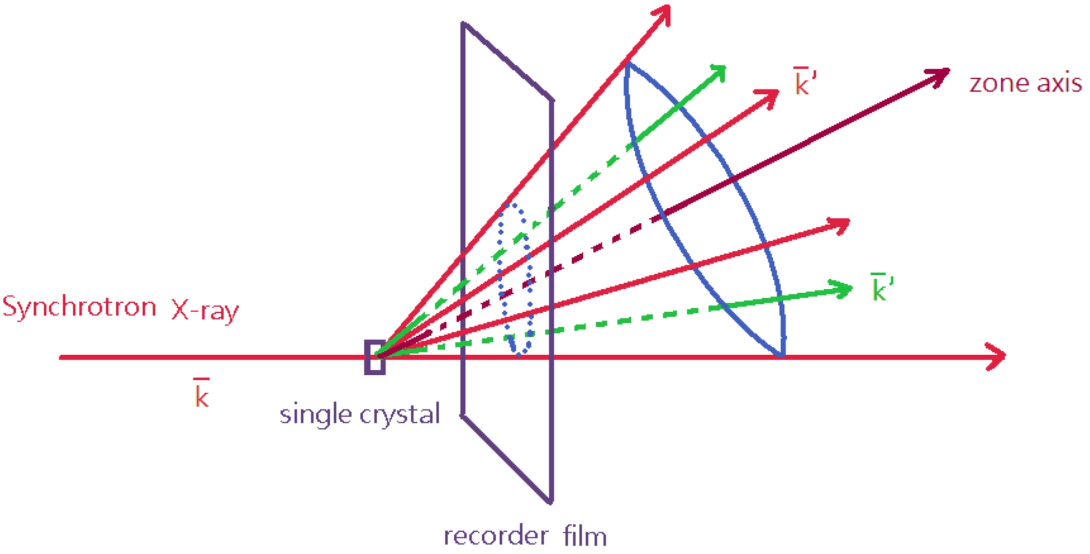
7-1-c X-ray diffractometer

--- structure characterization



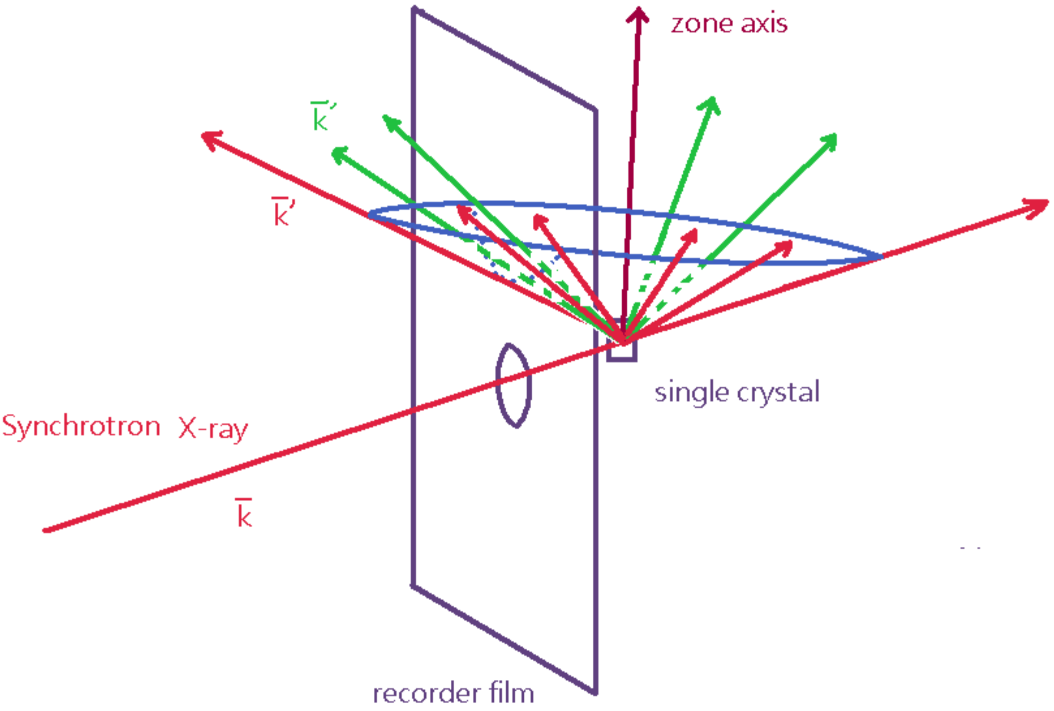
7-1-d X-ray topography

--- structural characterization



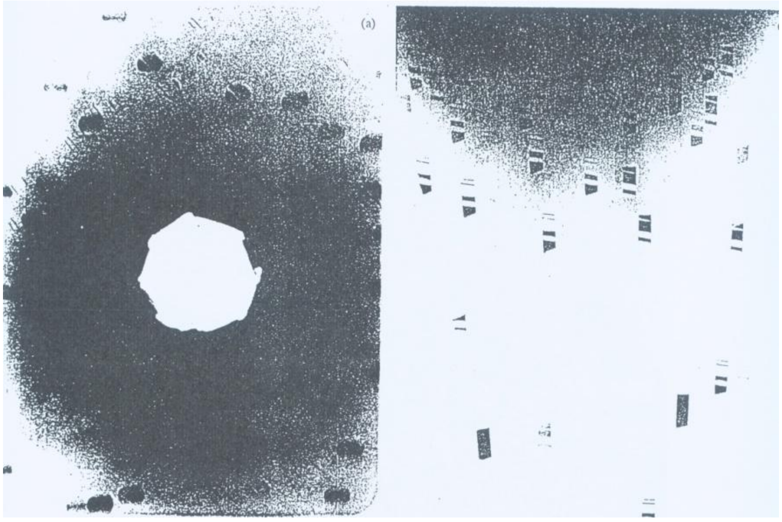
Laue spots on an ellipse

Synchrotron X-ray topography : transmission mode



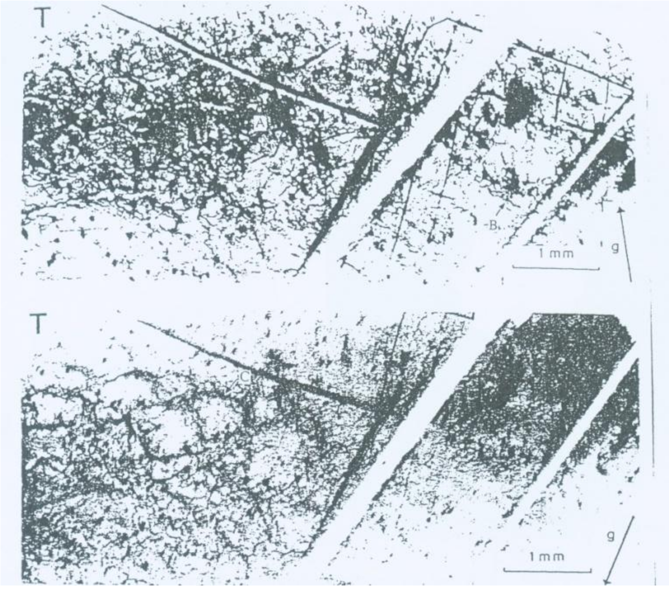
Laue spots on a hyperbola

Synchrotron X-ray topography : Reflection mode.



