Texture and Anisotroy

Part I:

Chapter 3. Application of diffraction to texture analysis

Wavelength for texture measurements

Texture analysis is based on the diffraction of radiation by a crystal lattice.
The wavelength of the incident radiation should be smaller than the lattice space.

TABLE 3.1

Average Diffraction Properties of Radiation Used for Texture Measurement by Diffraction

	Light	Neutrons	X-Rays	Electrons
Wavelength (nm)	400–700	0.05–0.3	0.05–0.3	0.001–0.01
Energy (eV)	1	10^{-2}	10^{4}	10^{5}
Charge (C)	0	0	0	-1.602×10^{-19}
Rest mass (g)	0	1.67×10^{-24}	0	9.11×10^{-28}
Penetration depth, absorption length (mm)	–	10–100	0.01–0.1	10^{-3}

Note: Light is included for comparison.

Diffraction of radiation

Electromagnetic radiation, such as light and X- and g-rays, is diffracted by elastic scattering of the incident waves at the atoms of the sample materials.

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{h}{\sqrt{2mE_{kin}}}$$

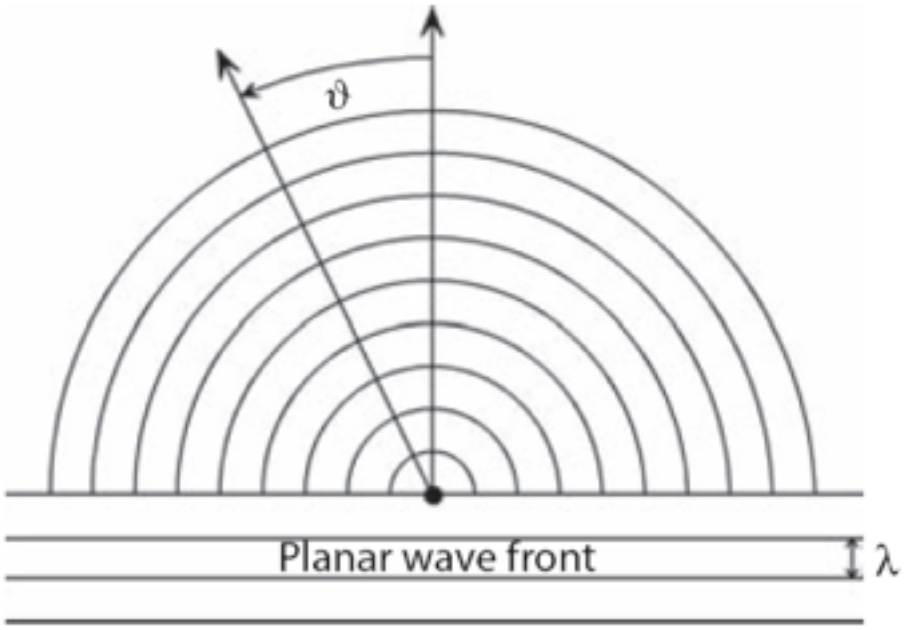


FIGURE 3.1
Scattering of a planar wave front at a point source giving rise to the formation of a Huygens spherical wave.

Diffraction of radiation-cont.

- **X-rays** are scattered by the shell electrons of the atoms.
- **Electrons** interact with both the shell electrons and the nucleus of the scattering atoms.
- **Neutrons** mainly interact with the nucleus of the atoms.

