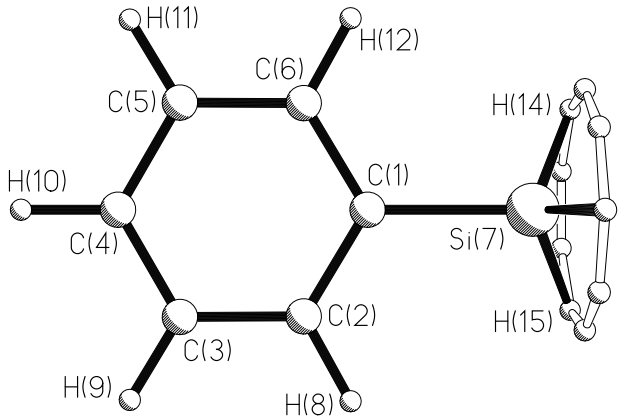
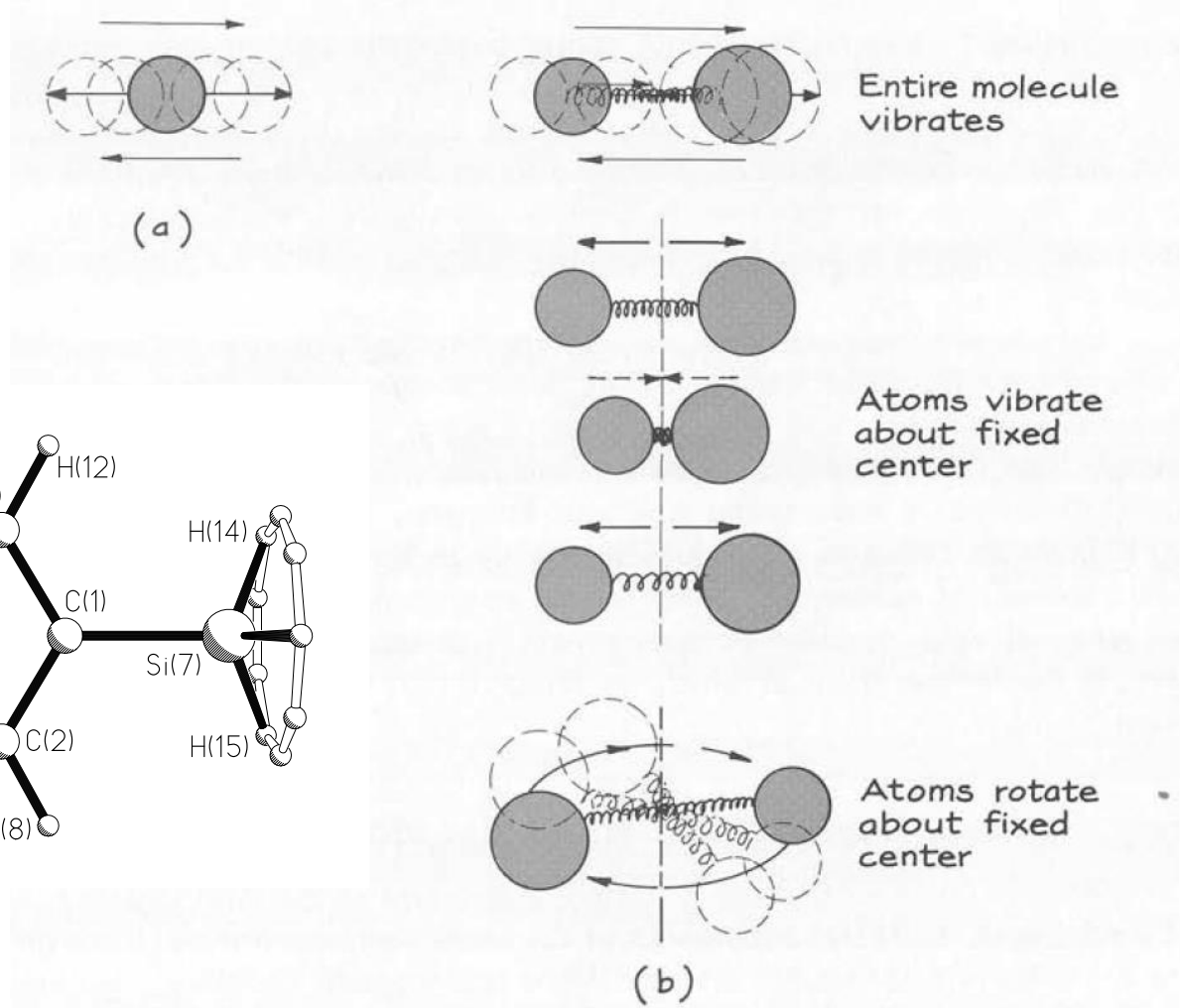
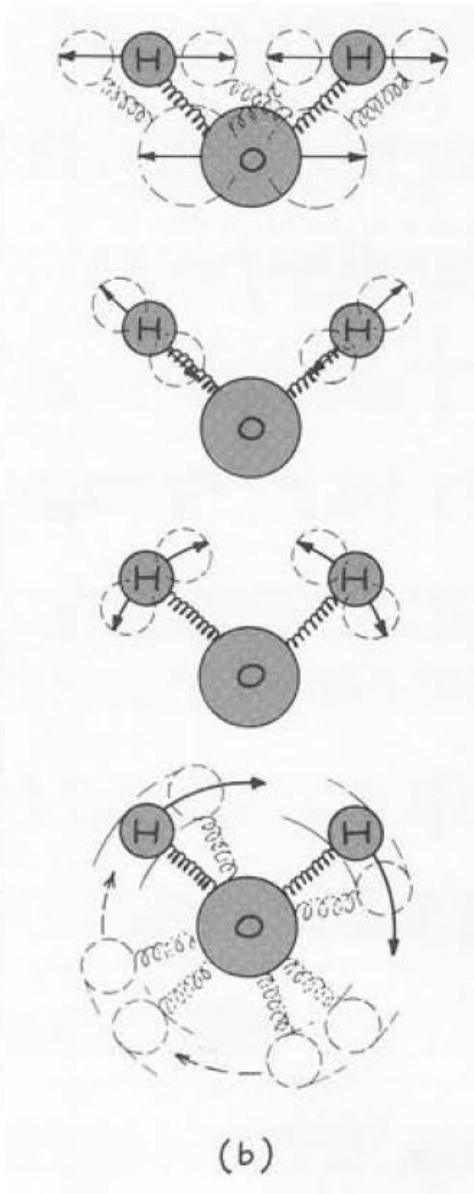
Structural Methods