X-ray films recording the diffraction patterns of CdTe in (a) transmission mode and (b) reflection mode. (adapted from Y. C. Liu, Ph.D. thesis, Stanford)

Each spot is actually a topograph after enlargement.

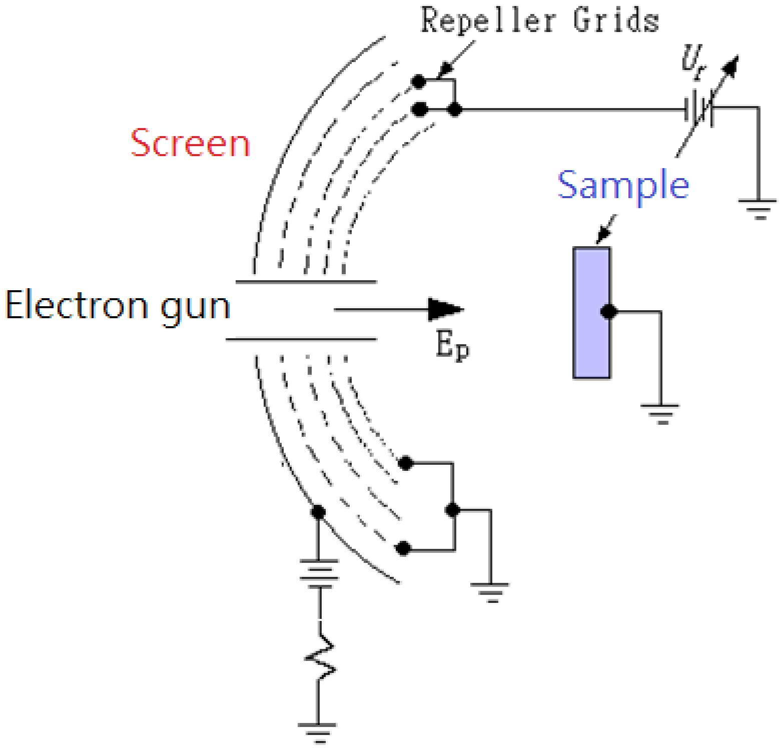


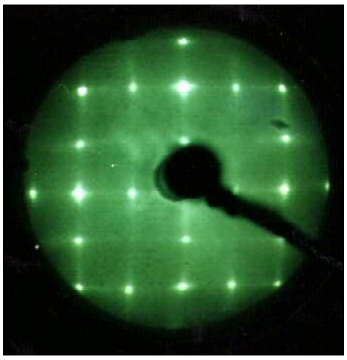
Tranmission tpograph of CdTe showing individual dislocation, dislocation tangling, and subcell structure. (adapted from Y. C. Liu, Ph.D. thesis, Stanford)

