Diffraction and Imaging part III

Duncan Alexander
EPFL-IPHYS-LSME

Diffraction and imaging III program

- Q and A from MOOC week 5 lectures and exercises
- Mini-lecture on:
  - Camera length
  - Structure factor
  - Zone axis SADP indexing
- JEMS tutorial

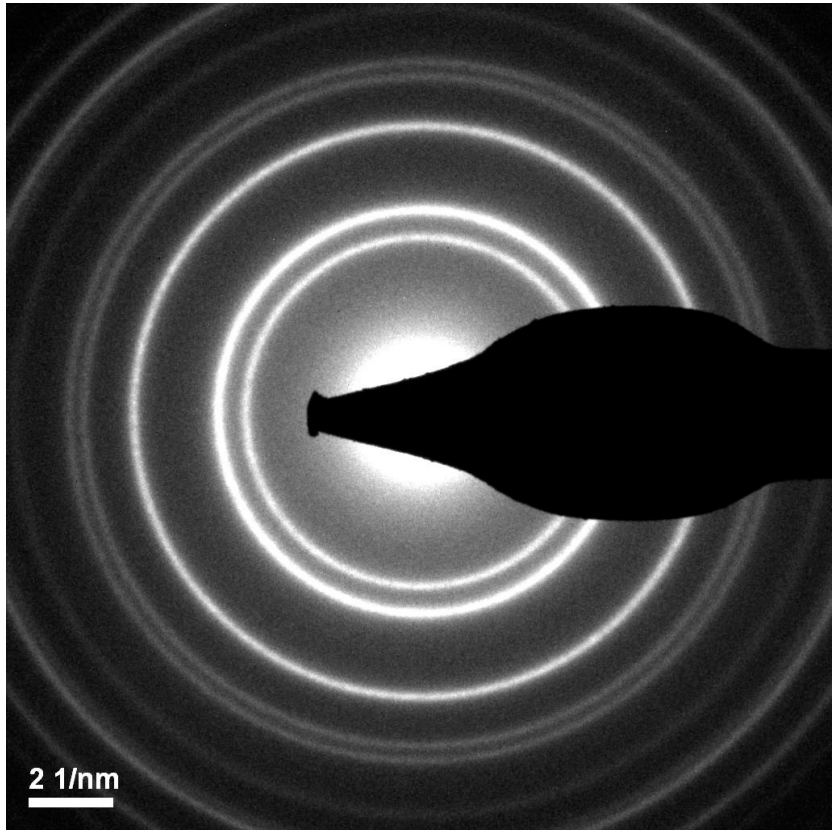
“Camera length” in TEM diffraction

Camera length in TEM diffraction

- Magnification in diffraction mode is called “camera length”
- Historically refers to virtual distance between diffracting object and screen when assuming Fraunhofer far-field diffraction
- Larger camera length $\Longrightarrow$ magnified diffraction pattern

Calibrating camera length

- Digital camera: pixels calibrated in reciprocal plane spacing (nm^{-1})
- To calibrate: record SADP from a known standard – e.g. NiO_x polycrystalline sample