Information	Gas	Liquid	Solid
Fingerprint	IR, (*MW**)	IR, Raman	IR, Raman
	MS, UV/Vis	MS, UV/Vis	MS, UV/Vis
	NMR		Pulver-XRD
Groups	IR, MS, NMR	IR, Raman	IR, Raman
		MS, NMR	MS, *S-NMR, (**Mössbr*.)
Molecular	IR, (**MW*)	IR, Raman	IR, Raman, S-NMR,
Symmetry	**GED	NMR	SC-XRD, (**NQR)
Lengths,	*MW, **GED	EXAFS***	SC-XRD,
Angles	IR, Raman	(*NMR*), (XRD)	***ND
Electronic	UV/Vis	UV/Vis	UV/Vis, PES, XPS, XRD
Structure	PES, ESR	ESR, (*XPS)	*Mössbr., ***ND
Electron density			SC-XRD

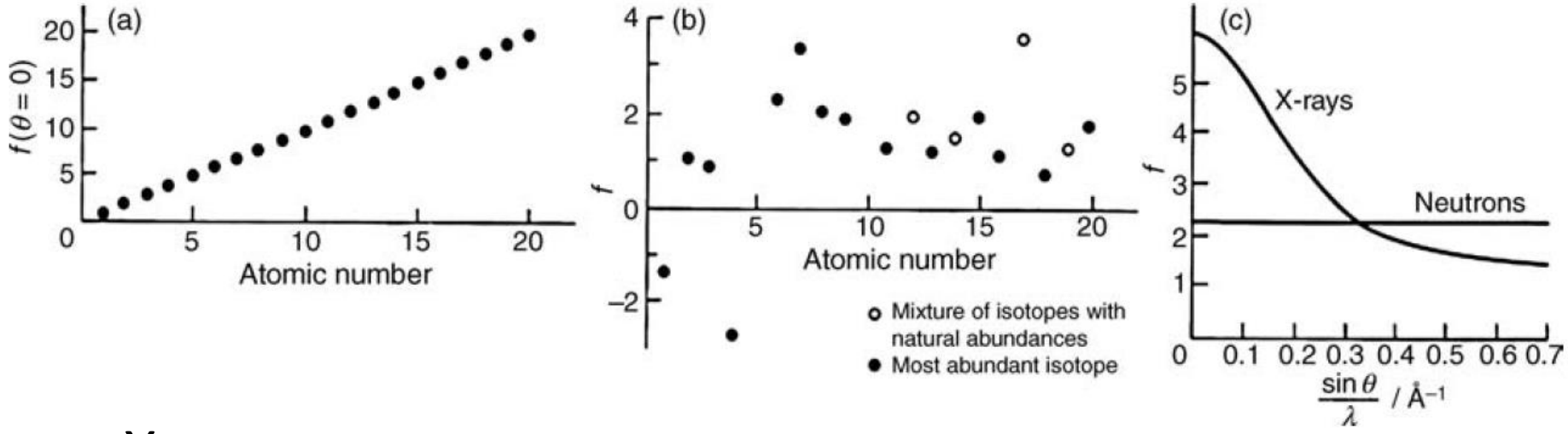
Vibrational Average in Single Crystal Determination





