Calculation of the zone axis

Université de Lorraine

CRM2 Cristallographie, Résonance Magnétique et Modélisations

cnrs

iJB Institut Jean Barriol

International Autumn School on Fundamental and Electron Crystallography (IASFEC)

8-13 October 2017, Sofia, Bulgaria

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BCS

Българско Кристалографско Дружество
Bulgarian Crystallographic Society
Основано 2009

БКД

MaThCryst

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Notation (reminder)

uvw: coordinates of a lattice nodes in direct space

[*uvw*]: direction indices in direct space

⟨*uvw*⟩: set of equivalent (symmetry-related) directions in direct space

(*hkl*): Miller indices of a lattice plane in direct space

{*hkl*}: crystal form (set of crystal faces equivalent by symmetry). By extension, also set of equivalent (symmetry-related) lattice planes in direct space

hkl: coordinates of a lattice node in reciprocal space; also, Laue indices of a diffraction

[*hkl*]*: direction indices in reciprocal space

⟨*hkl*⟩*: set of equivalent directions in reciprocal space

(*hkl*)*: Miller indices of a lattice plane in reciprocal space

{*hkl*}*: set of equivalent lattice planes in reciprocal space

Zone axis: formal definition

A zone axis is a lattice row parallel to the intersection of two (or more) families of lattices planes. It is denoted by [*u v w*]. A zone axis [*u v w*] is parallel to a family of lattice planes of Miller indices (*hkl*) if (Weiss law):

$$uh + vk + wl = 0$$

The indices of the zone axis defined by two lattice planes (h_1,k_1,l_1), (h_2,k_2,l_2) are given by:

$$\frac{u}{\begin{vmatrix} k_1 & l_1 \\ k_2 & l_2 \end{vmatrix}} = \frac{v}{\begin{vmatrix} l_1 & h_1 \\ l_2 & h_2 \end{vmatrix}} = \frac{w}{\begin{vmatrix} h_1 & k_1 \\ h_2 & k_2 \end{vmatrix}}$$

Conversely, any crystal face can be determined if one knows two zone axes parallel to it (**zone law**)

Three lattice planes have a common zone axis (are in zone) if their Miller indices (h_1,k_1,l_1), (h_2,k_2,l_2), (h_3,k_3,l_3) satisfy the relation:

$$\begin{vmatrix} h_1 & k_1 & l_1 \\ h_2 & k_2 & l_2 \\ h_3 & k_3 & l_3 \end{vmatrix} = 0$$

Compute the zone axis

Let the Miller indices of two lattice planes be (h_1,k_1,l_1), (h_2,k_2,l_2).

$$\begin{array}{c|cccc|c} h_1 & k_1 & l_1 & h_1 & k_1 & l_1 \\ h_2 & k_2 & l_2 & h_2 & k_2 & l_2 \\ \hline & & u \quad v \quad w & & & \end{array}$$

Remove common factor, if any

$+$ $-$

Exercise: zone axis for faces (001) and (101)

$$\begin{array}{c|cccc|c} 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ \hline & & 0 \quad 1 \quad 0 & & & \end{array}$$

Exercise: zone axis for faces (231) and (362)

$$\begin{array}{c|cccc|c} 2 & 3 & 1 & 2 & 3 & 1 \\ 3 & 6 & 2 & 3 & 6 & 2 \\ \hline & & 0 \quad \bar{1} \quad 3 & & & \end{array}$$

