
Dynamical effects in diffraction patterns

Lecture 7

Outline

Dynamic diffraction - the idea

Origin of Kikuchi maps

Examples of Kikuchi maps

Using Kikuchi maps:

- Precise orientation determination
- Setting the value of \vec{s}

Double diffraction

Forbidden reflections

Dynamical diffraction

Radiation	Elastic Mean Free Path (Å)	Absorption Length (Å)
Neutrons	10^8	10^9
X-rays	10^4	10^6
Electrons	10^2	10^3

Electrons interact strongly with matter

Mean free path before interaction is $\approx 100\text{\AA}$

We have been considering only ‘kinematical’ diffraction to date

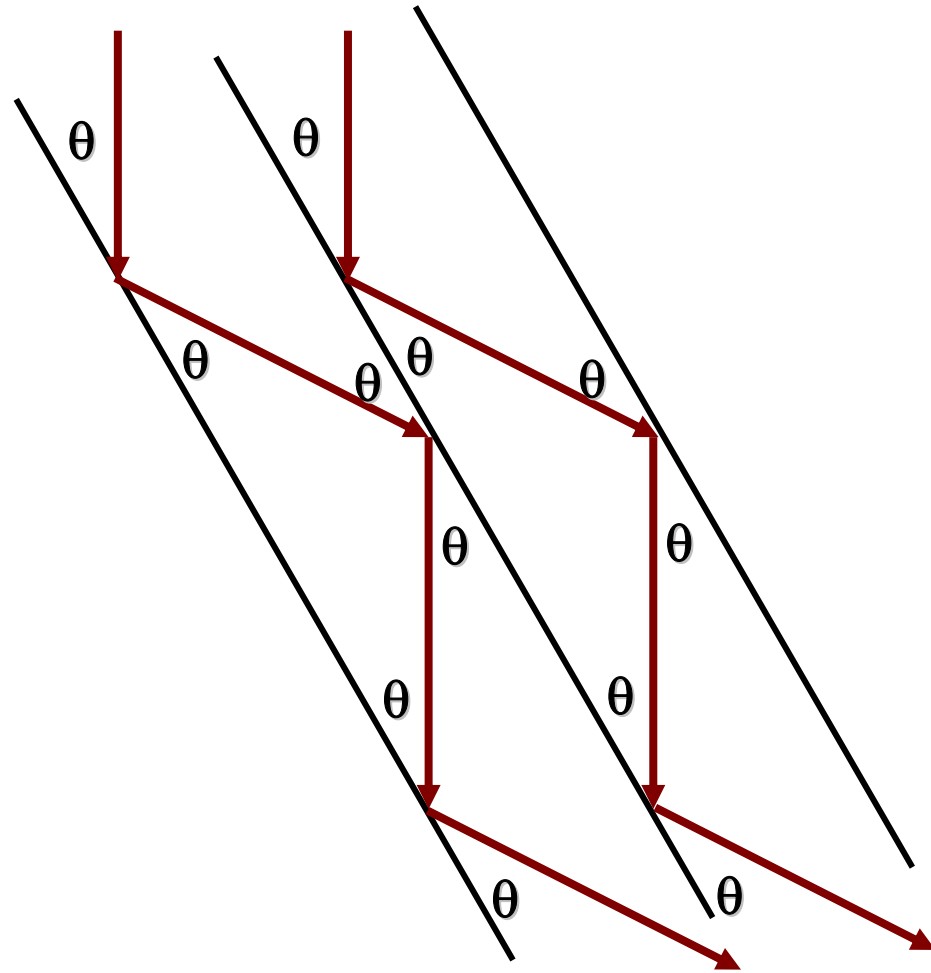
- Single diffraction events
- ‘First Born approximation’

Dynamical diffraction

In reality, have dynamical diffraction conditions in nearly all cases

Has important effects on:

- Diffraction intensities
- Image contrast
- Features in diffraction patterns

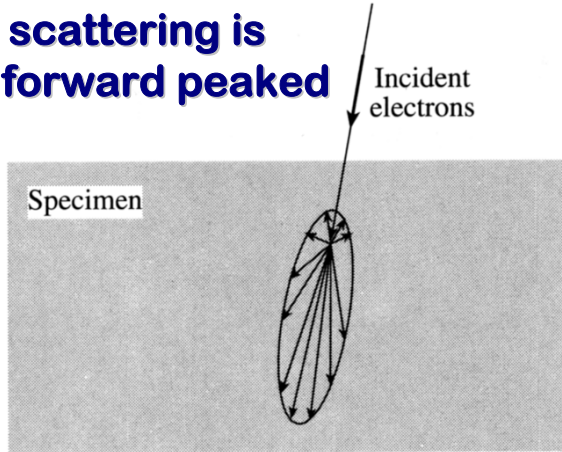


Simplified schematic of dynamical scattering

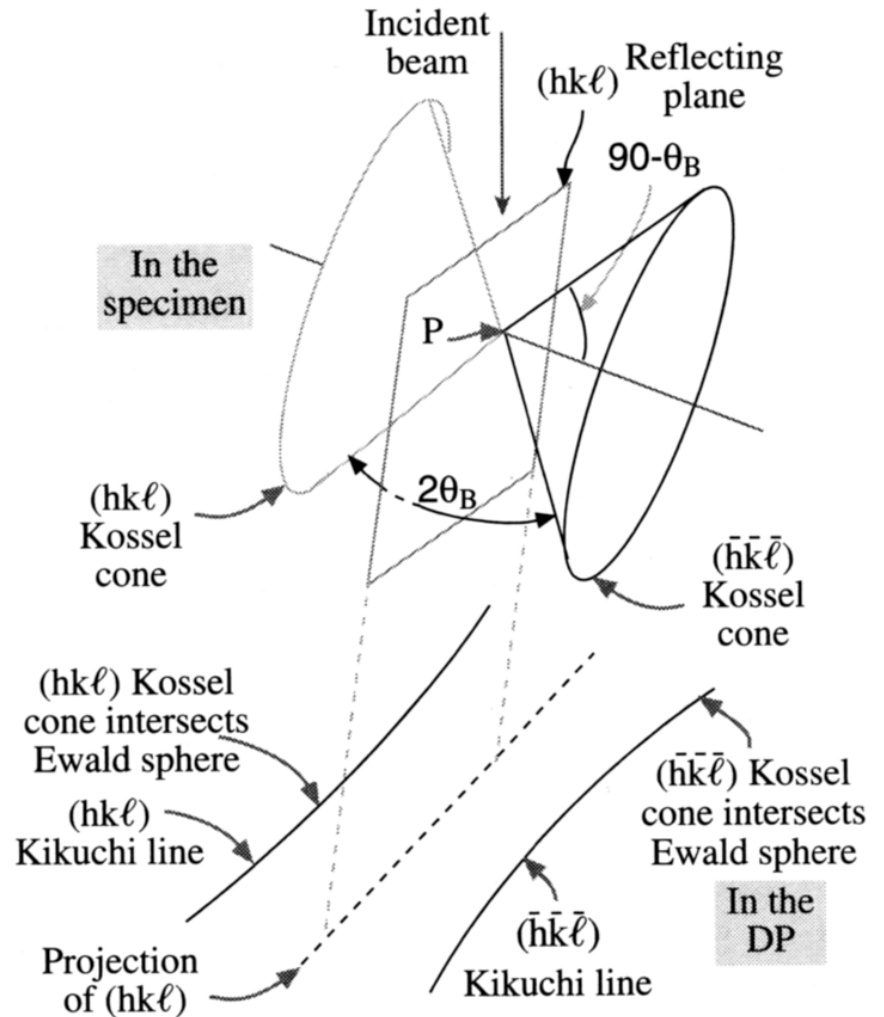
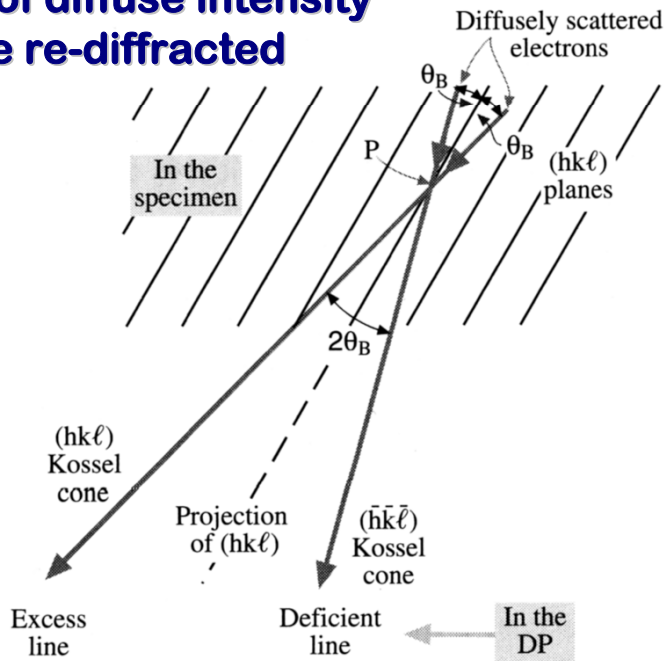
Kikuchi lines