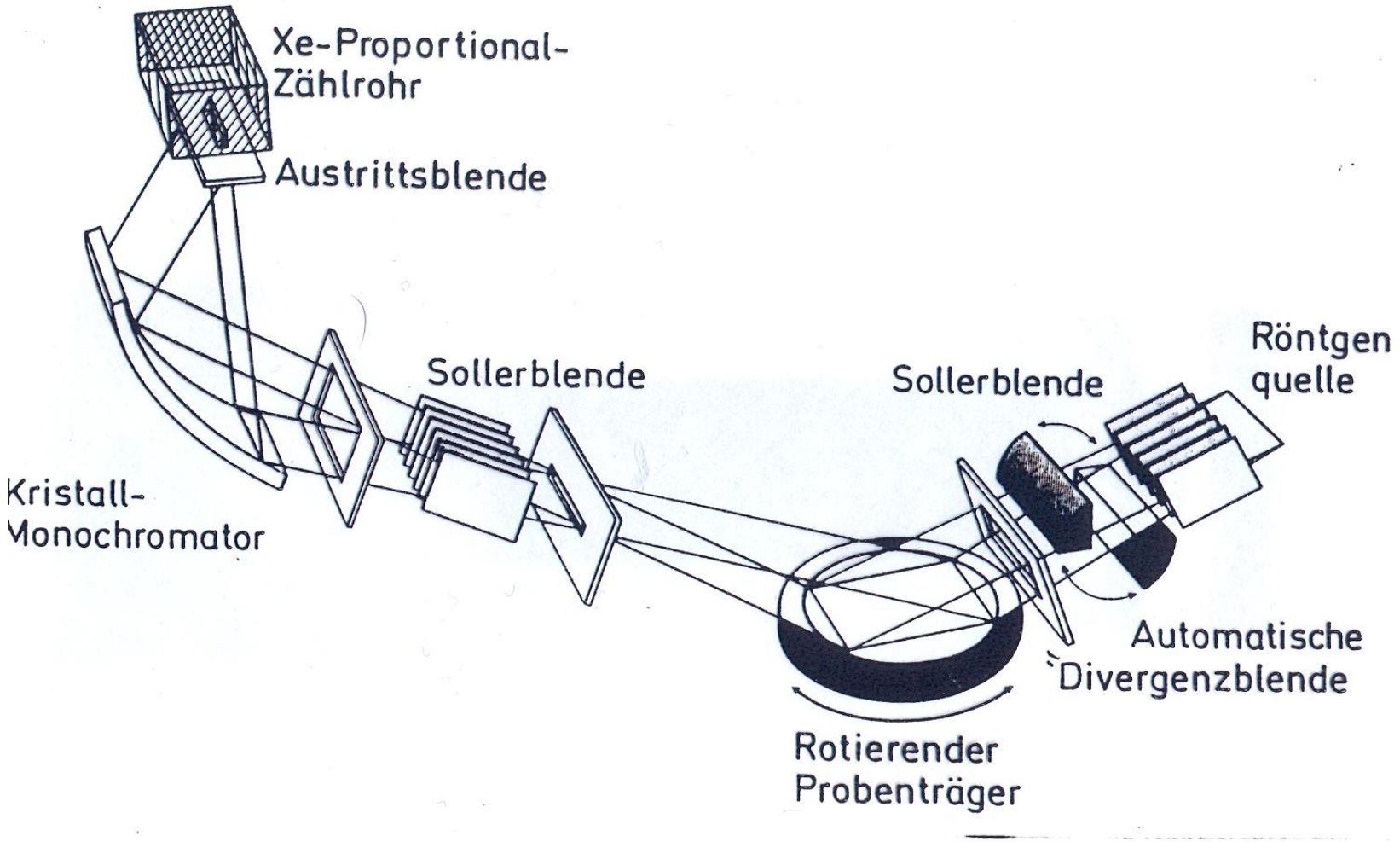


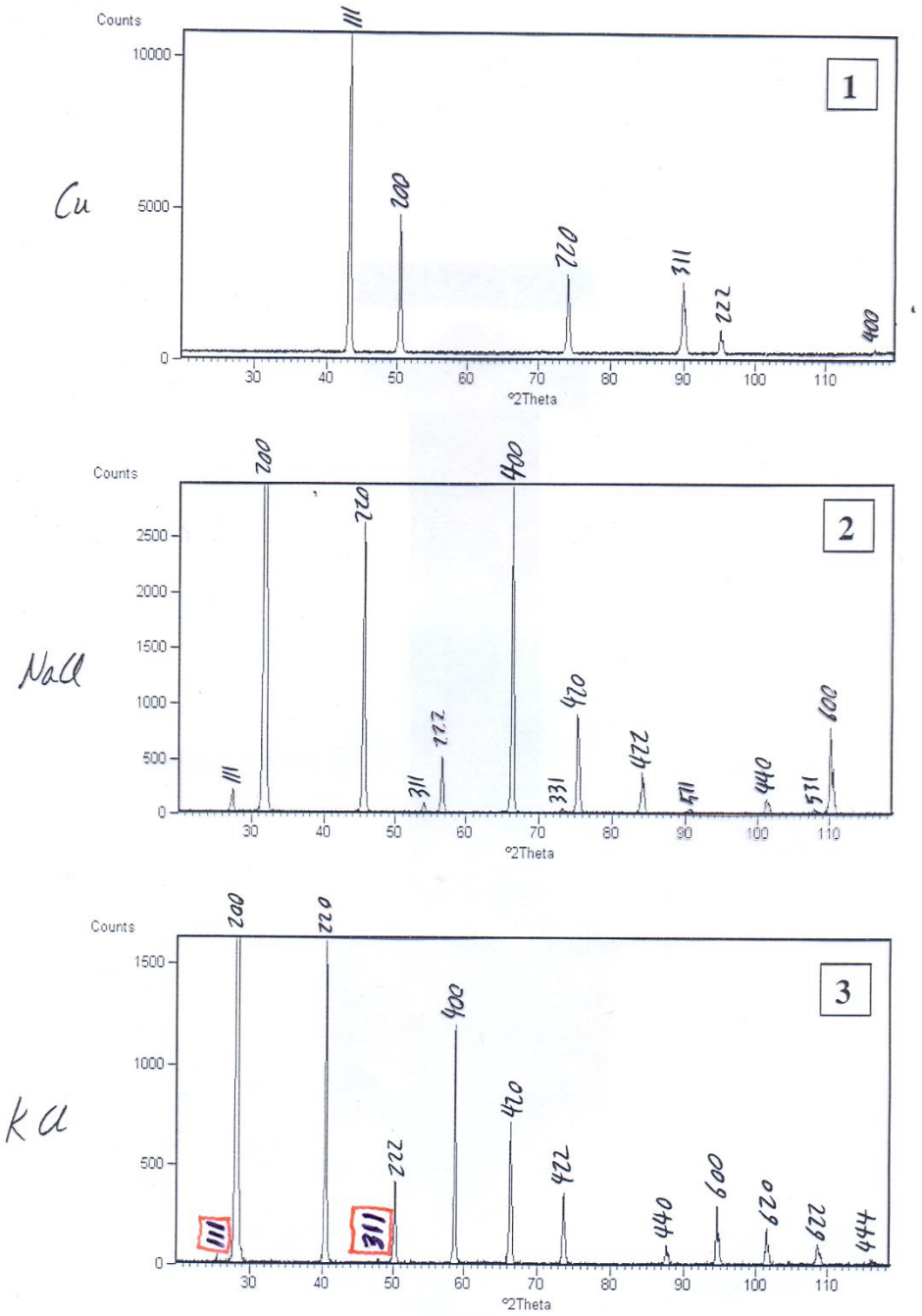
Variation of the scattering power scattering amplitude *f* with the atomic number