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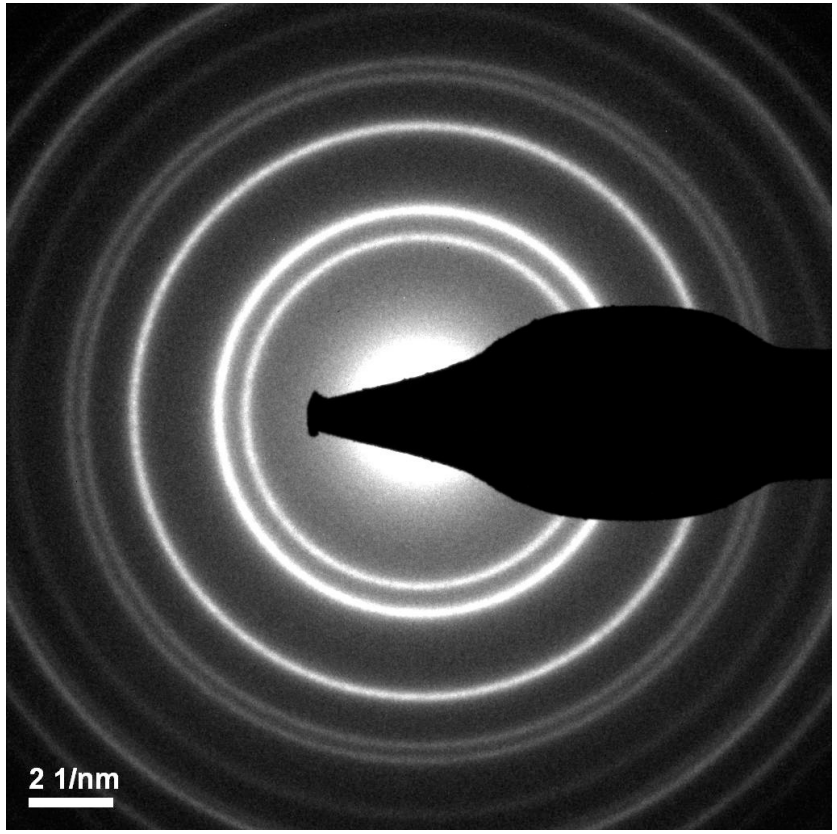


$$(D/2)C = d_{hkl}^{-1}$$

D: diameter of ring (pixels)
C: calibration (nm^{-1} per pixel)
d_{hkl}^{-1}: reciprocal plane spacing (nm^{-1})

The structure factor

Structure factor

- Position dependent wave function for incident plane wave:

$$\psi(\vec{r}) = \psi_0 \exp\left(-2\pi i \vec{k}.\vec{r}\right)$$

- Scattered by individual atom gives spherical scattered wave:

$$\psi_{\text{atom}}(\vec{r}) = \frac{\exp\{-2\pi ikr\}}{r} f\left(\overrightarrow{K}\right)$$

- Consider assembly of atoms into a unit cell. Total scattered wave is:

$$\psi_s(\vec{r}) = \frac{\exp\{-2\pi \mathrm{i}kr\}}{r} \sum_j f_j \exp\left(2\pi i \overrightarrow{K} \cdot \vec{r}_j\right)$$

- Define structure factor for unit cell: $F\left(\overrightarrow{K}\right) = \sum_j f_j \exp\left(2\pi i \overrightarrow{K} \cdot \vec{r}_j\right)$

Structure factor

- Scattered wave given by: $\psi_s(\vec{r}) = \frac{\exp\{-2\pi i k r\}}{r} F(\vec{K})$
- At Bragg condition: $\vec{K} = \vec{g} = h\boldsymbol{a}^* + k\boldsymbol{b}^* + l\boldsymbol{c}^*$
- Position of each atom in unit cell: $\vec{r}_j = x_j\boldsymbol{a} + y_j\boldsymbol{b} + z_j\boldsymbol{c}$
- Structure factor for reflection $\vec{g}$: $F_g = \sum_j f_j \exp\left[2\pi i\left(hx_j + ky_j + lz_j\right)\right]$
- Add up scattering from all unit cells across a sample of thickness t find intensity of scattered beam:

$$I_g = \left[\frac{\sin(\pi t s)}{\xi_g s}\right]^2 \qquad \text{where:} \qquad \xi_g = \frac{\pi k V_0 \cos\theta_B}{F_g}$$

Systematic absences

- Depending on symmetry of a structure, certain planes can have structure factor $F_g = 0$
- If so, intensity of diffracted beam $I_g = 0 \Longrightarrow$ “systematic absence”/“forbidden reflection”
- Example: face-centred cubic lattice (FCC)

  Lattice point positions: $x,y,z = \quad 0,0,0; \quad \frac{1}{2},\frac{1}{2},0; \quad \frac{1}{2},0,\frac{1}{2}; \quad 0,\frac{1}{2},\frac{1}{2}$

$$F_g = \sum_j f_j \exp\left[2\pi i\left(hx_j + ky_j + lz_j\right)\right]$$

Systematic absences

- FCC: planes with indices h,k,l mixed odd and even are *absent*

- How about body centred cubic (BCC), with lattice points: $x,y,z = 0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}$