origin

Inelastic scattering is strongly forward peaked

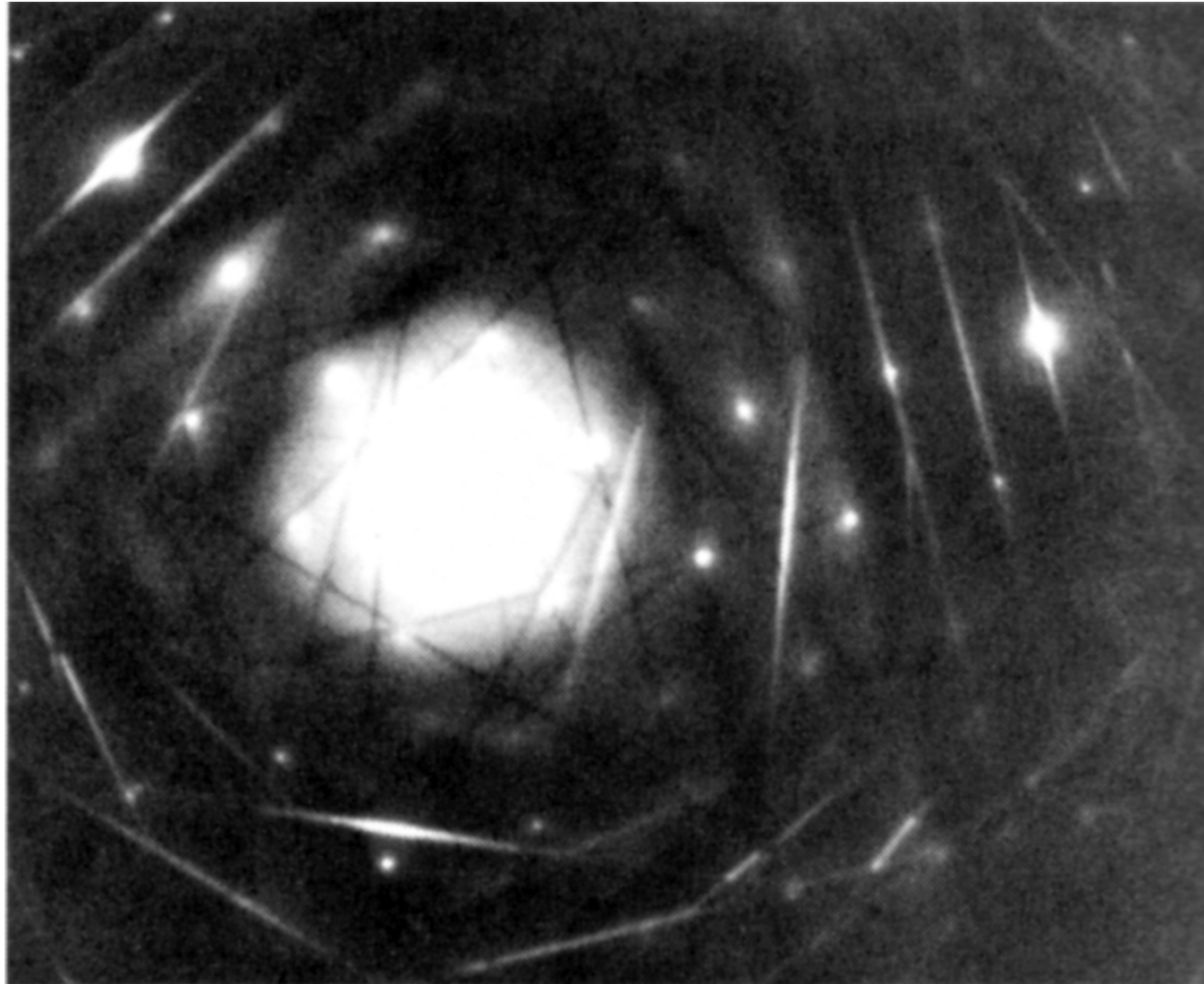


Cone of diffuse intensity can be re-diffracted



Results in a cone of diffracted intensity, which intersects Ewald sphere as hyperbolae