X-rays neutrons

Pulverdiffraktometer





Diffraktogramme von Cu, NaCl und KCl

Diffraktogramme von Phasengemischen

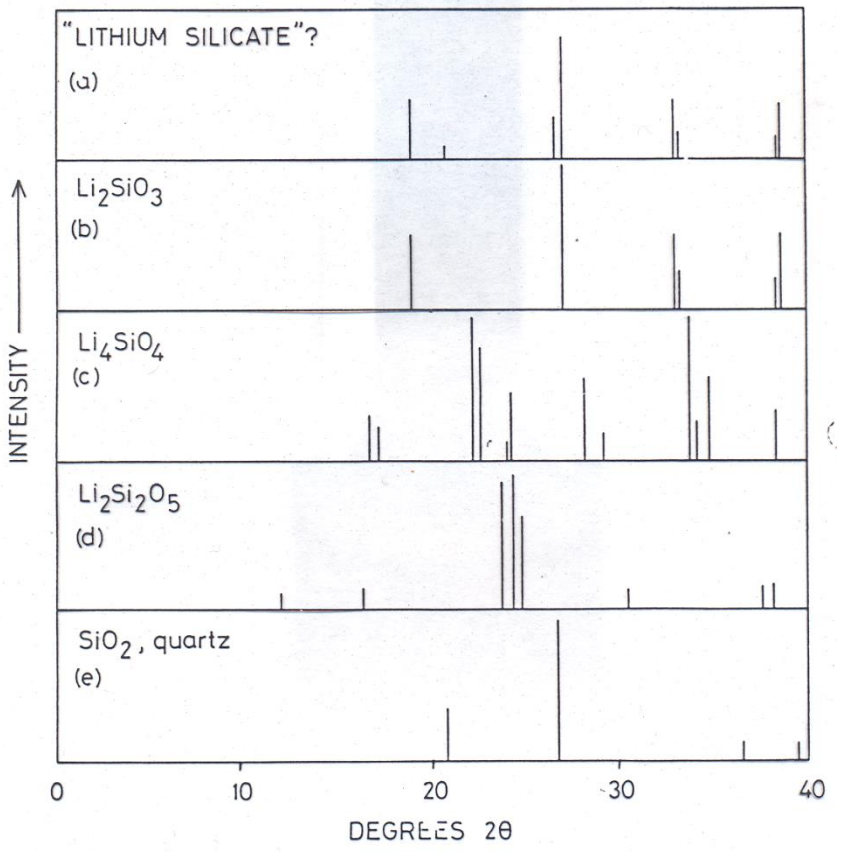


Fig. 5.47 Powder patterns of (a) a bottle labelled 'lithium silicate' and (b) to (e) standard lithium silicate and silica phases