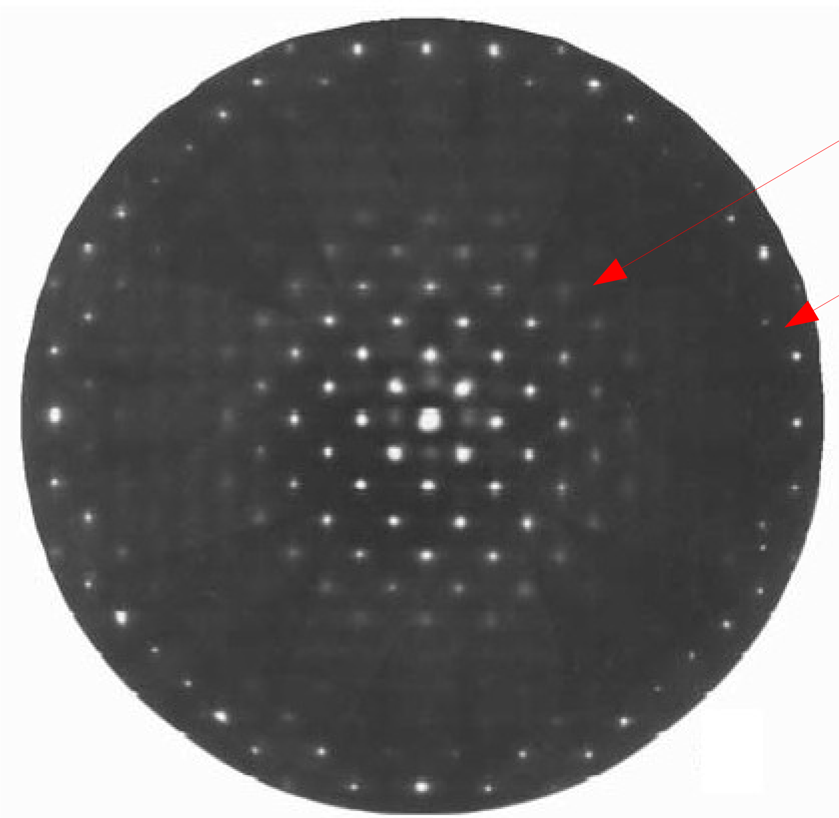
Low-index zone axes correspond to lattice rows parallel to several lattice planes

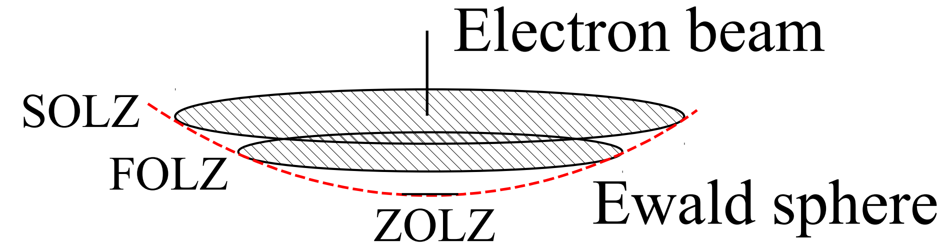
$$\begin{array}{c|cccc|c} h_1 & 0 & l_1 & h_1 & 0 & l_1 \\ h_2 & 0 & l_2 & h_2 & 0 & l_2 \\ \hline & & 0 \quad n \quad 0 & & & \end{array}$$

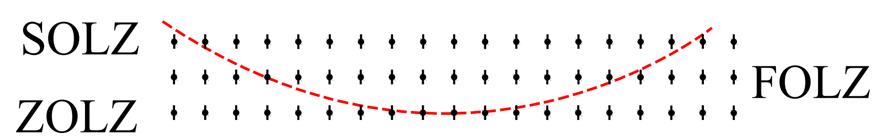
$$n = l_1h_2 - l_2h_1$$

Zone axis pattern in electron diffraction

A **Zone-Axis Pattern** (ZAP) is observed when a high symmetry [*uvw*] direction of the crystal is parallel to the incident beam.
The diffraction spots on the pattern are arranged along **Laue zones**.