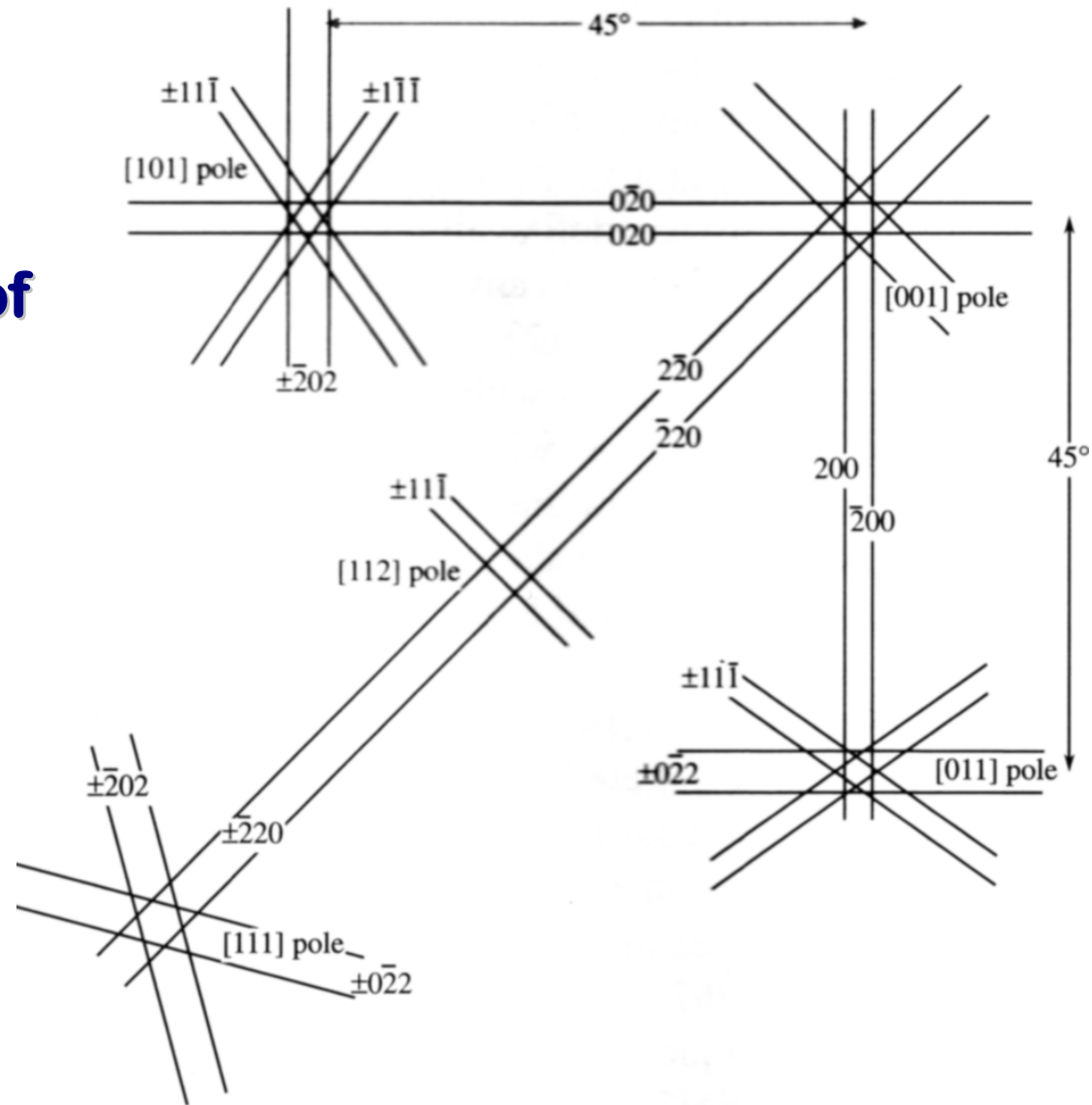
Example Kikuchi pattern



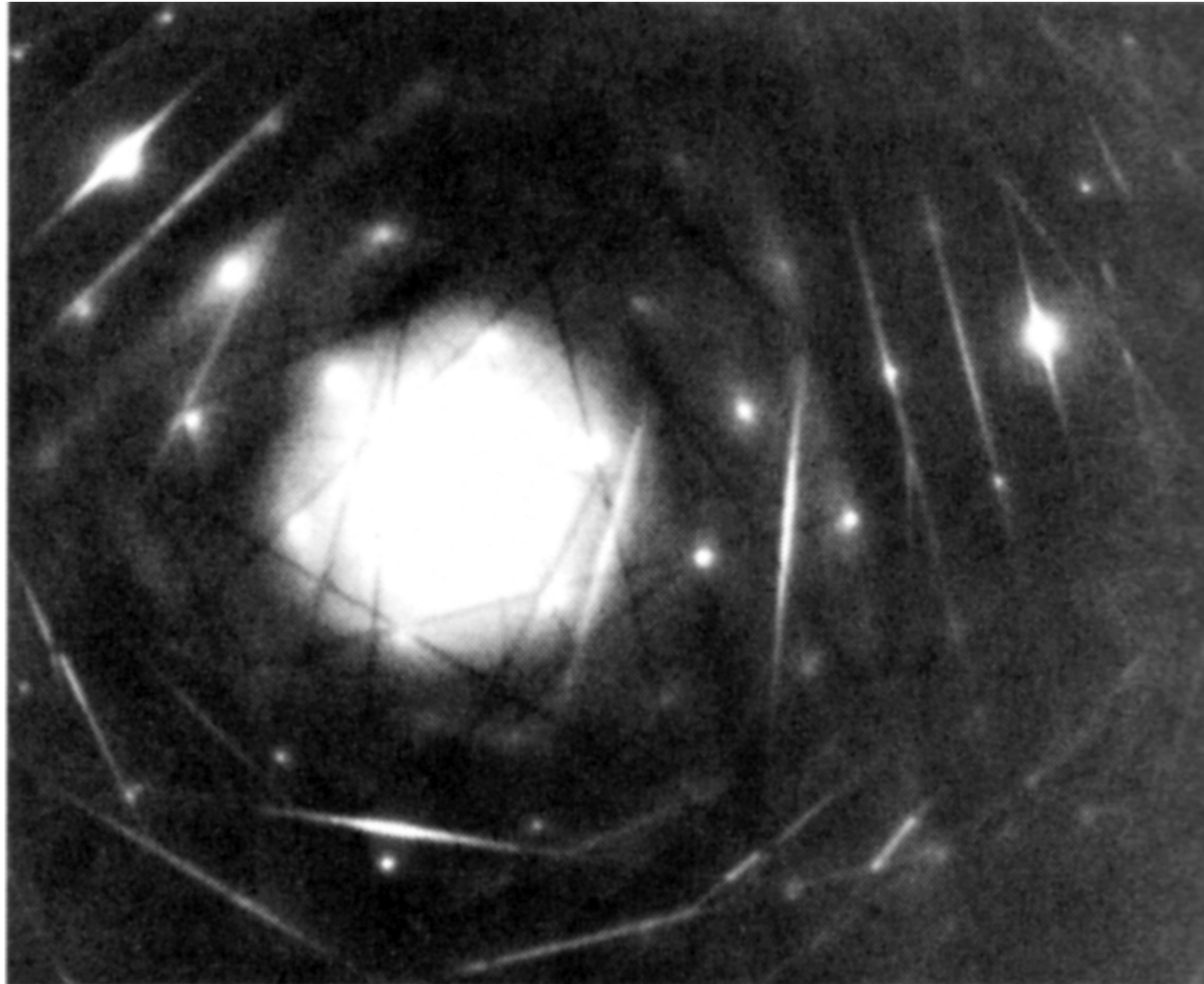
Kikuchi lines

Kikuchi lines connect zone axes that share a family of planes

Provide a “road map” of reciprocal space