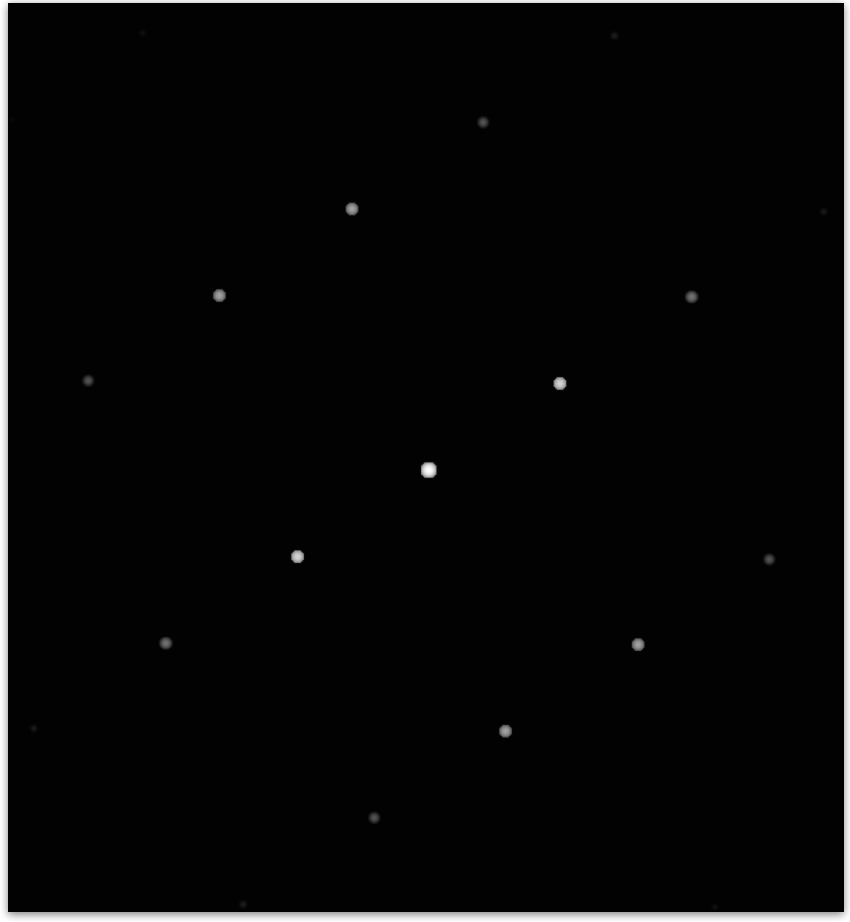
Indexing diffraction patterns

How do we analyse a zone axis SADP?

- Weiss zone law applies:
  $hU + kV + lW = 0$
- Angles between planes in real space =
  angle between their diffraction spots
- For indexing, choose two potential, non-parallel planes(h_1 k_1 l_1) and (h_2 k_2 l_2).
  Then determine zone axis [U V W] as cross product:

$$U = k_1 l_2 - k_2 l_1$$
$$V = l_1 h_2 - l_2 h_1$$
$$W = h_1 k_2 - h_2 k_1$$

- Index two reflections that have correct plane spacings, making sure that angle between planes is correct
- Go from there using vectorial addition, choice of planes that are consistent with [U V W]