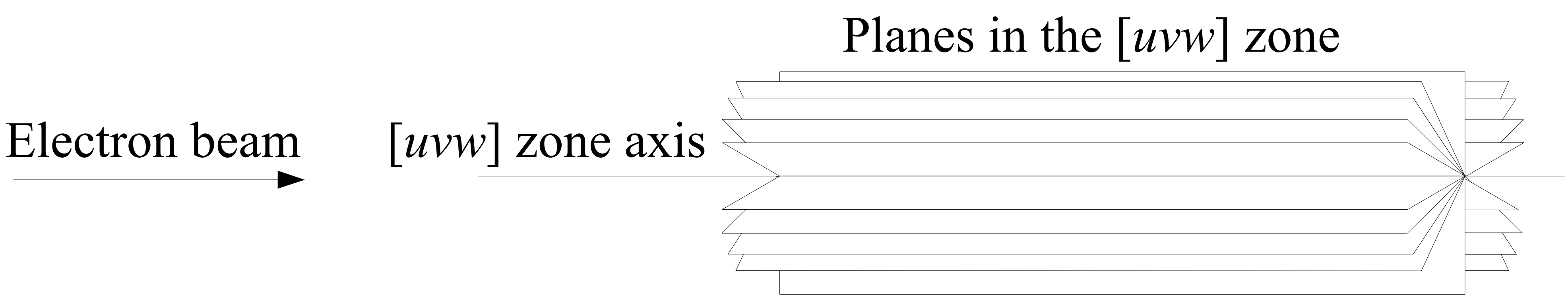






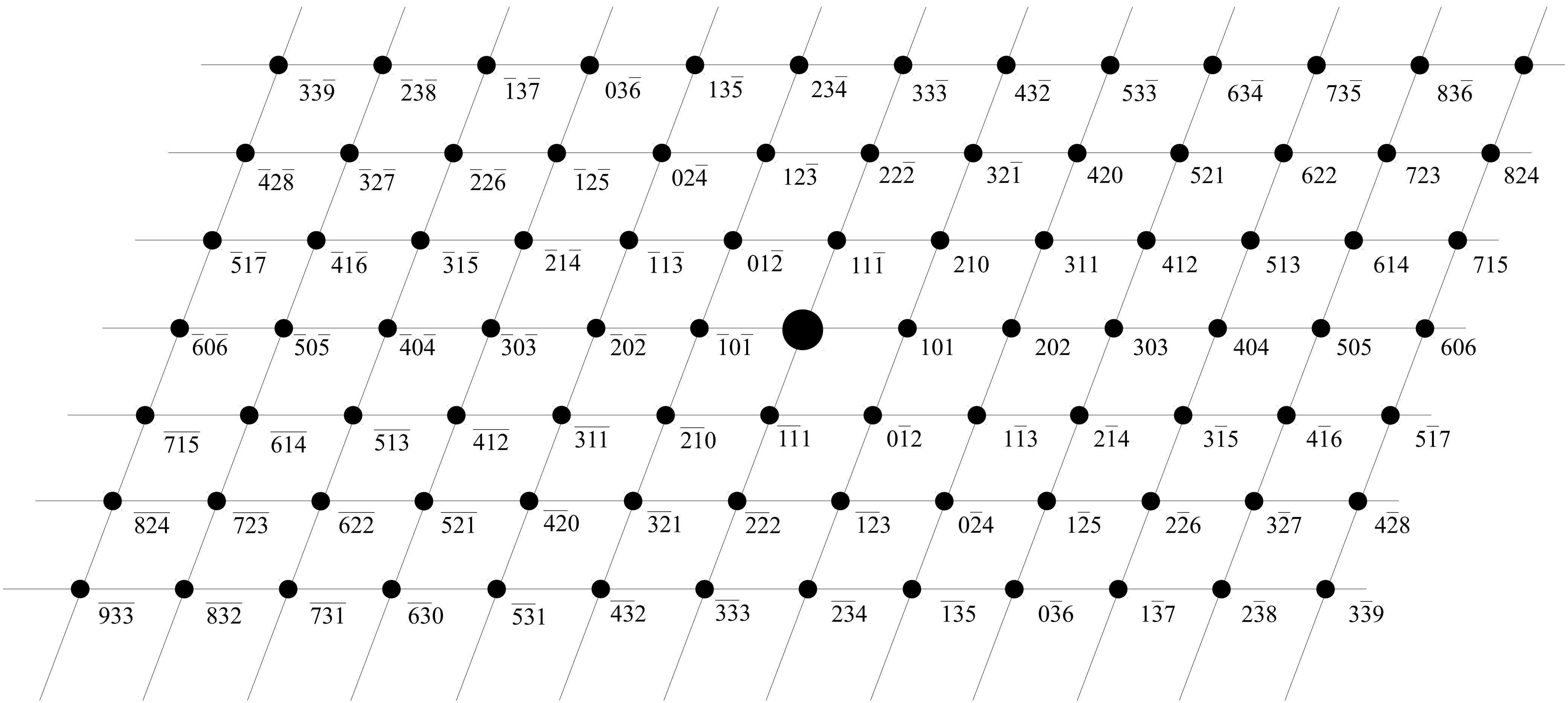
Zone axis pattern in electron diffraction