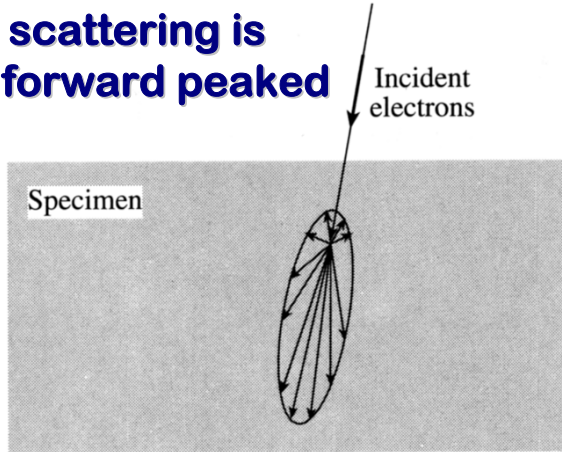
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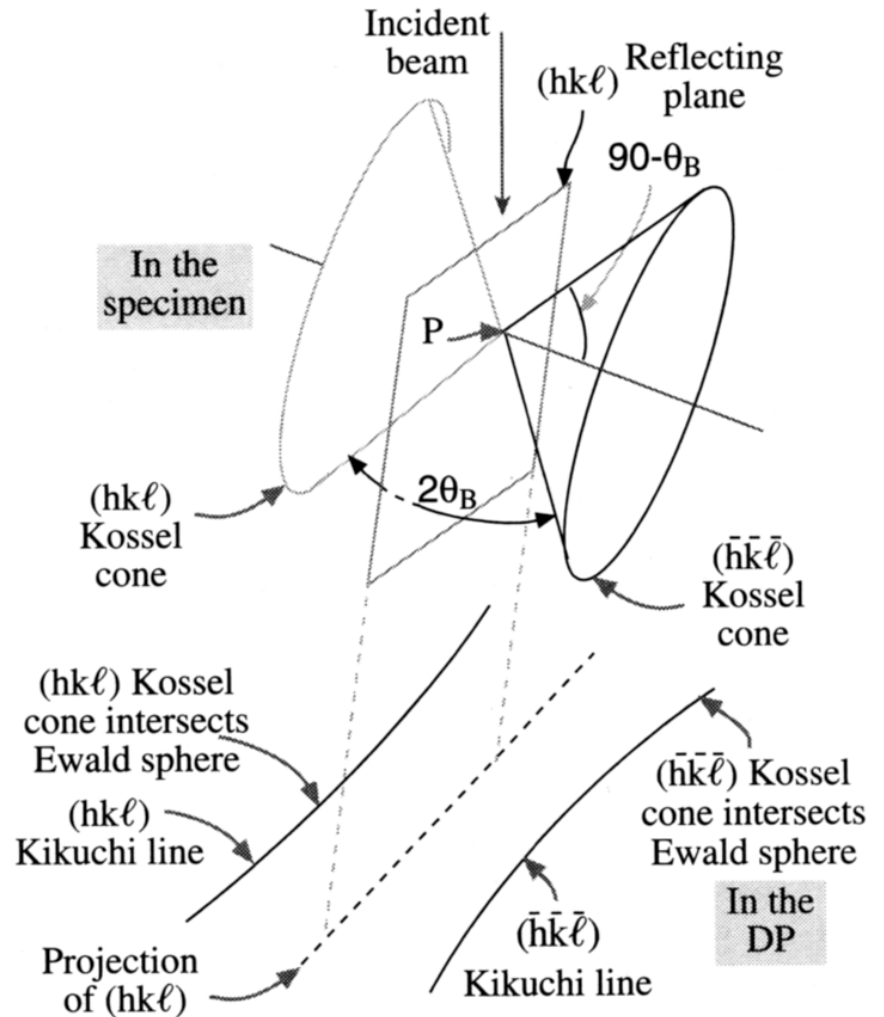
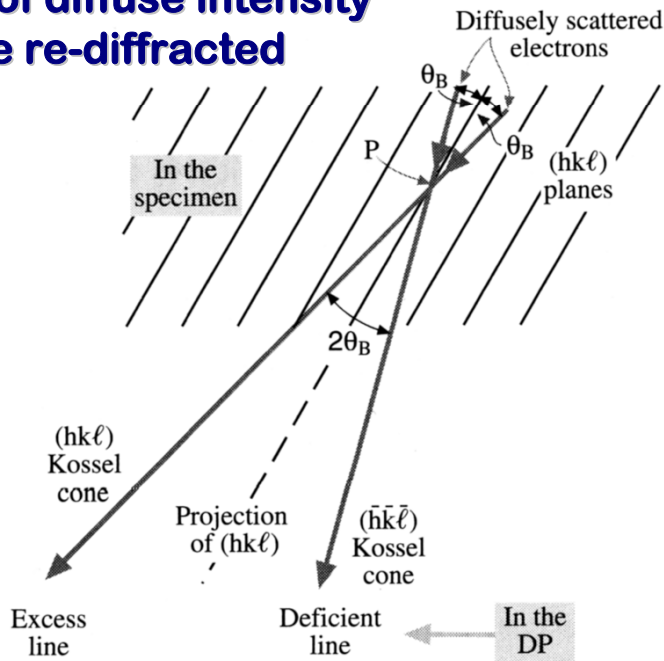
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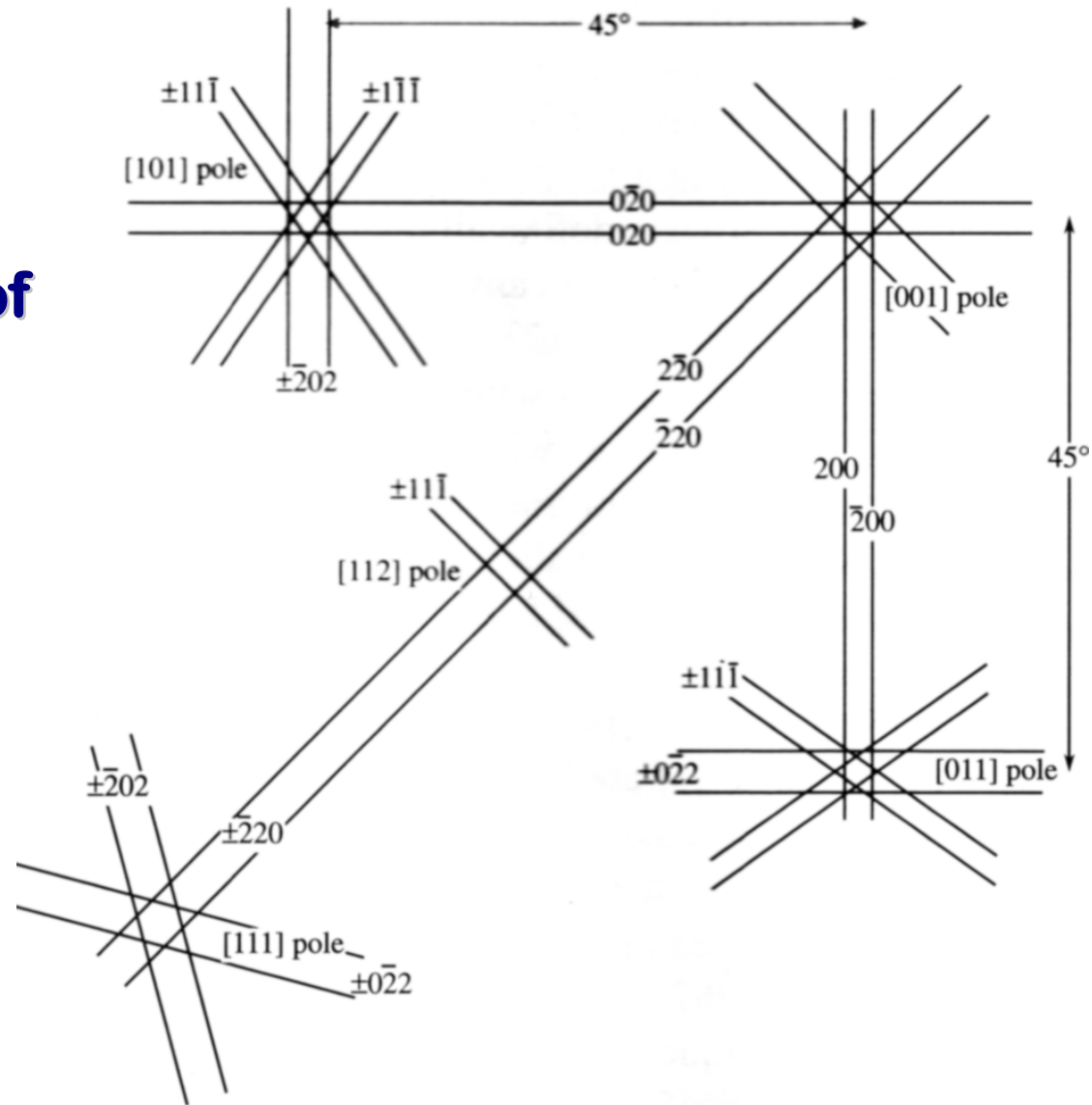