Tutorial #1

Fe (BCC)
a = 0.286 nm

(h,k,l)	d / nm
(0, 0, 0)	
(1, 1, 0)	0.20216
(2, 0, 0)	0.14295
(2, 1, 1)	0.11672
(2, 2, 0)	0.10108
(3, 1, 0)	0.09041
(2, 2, 2)	0.08253
(3, 2, 1)	0.07641
(4, 0, 0)	0.07147
(3, 3, 0)	0.06739
(4, 1, 1)	0.06739
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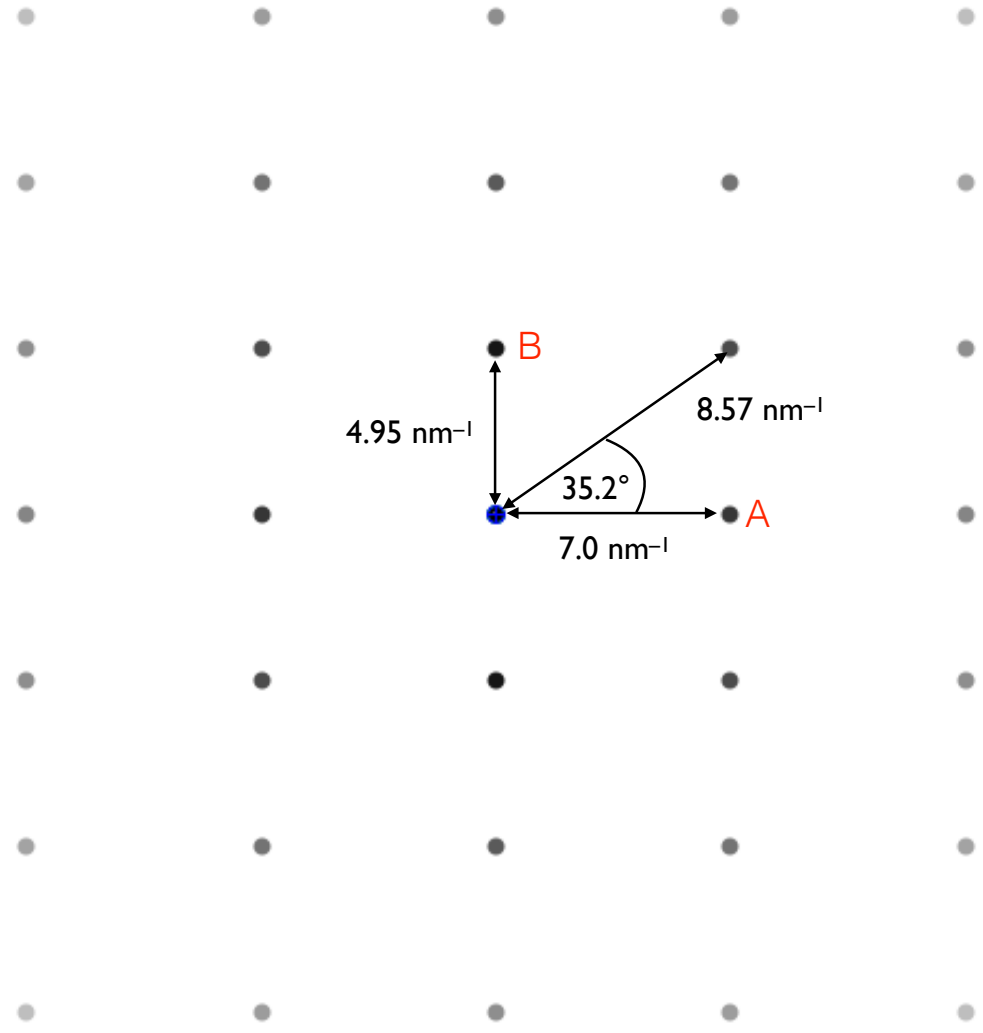