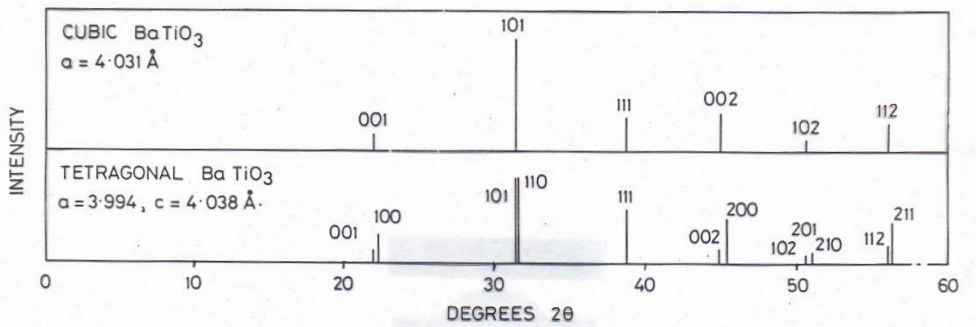
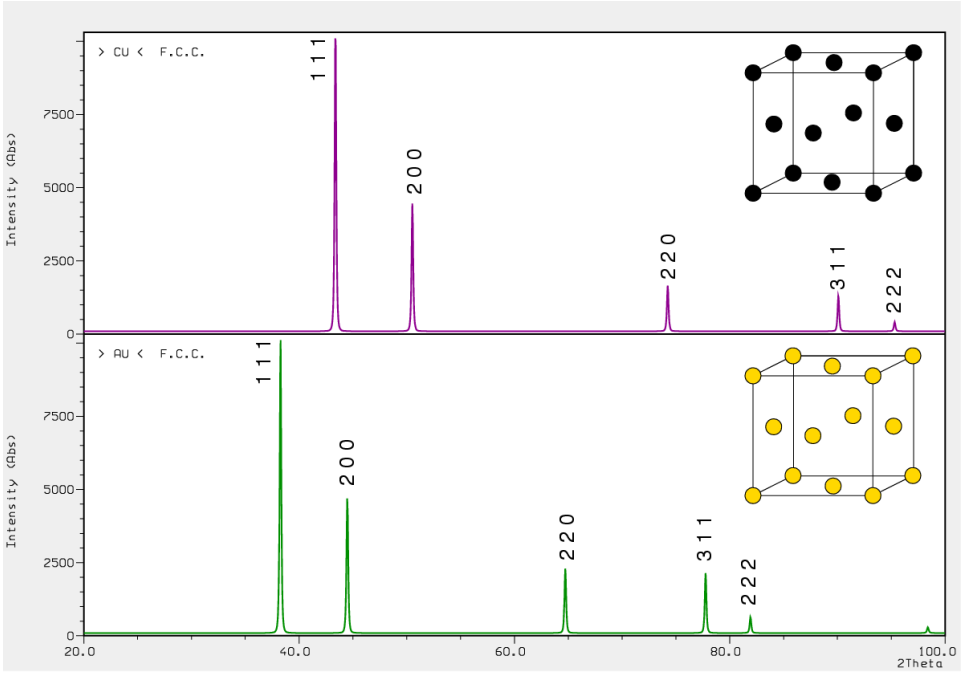


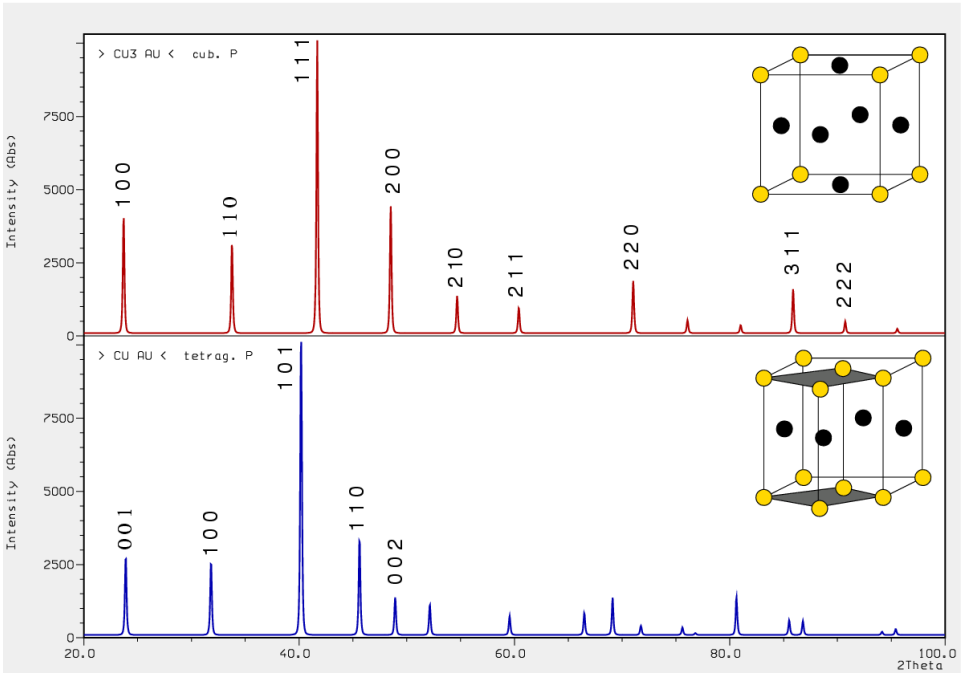
Fig. 5.46 Powder patterns of cubic and tetragonal $BaTiO_3$ showing the influence of crystal symmetry and multiplicities on the number of lines that are observed.

Pulverdiagramme des Systems Cu/Au

ruby.chemie.uni-freiburg.de/Vorlesung/methoden_II_4.xhtml



- Kupfer (fcc / kdp)
- Gold (fcc / kdp)



- Cu_3Au (Kub. P)
- CuAu (tetr. P)

Monoklin

$$\sin^2\theta = \frac{\lambda^2}{4}\left[\frac{h^2}{a^2\sin^2\beta} + \frac{k^2}{b^2} + \frac{l^2}{c^2\sin^2\beta} - \frac{2hl\cos\beta}{ac\sin^2\beta}\right]$$

Orthorhombisch

$$\sin^2\theta = \frac{\lambda^2}{4}\left[\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}\right]$$

Tetragonal

$$\sin^2\theta = \frac{\lambda^2}{4a^2}\left[h^2 + k^2 + \left(\frac{a}{c}\right)^2 l^2\right]$$