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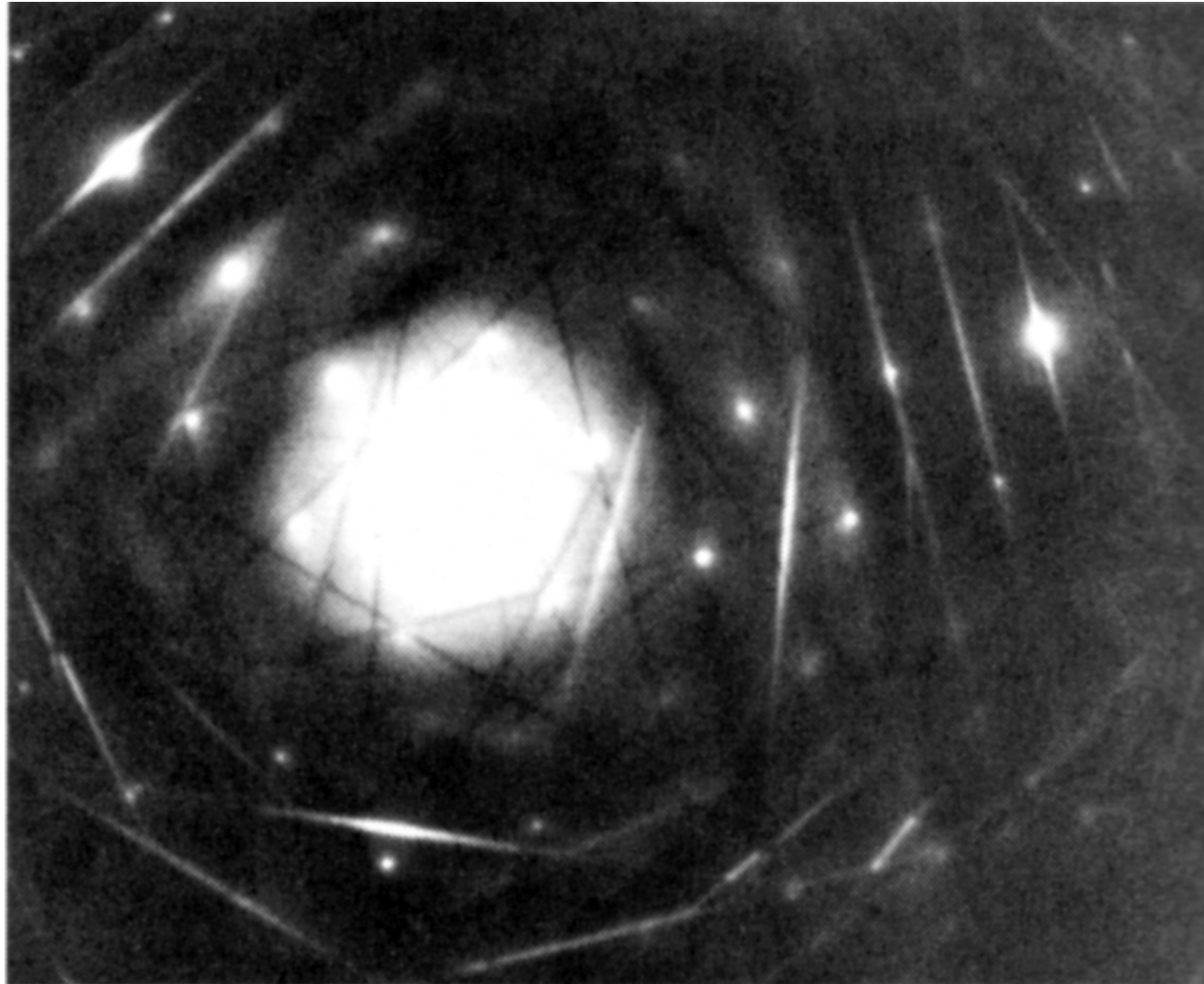
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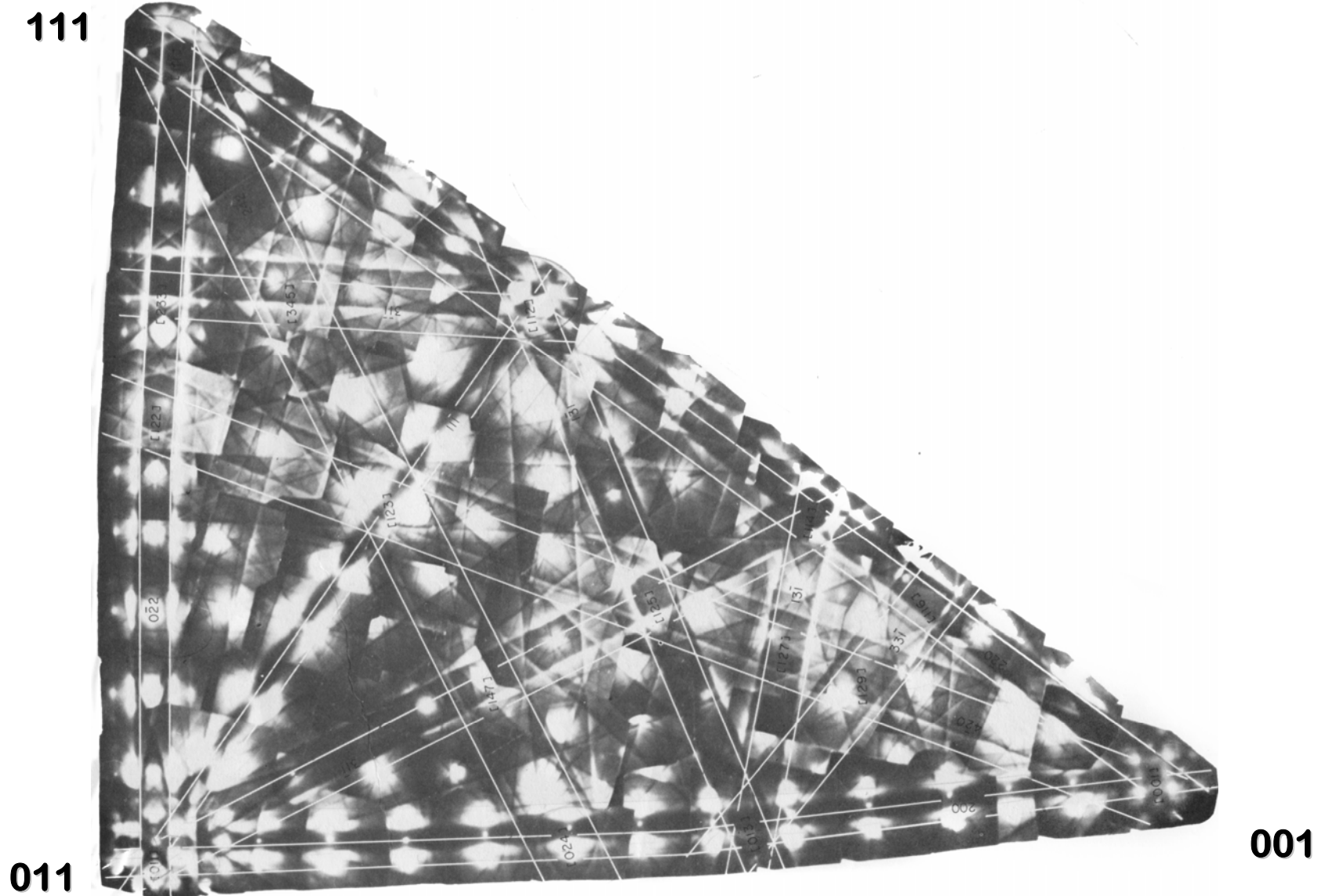