Zone-Axis Pattern obtained along the [*uvw*] zone axis.
The diffraction pattern shows the (*uvw*)* reciprocal lattice plane.
This pattern is produced from direct lattice planes in the [uvw] zone, *i.e.* "vertical" in the microscope and (almost) parallel to the electron beam.
If the Laue indices are known, then the indices of the zone axis are easily obtained.

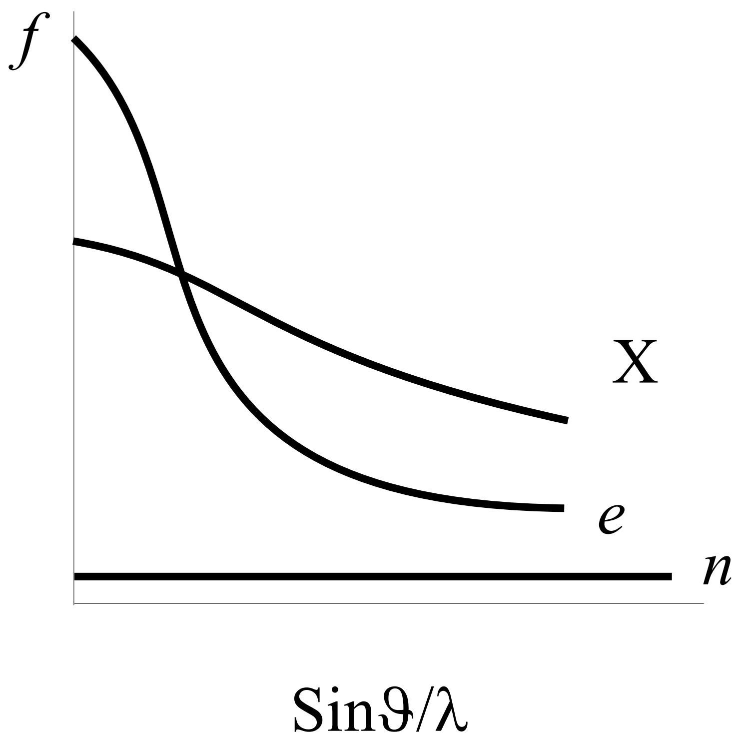


Exercise

Find the zone axis from the following 2D diffraction pattern (no intensity shown)



How to choose a suitable zone axis for EM?



Zone axes [*uvw*] of interest in EM correspond to lattice plane (*hkl*) of small larger interplanar distance *d*(*hkl*), *i.e.* of high reticular density, which means small Miller indices.

$$d(hkl) = 1/\|\mathbf{r}^*(hkl)\| = (hkl|\mathbf{G}^*|hkl)^{1/2}$$

Perpendicularity between lattice directions [*uvw*] and lattice planes (*hkl*)

The perpendicularity between a lattice direction [*uvw*] and a lattice plane (*hkl*) depends on the symmetry of the lattice – which on its turn depends on the presence or absence of metric specialisation.

Lattice symmetry	lattice plane	lattice direction
$\bar{1}$	---	---
2/*m* (*b*-unique)	(010)	[010]
2/*m* 2/*m* 2/*m*	(100) (010) (001)	[100] [010] [001]
4/*m* 2/*m* 2/*m*	(001) (*hkl*)	[001] [*hkl*]
$\bar{3}$ 2/*m* and 6/*m* 2/*m* 2/*m* (hexagonal axes)	(001) (*hki*)	[001] [2*h*+*k*,*h*+2*k*,0]
4/*m* $\bar{3}$ 2/*m*	(*hkl*)	[*hkl*]