Tutorial #2

Fe (BCC)
a = 0.286 nm

(h,k,l)	d / nm
(0, 0, 0)	
(1, 1, 0)	0.20216
(2, 0, 0)	0.14295
(2, 1, 1)	0.11672
(2, 2, 0)	0.10108
(3, 1, 0)	0.09041
(2, 2, 2)	0.08253
(3, 2, 1)	0.07641
(4, 0, 0)	0.07147
(3, 3, 0)	0.06739
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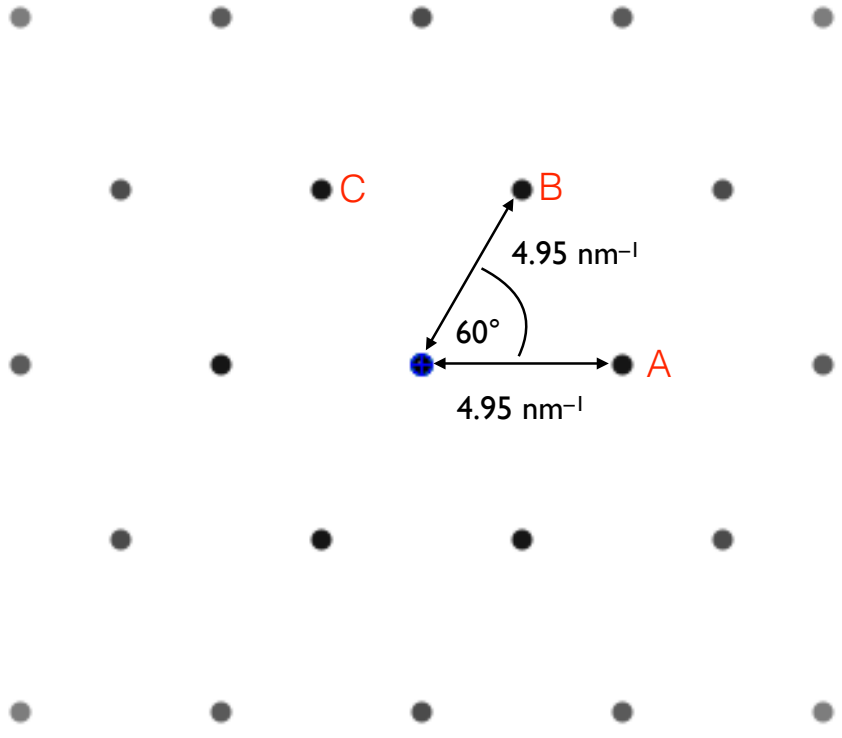
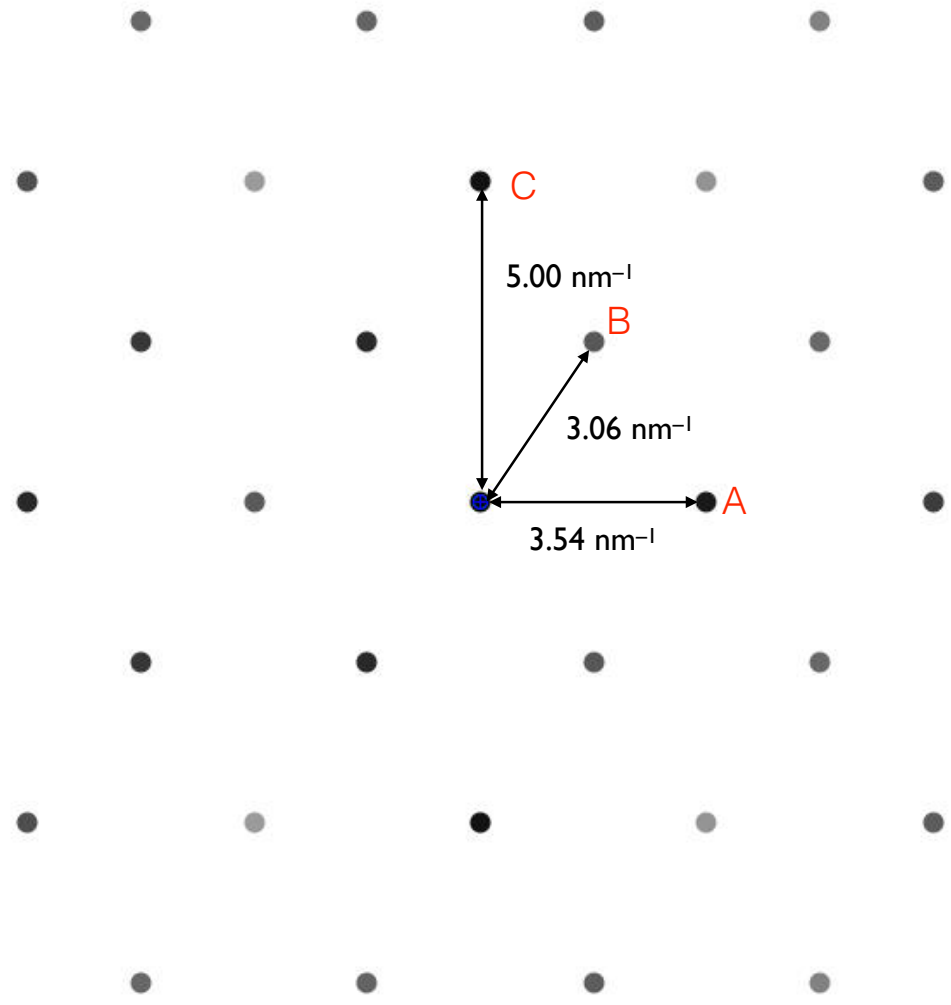