Example Kikuchi pattern



Kikuchi lines & maps

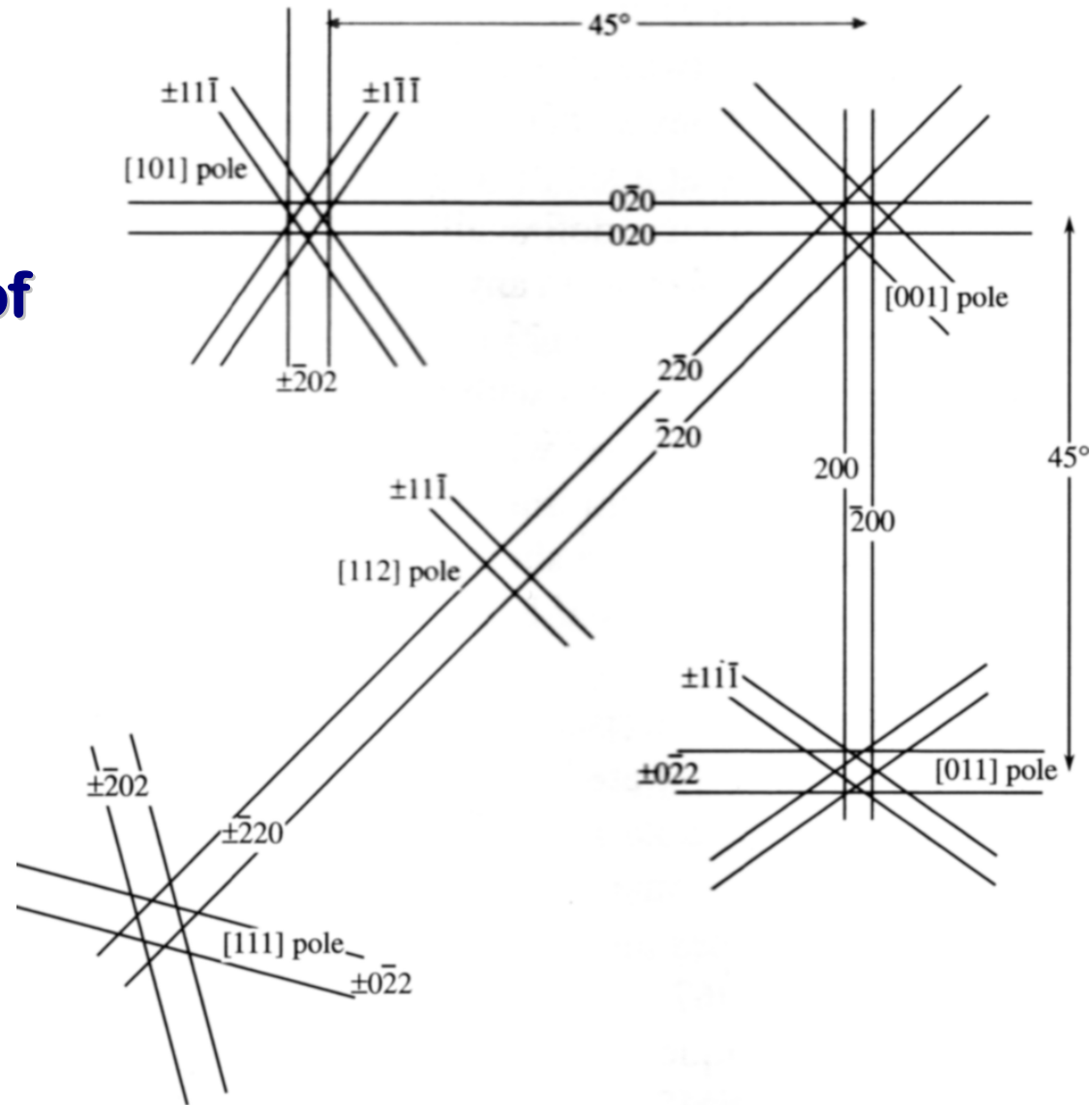
example: fcc



Kikuchi lines

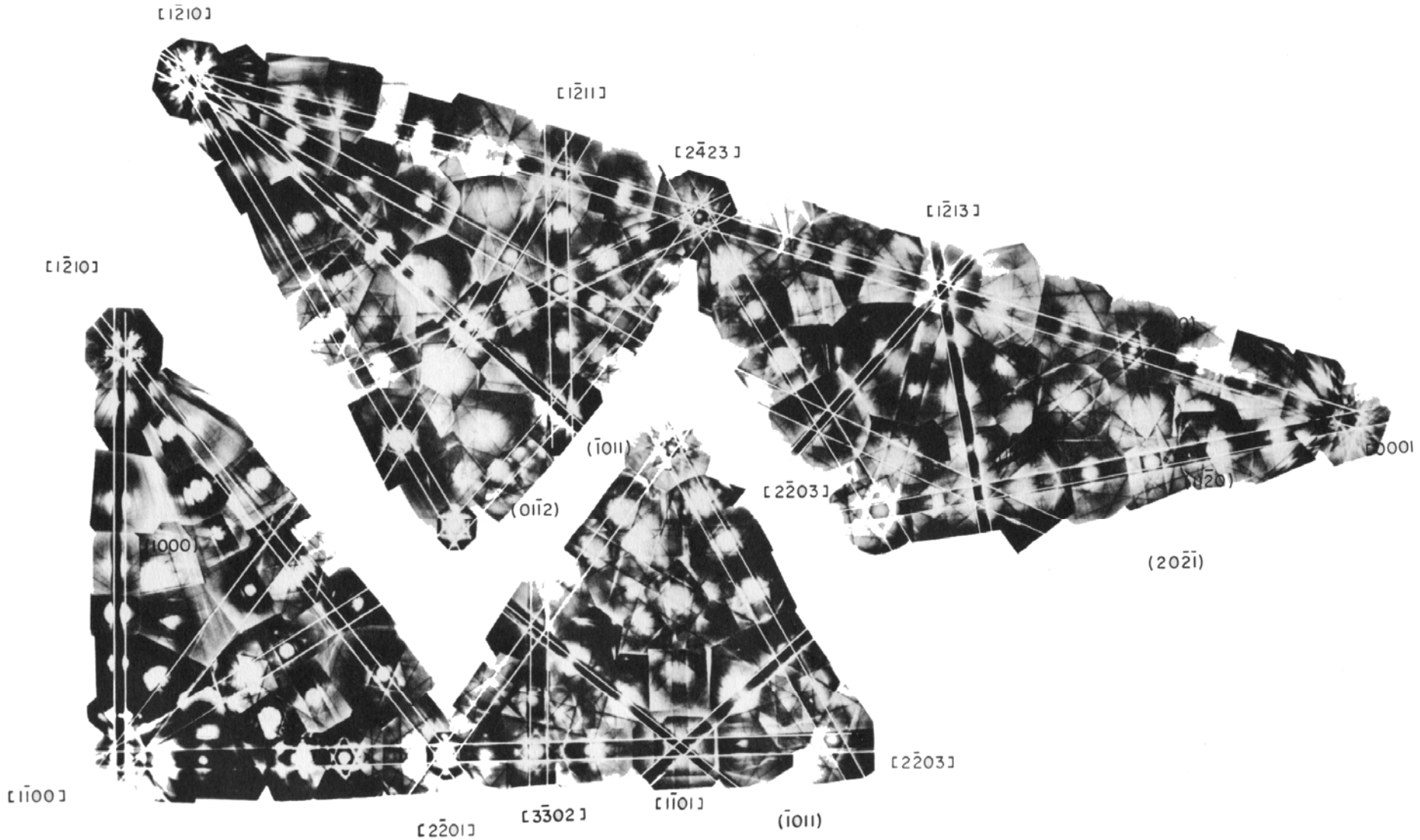
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Provide a “road map” of reciprocal space



Kikuchi lines

example: hcp



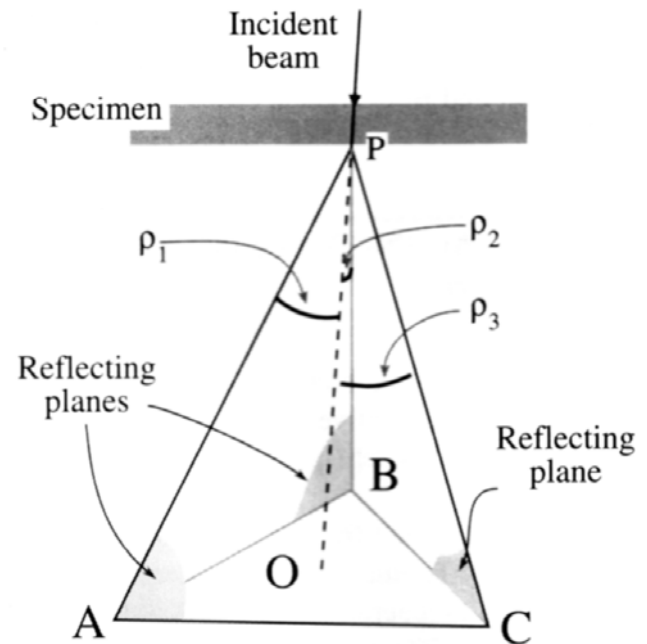
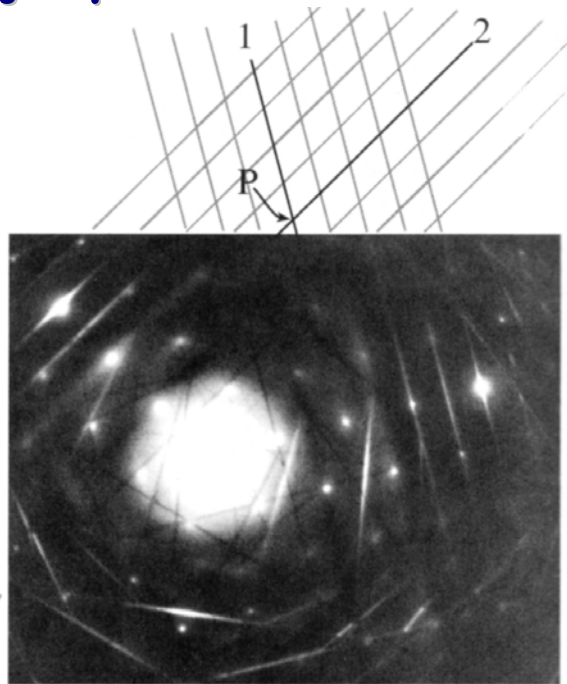
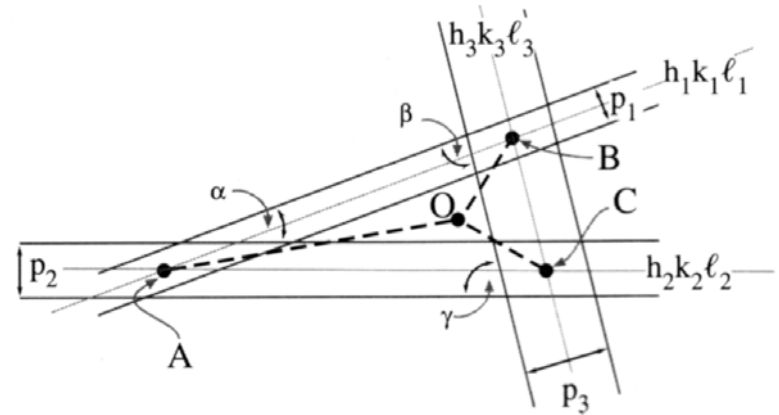
Kikuchi lines