Hexagonal und trigonal

$$\sin^2\theta = \frac{\lambda^2}{4a^2}\left[\frac{4}{3}(h^2 + k^2 + hk) + \left(\frac{a}{c}\right)^2 l^2\right]$$

Kubisch

$$\sin^2\theta = \frac{\lambda^2}{4a^2}\left[h^2 + k^2 + l^2\right]$$

Triklin

$$\sin^2\theta = \frac{\lambda^2}{4}\left[h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2klb^*c^*\cos\alpha^* + 2lhc^*a^*\cos\beta^* + 2hka^*b^*\cos\gamma^*\right]$$

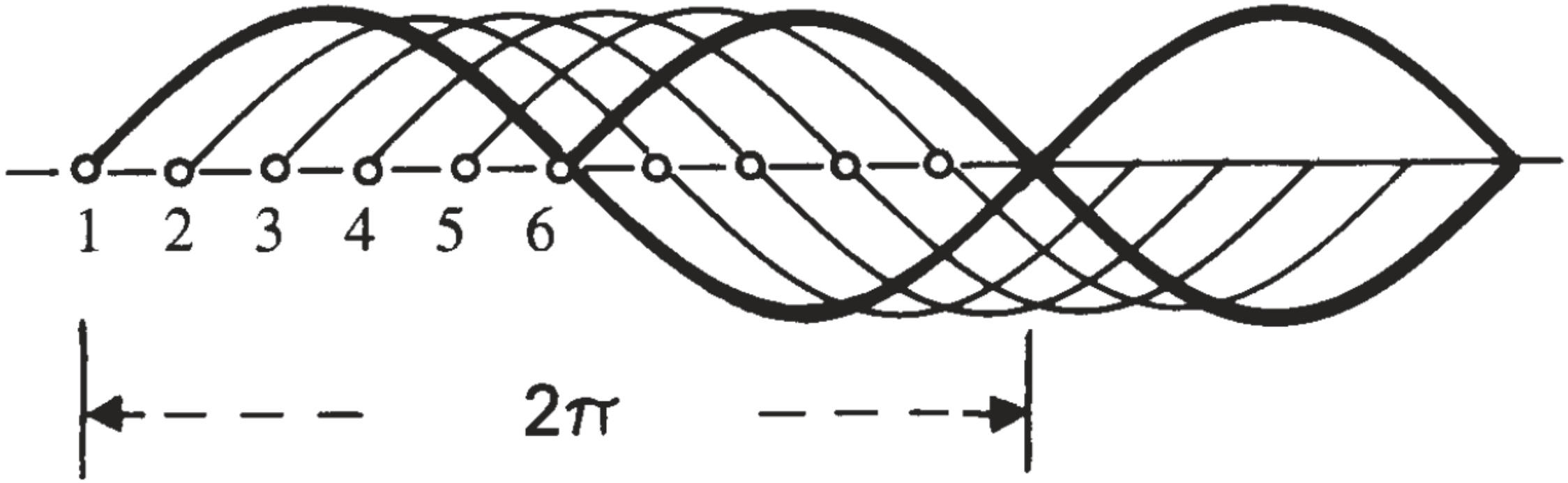
$$a^* = \frac{1}{V}bc\sin\alpha, \qquad \cos\alpha^* = \frac{\cos\beta\cos\gamma - \cos\alpha}{\sin\beta\sin\gamma}$$