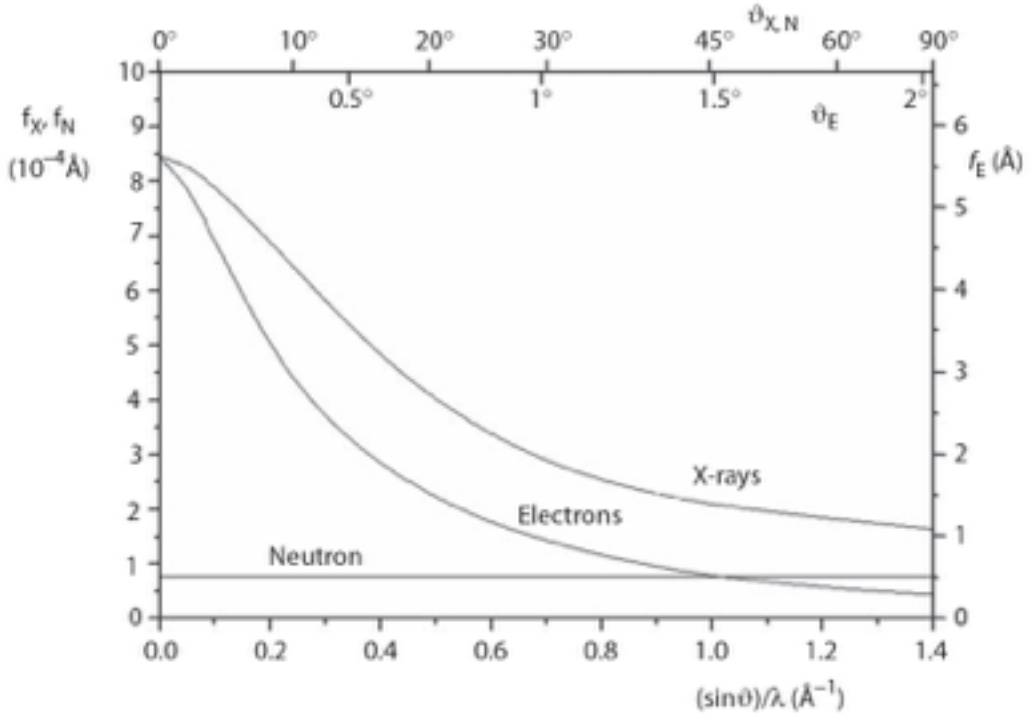
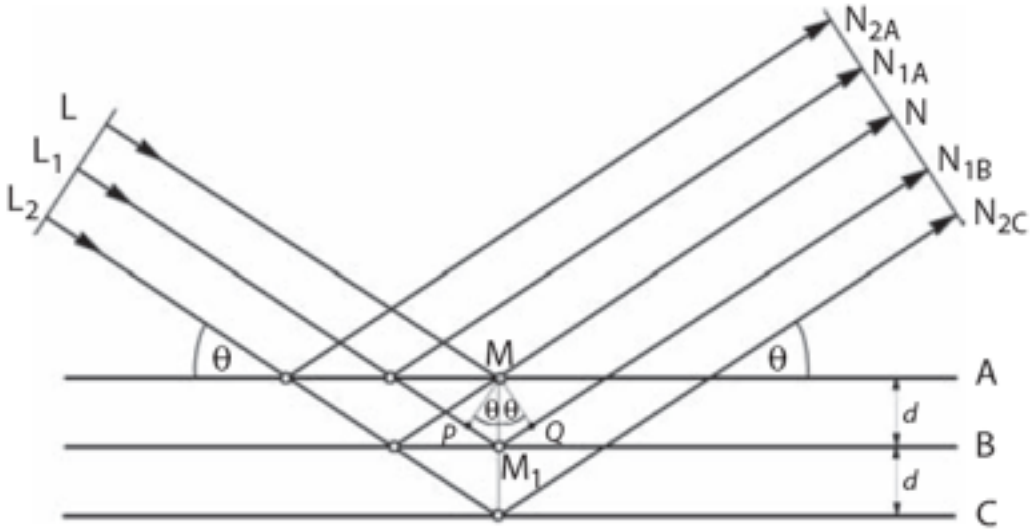


FIGURE 3.2
Angular variation of the atomic scattering amplitude *f* of copper for x-rays, electrons, and neutrons (note different scales for electrons). The reflection angles of the upper axis were calculated with $\lambda = 0.07107$ nm for x-rays and neutrons, and with $\lambda = 0.00251$ nm for electrons (see Table

