Summary of lecture from 09.03.2018

Structure factors, systematic abscences, and XRD plots

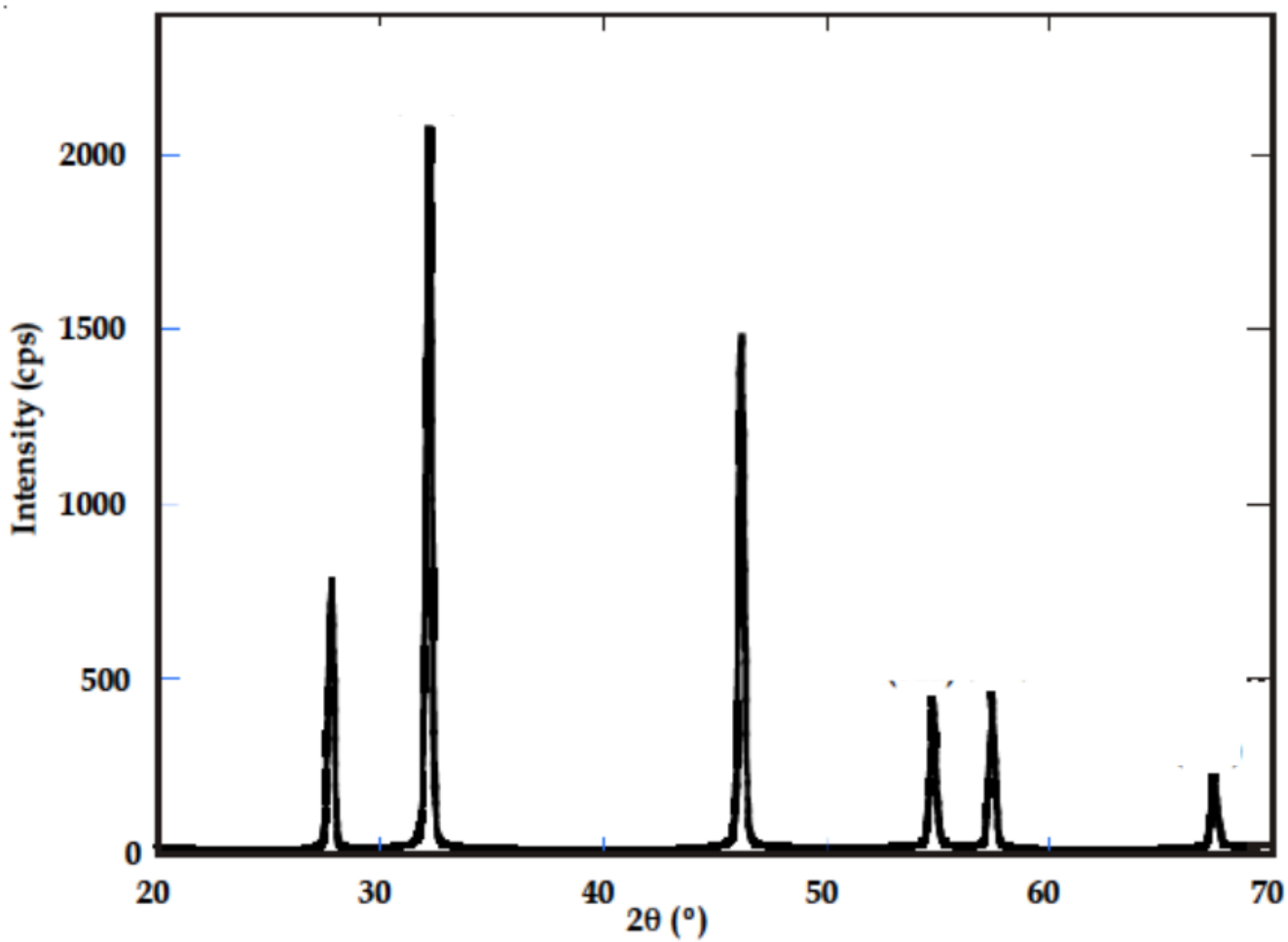

Fig. 9. X-Ray diffraction pattern of silver chloride nanoparticles

Form factor and structure factor

- Structure factor

$$S_k = \sum_{\text{atom } j \in \text{ unit cell}} f_j(k)\, e^{ik \cdot r_j}$$

  Proportional to peak intensity: $|S_k|^2 \propto I_k$

- Atomic form factor $f_j(k)$
  "Strength of scattering from atom j"

$$f_j(k) = \int e^{ik \cdot r} V_j(r)\, \mathrm{d}r$$

  Fourier transform of scattering potential $V_j(r)$

Monoatomic bases

$$S_k = j \cdot f(k) \sum_j e^{ik \cdot r_j} = j \cdot f(k) \sum_j e^{i2\pi\left(hx_j + ky_j + lz_j\right)} = j \cdot f \cdot S_k^{\text{lattice}}$$

with $S_k^{\text{lattice}} = \sum_j e^{ik \cdot r_j}$ the structure factor for the lattice
and $f(k)$ the form factor

	lattice points	S_k^{lattice}	systematic absence
sc	$[0, 0, 0]$	1	all h, k, l allowed
bcc	$[0, 0, 0]$ $\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	2	$h + k + l$ must be even
fcc	$[0, 0, 0]$ $\left[\frac{1}{2}, \frac{1}{2}, 0\right]$ $\left[\frac{1}{2}, 0, \frac{1}{2}\right]$ $\left[0, \frac{1}{2}, \frac{1}{2}\right]$	4	h, k, l all even or all odd

Systematic absences

- For some combinations of h, k, l: $S_k = 0$
- (hkl) not allowed: destructive interference
- absence of peak

Polyatomic bases

$$S_k = S_k^{\text{lattice}} \cdot S_k^{\text{basis}}$$

example	crystal	basis	S^{lattice}	S^{basis}
CsCl	sc	Cs: $[0, 0, 0]$ Cl: $\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	1	$f_{Cs} + f_{Cl}\,(-1)^{h+k+l}$
NaCl	fcc	Na: $[0, 0, 0]$ Cl: $\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	4	$f_{Na} + f_{Cl}\,(-1)^{h+k+l}$

If $f_A \neq f_B$ systematic absences same as for S_k^{lattice}