precise orientation determination

Can determine orientation to 0.1°

Simple exercise in geometry

Generally, not needed, as you use Kikuchi lines to help you tilt to major poles



Kikuchi lines

precise orientation determination

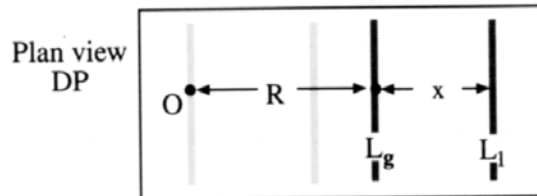
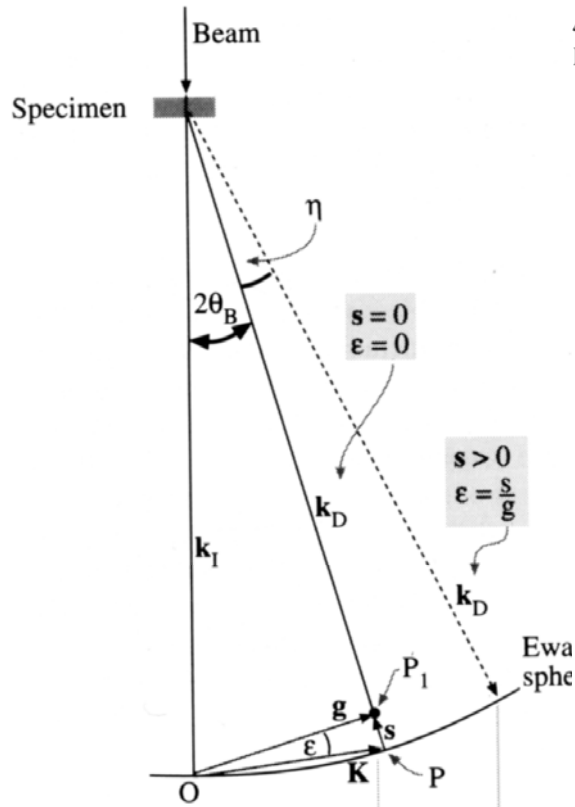
Magnitude & sign of s important in image

Kikuchi lines used to 'set' s

If excess line between g & 0 , s is negative

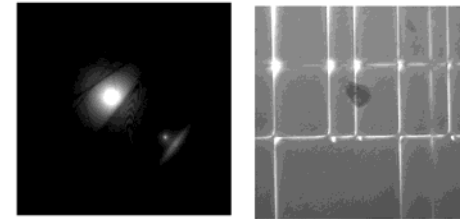
If excess line on opposite side of g , s is positive

$$s = \frac{x}{R} \lambda |g|^2$$

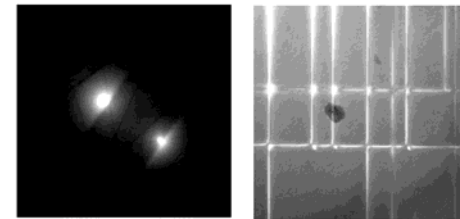


400 two beam condition
Images are axial dark field

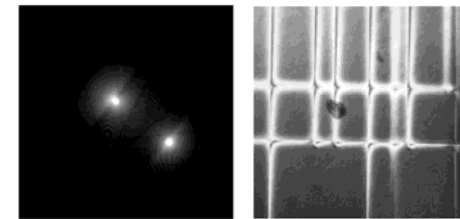
$s \gg 0$



$s > 0$



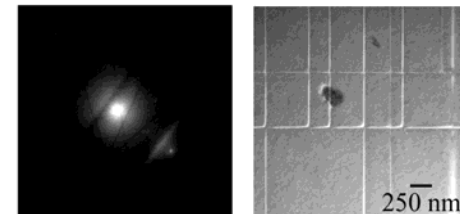
$s = 0$



$s < 0$



$s \ll 0$

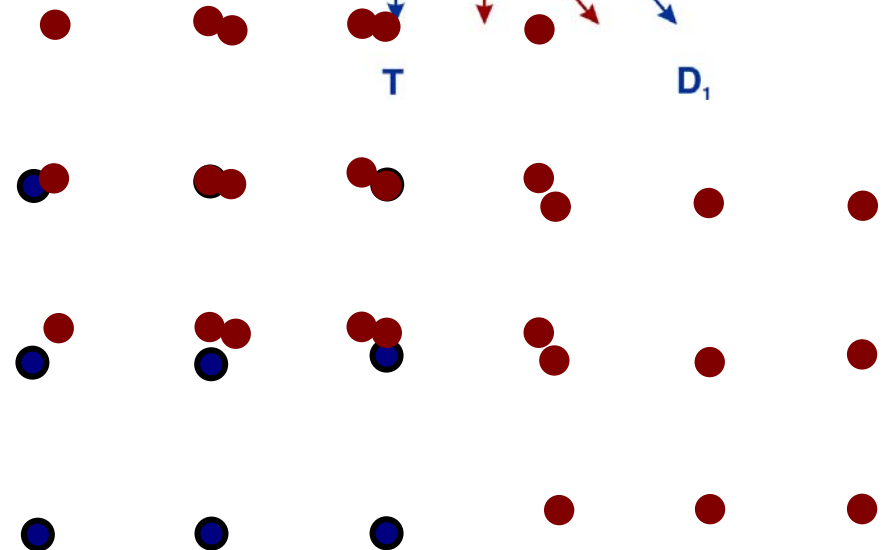
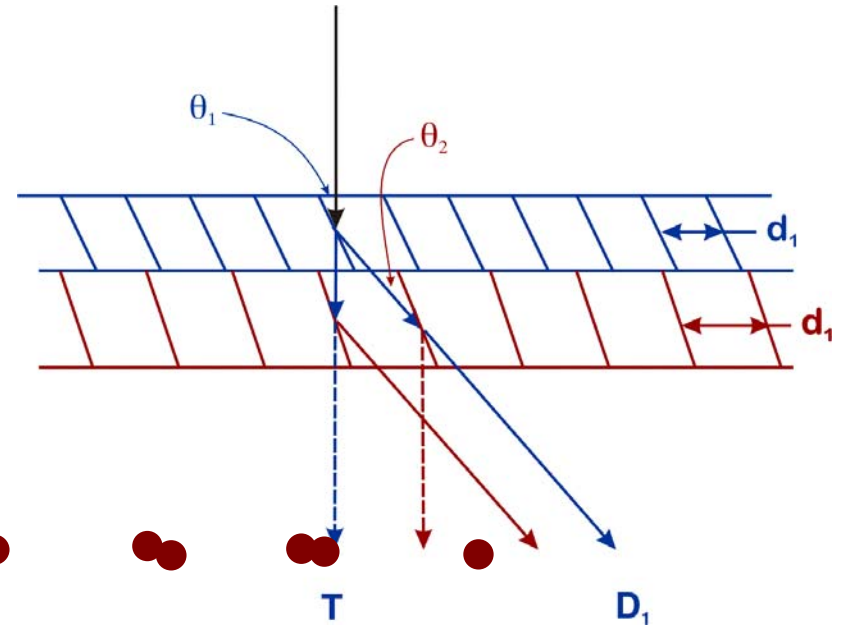


Double diffraction

Frequent cause of extra spots, esp in thin films on substrates

Each diffraction spot from top crystal becomes direct beam for second diffraction event

Note a great way to check for this / eliminate it, is to turn the sample upside down!