Bragg's law

$$2d_{hkl}\sin\theta = n\lambda$$



For cubic

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

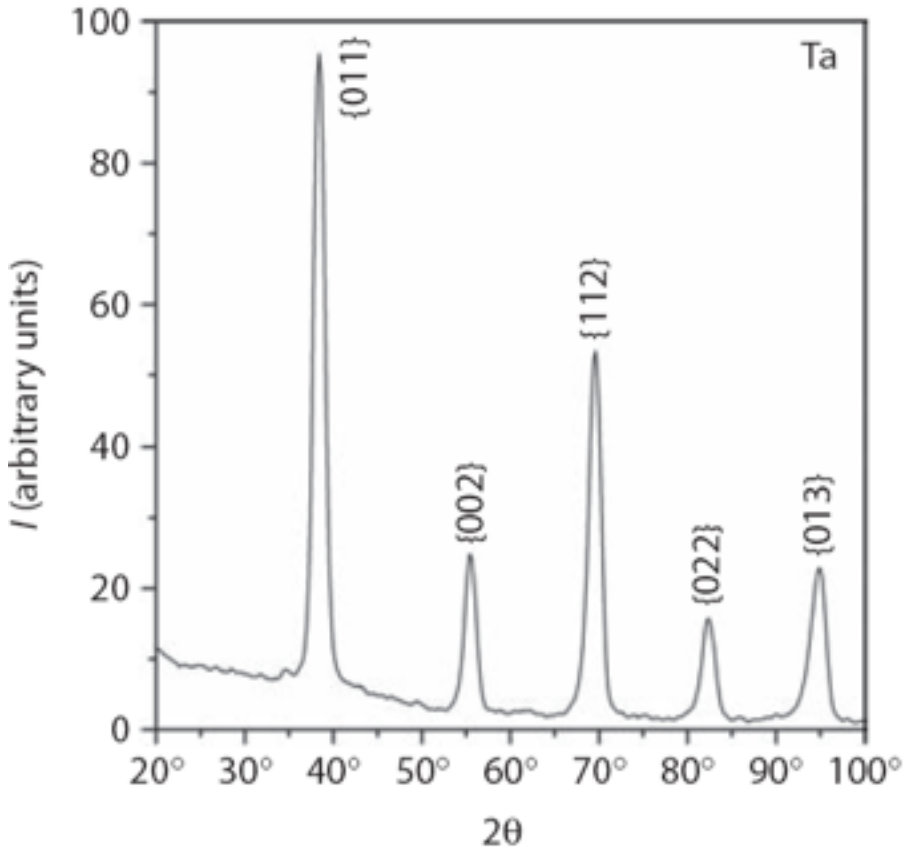
For orthorhombic

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

For hcp

$$\frac{1}{d_{hkl}^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

Determination of lattice planes



$$h + k + l = even$$

TABLE 3.2

Bragg Angles θ for Diffraction of Radiation at Different Reflectors *hkl* in Tantalum

hkl	$h^2 + k^2 + l^2$	2θ
100	1	26.9
110	2	38.5
111	3	47.6
200	4	55.5
210	5	62.8
211	6	69.6
220	8	82.4
221/300	9	88.6
310	10	94.9
311	11	101.1
222	12	107.6

Note: Body-centered cubic: $a = 0.331$ nm, $\lambda = 0.15418$ nm.

FIGURE 3.5
θ/2θ diffraction spectrum of a bcc tantalum powder sample (x-ray CuKα radiation).