7-2 Low energy electron diffraction (LEED)

--- surface structure determination

--- in UHV (ultra-high vacuum)

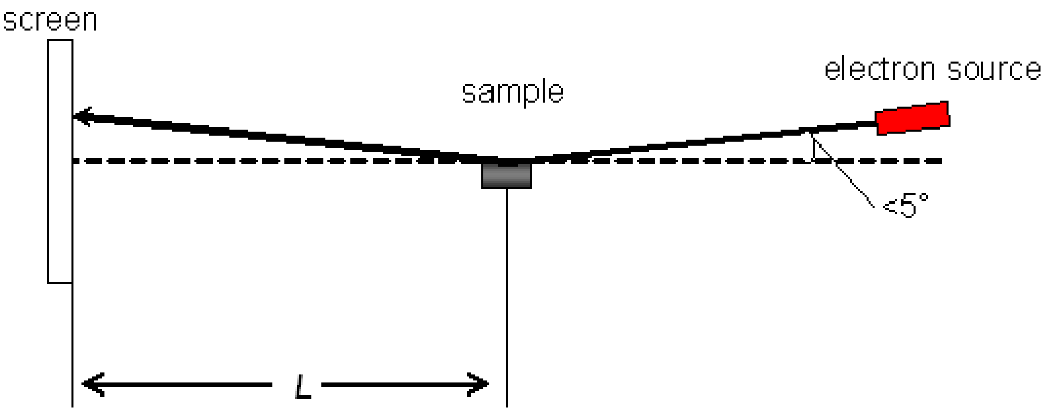


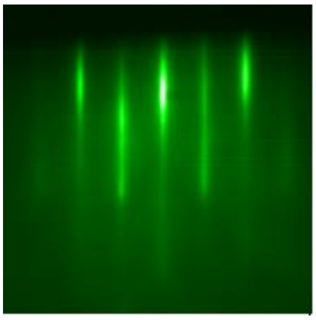


LEED pattern of Si(100)2x1

7-3 Reflection high energy electron diffraction (RHEED)

--- used in MBE (molecular beam epitaxy)

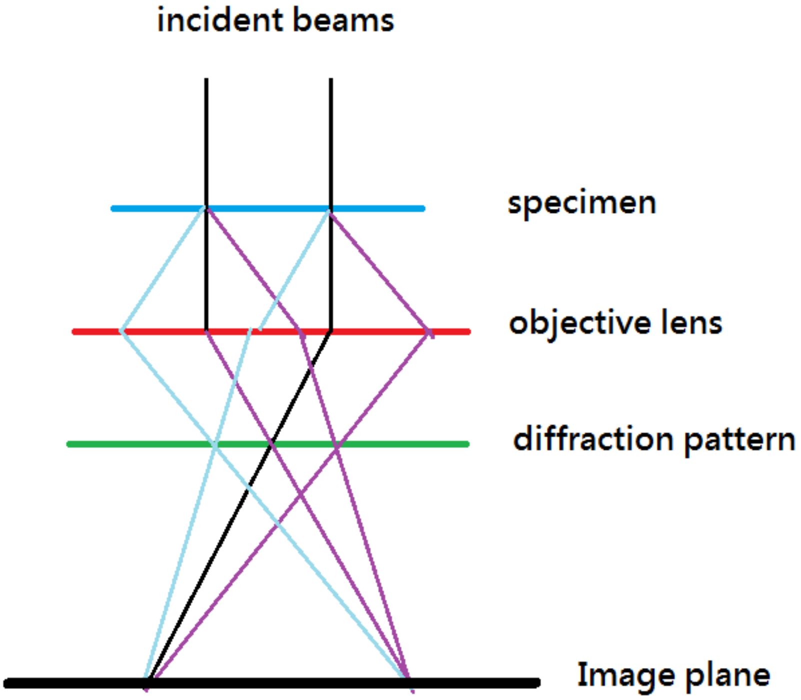




Streaky RHEED pattern of an epitaxial layer

Schematic of a RHEED setup. The distance from sample to screen, L, and the energy of the electron beam must be known to derive the lattice spacings of the crystal

7-4 Transmission electron microscope (TEM) --- structure, morphology, and chemical determination



This is a simple sketch of the beam path of the electrons in a TEM after the illumination system. A parallel beam of electrons enters the specimen and are scattered in various directions. The objective lens is used to collect all scattered beams originating from the same point on the sample in one point in the image plane (bottom). Note also that in the back focal plane (marked 'diffraction pattern') electrons originating at different point on the sample, but scattered in the same direction, are collected. Observing the electrons in this plane gives the diffraction pattern, containing information on the angular scattering distribution of the electrons. The diffraction pattern and the image are related through a Fourier transform.

Electron diffraction in TEM
Example:

Polycrystalline PtSi/Si(100)