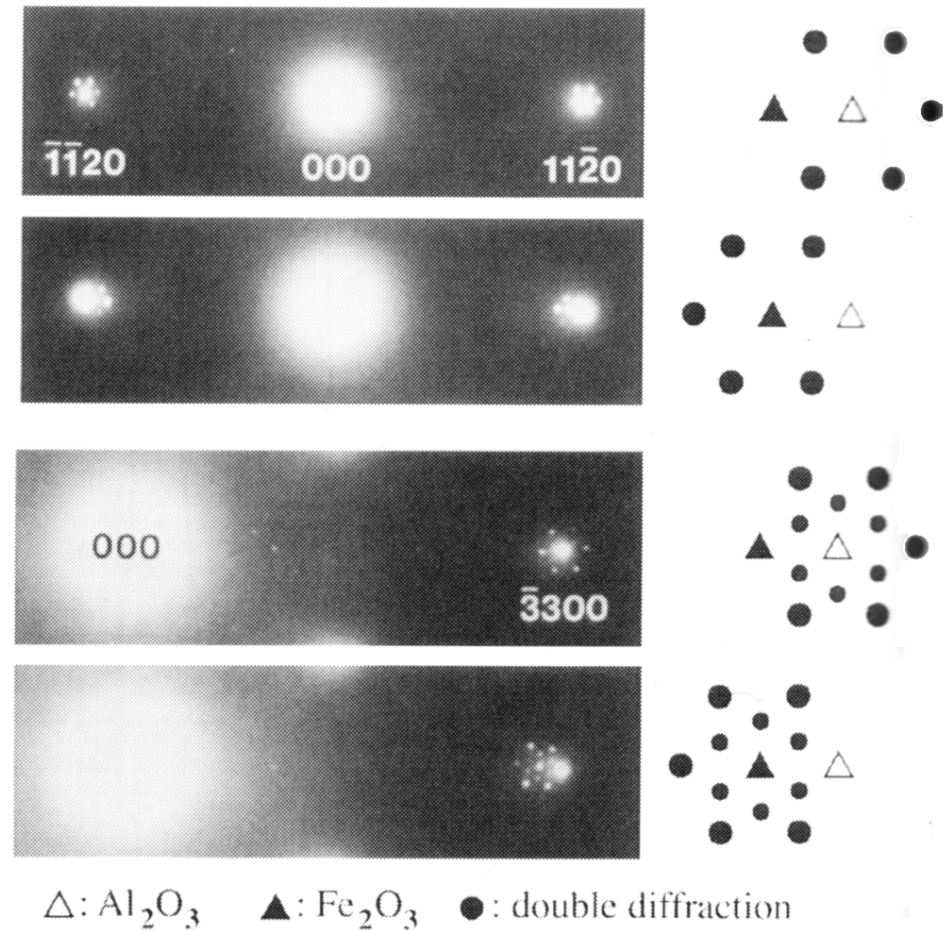


Double diffraction

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Forbidden Reflections

Can have 'forbidden reflections' in a diffraction pattern if dynamical scattering occurs.

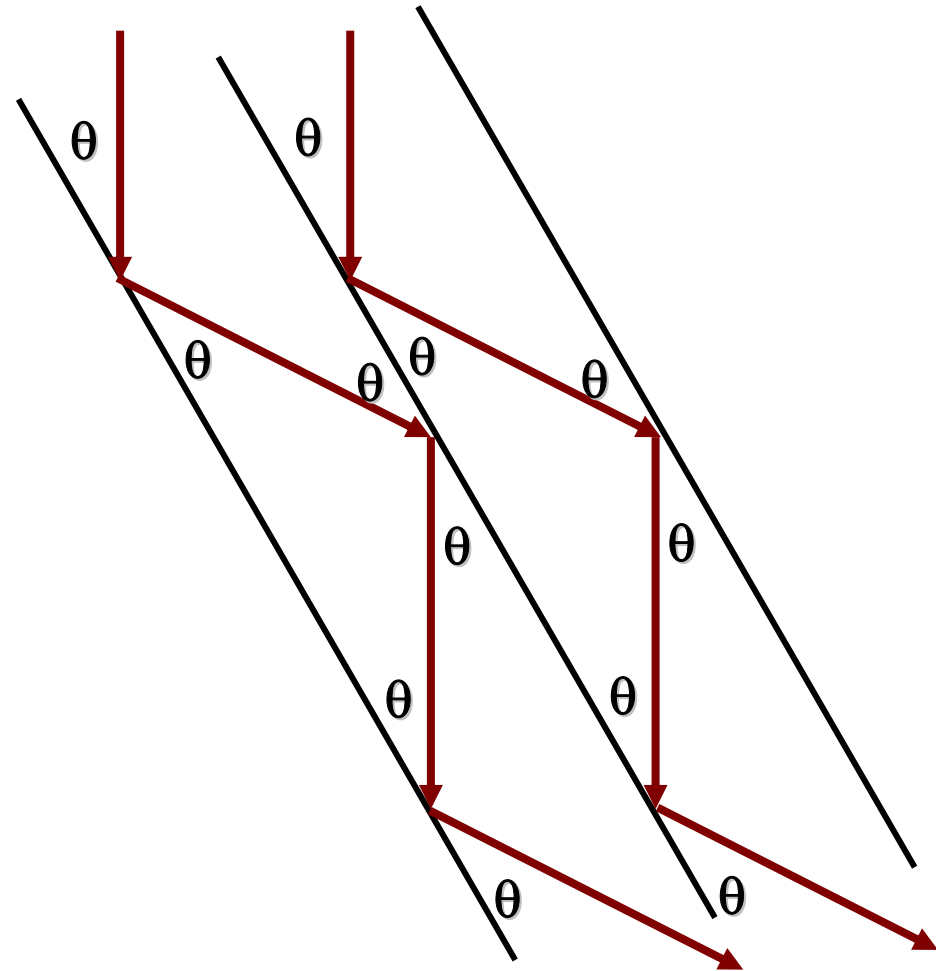
Must have a vector addition to get the beam.

Example

- Can see 200 in silicon 110 zone axis

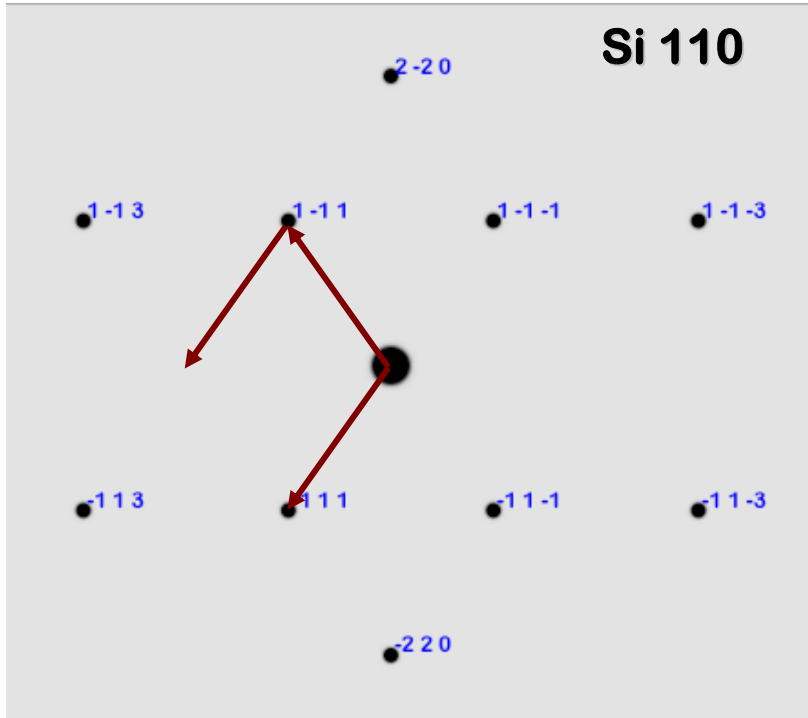
$$1\bar{1}\bar{1} + 1\bar{1}\bar{1} = 200$$

- Cannot see 200 in 100 zone axis - $1\bar{1}\bar{1}$'s not present



Simplified schematic of dynamical scattering

Forbidden Reflections



$$11\bar{1} + 1\bar{1}1 = 200$$

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