Example 1 of structure factor

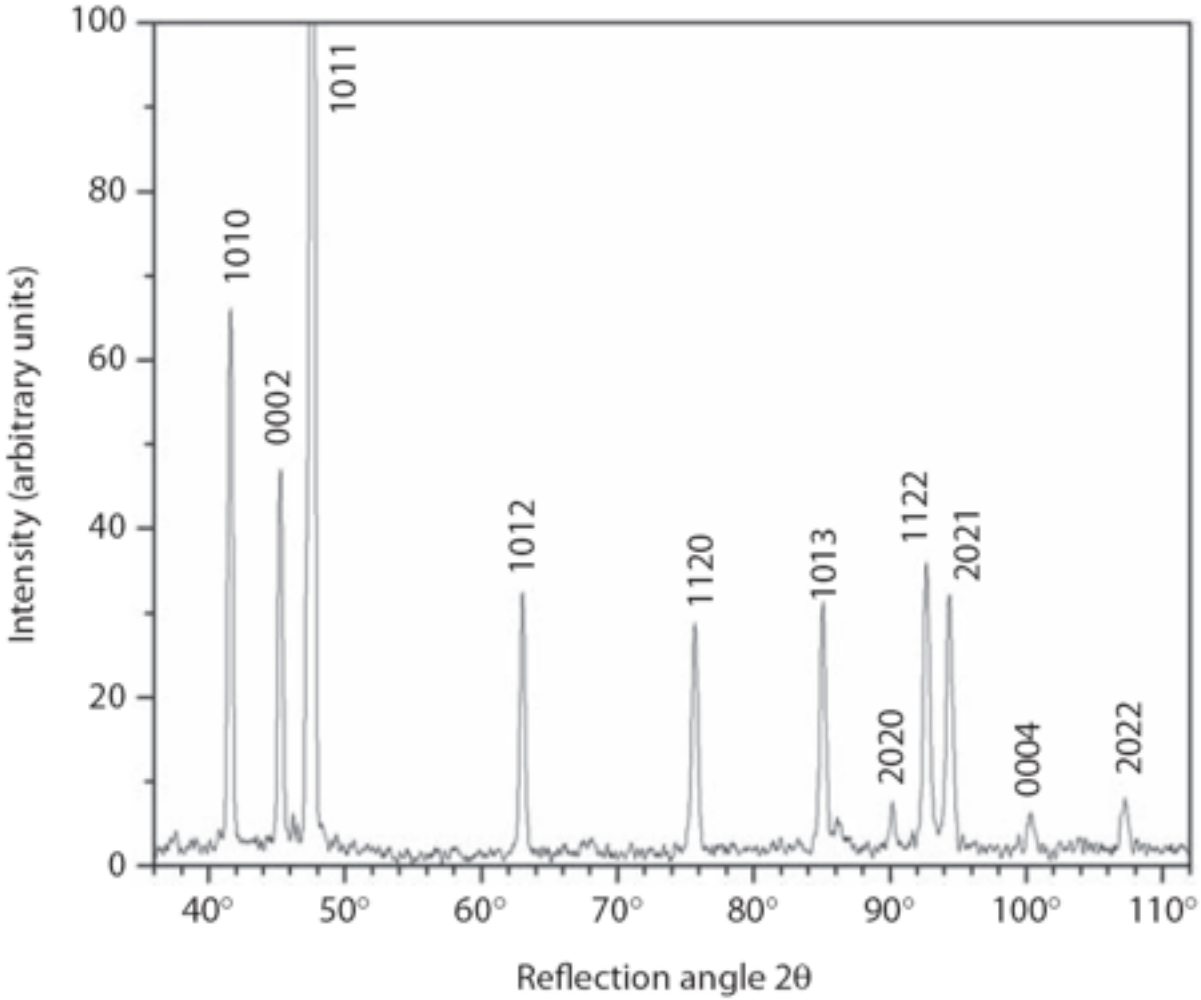


FIGURE 3.7
θ/2θ diffraction spectrum of a hexagonal titanium powder sample (x-ray CoKα radiation).