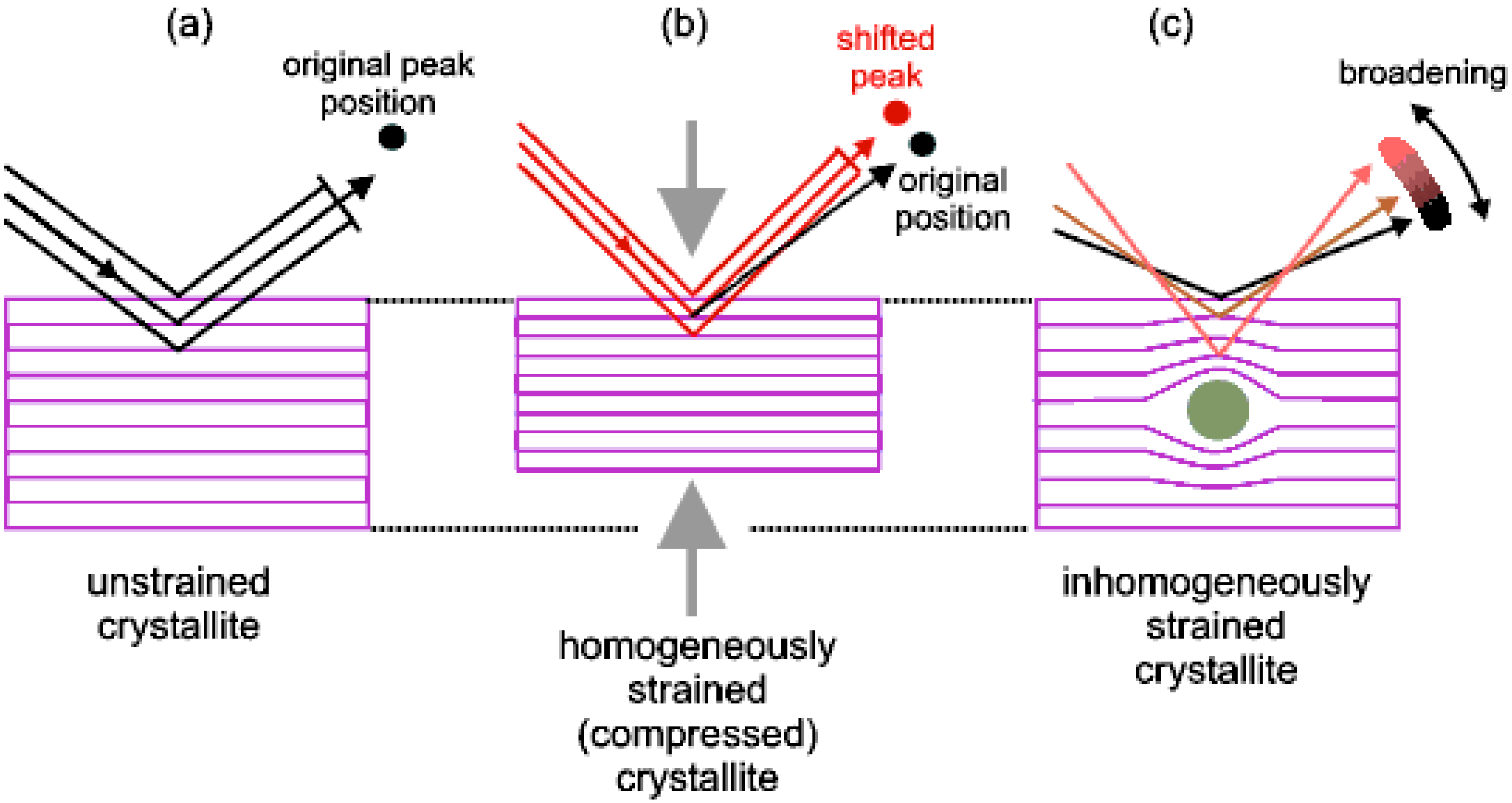
$$b^* = \frac{1}{V}ca\sin\beta, \qquad \cos\beta^* = \frac{\cos\gamma\cos\alpha - \cos\beta}{\sin\gamma\sin\alpha}$$

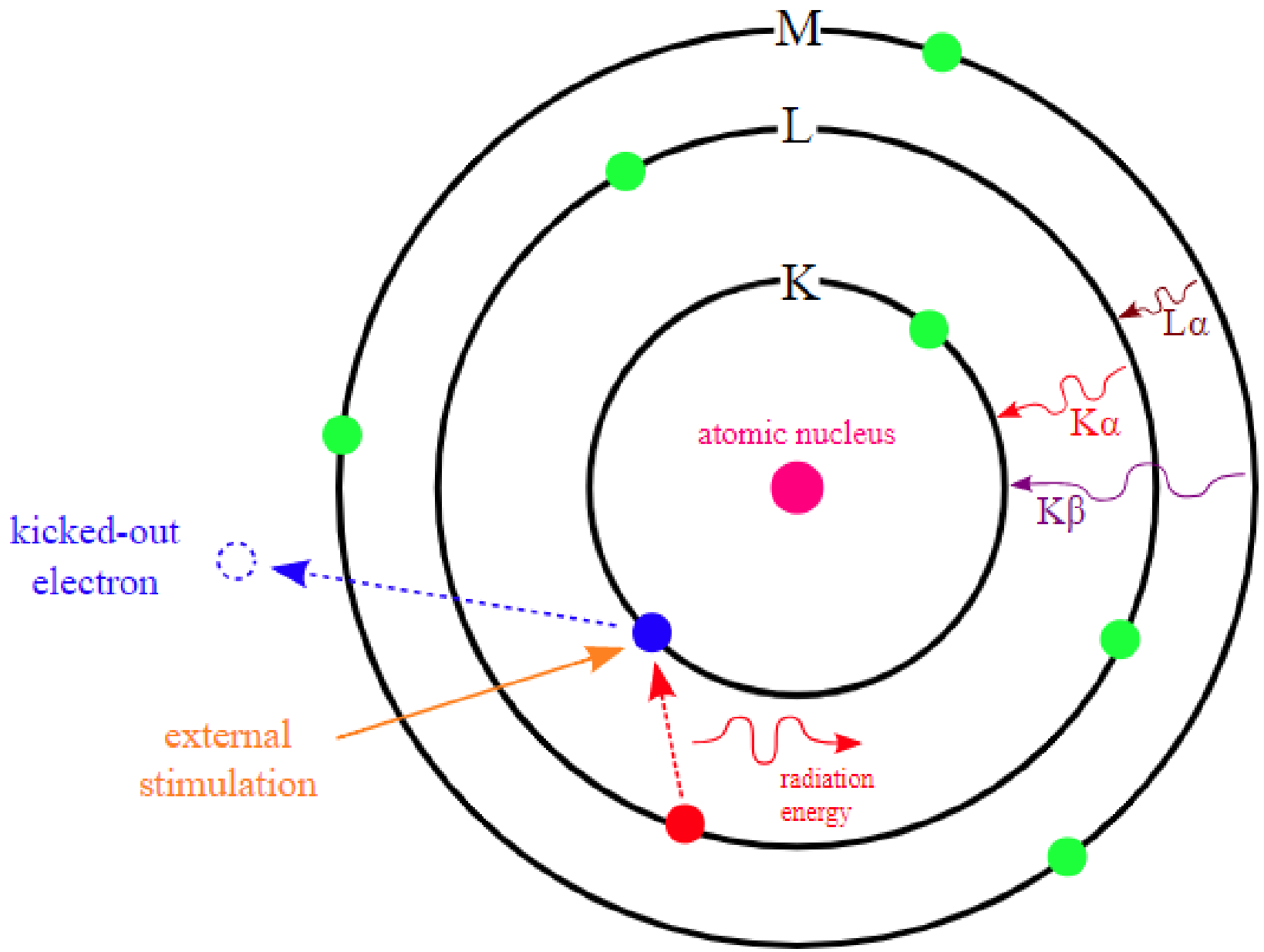
$$c^* = \frac{1}{V}ab\sin\gamma, \qquad \cos\gamma^* = \frac{\cos\alpha\cos\beta - \cos\gamma}{\sin\alpha\sin\beta}$$