Tutorial #3

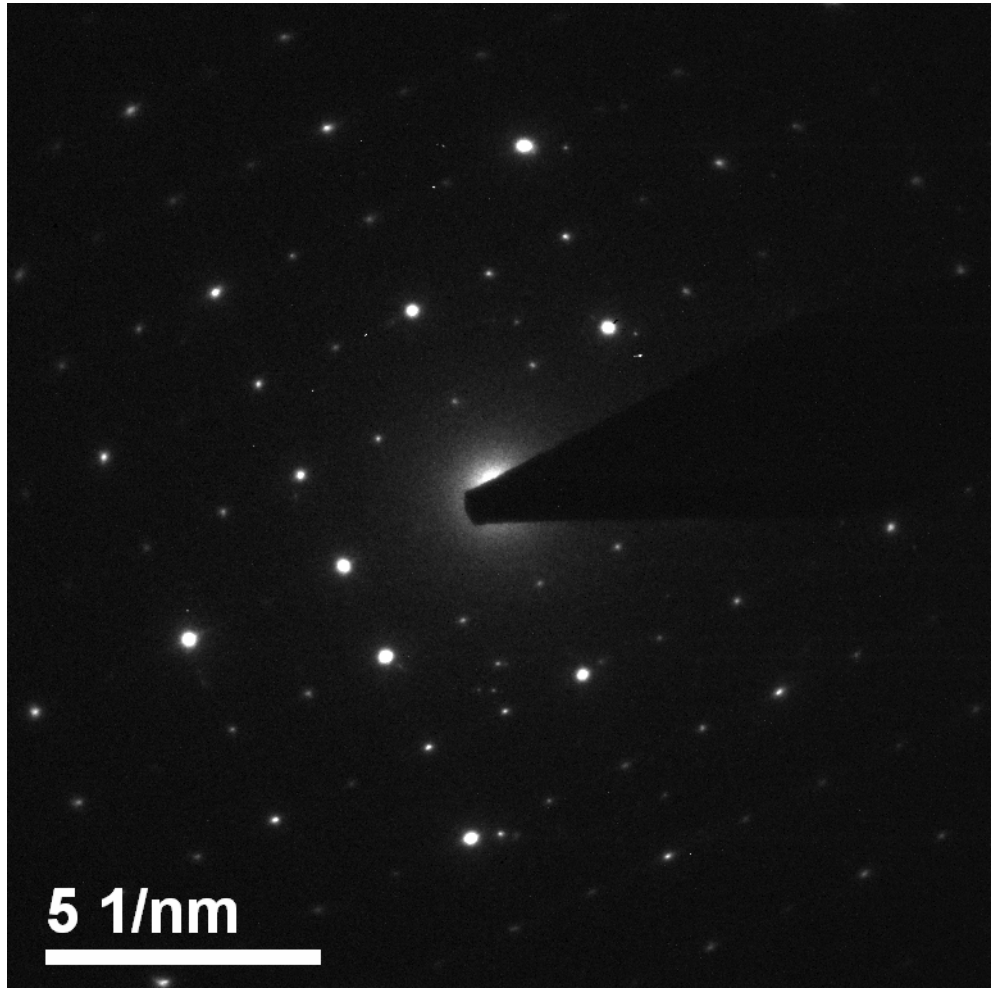
GaAs (zinc blende FCC)
a = 0.565 nm

(h,k,l)	d / nm
(0, 0, 0)	
(1, 1, 1)	0.32632
(2, 0, 0)	0.2826
(2, 2, 0)	0.19983
(3, 1, 1)	0.17041
(2, 2, 2)	0.16316
(4, 0, 0)	0.1413
(3, 3, 1)	0.12967
(4, 2, 0)	0.12638
(4, 2, 2)	0.11537
(3, 3, 3)	0.10877



Fitting by simulation

- Can use e.g. Stadelmann's JEMS software to simulate diffraction patterns for known crystal structure(s), and fit to experimental data
- JEMS can also do "active" fitting from measured reciprocal lattice spacings and angles



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