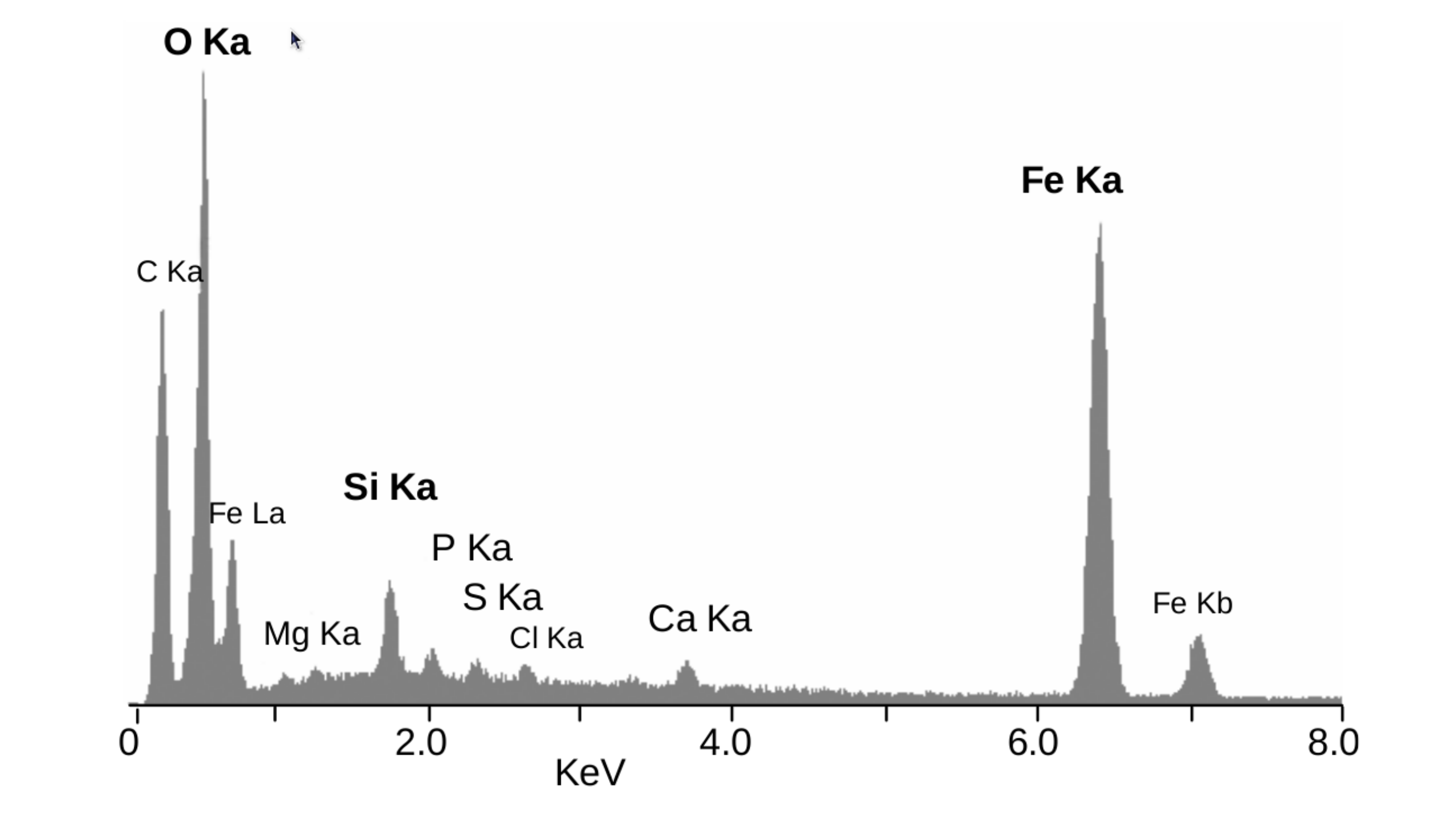
$$\mathrm{V} = abc\sqrt{1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma}$$

$\Delta = \lambda/10$




(a)
original peak position
(b)
shifted peak
original position
(c)
broadening
unstrained crystallite
homogeneously strained (compressed) crystallite
inhomogeneously strained crystallite


M
L
K
Lα
Kα
Kβ
atomic nucleus
kicked-out
electron
external
stimulation
radiation
energy


O Ka
C Ka
Fe La
Si Ka
P Ka
S Ka
Mg Ka
Cl Ka
Ca Ka
Fe Ka
Fe Kb
0
2.0
4.0
6.0
8.0
KeV