Example 2 of structure factor

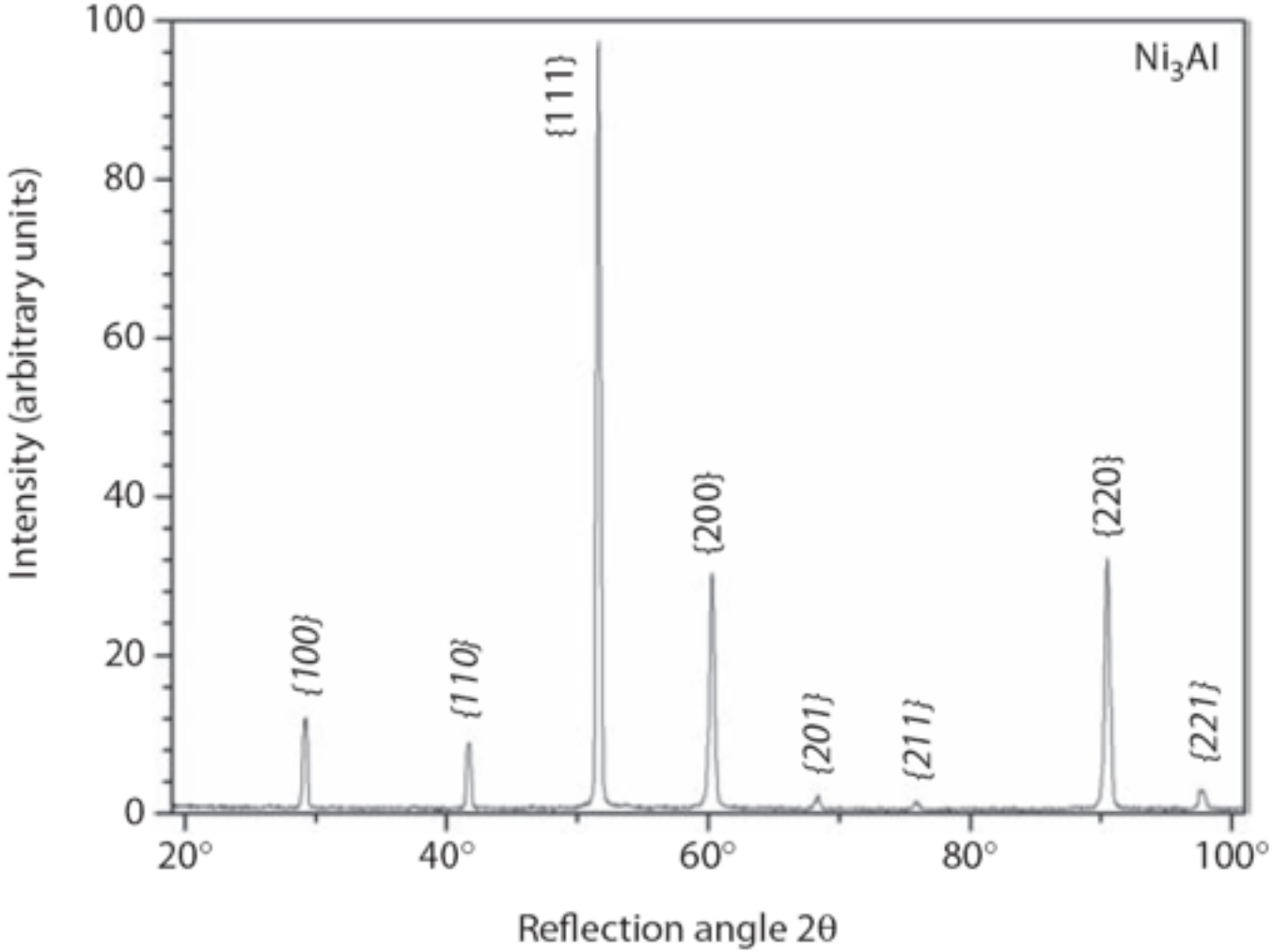


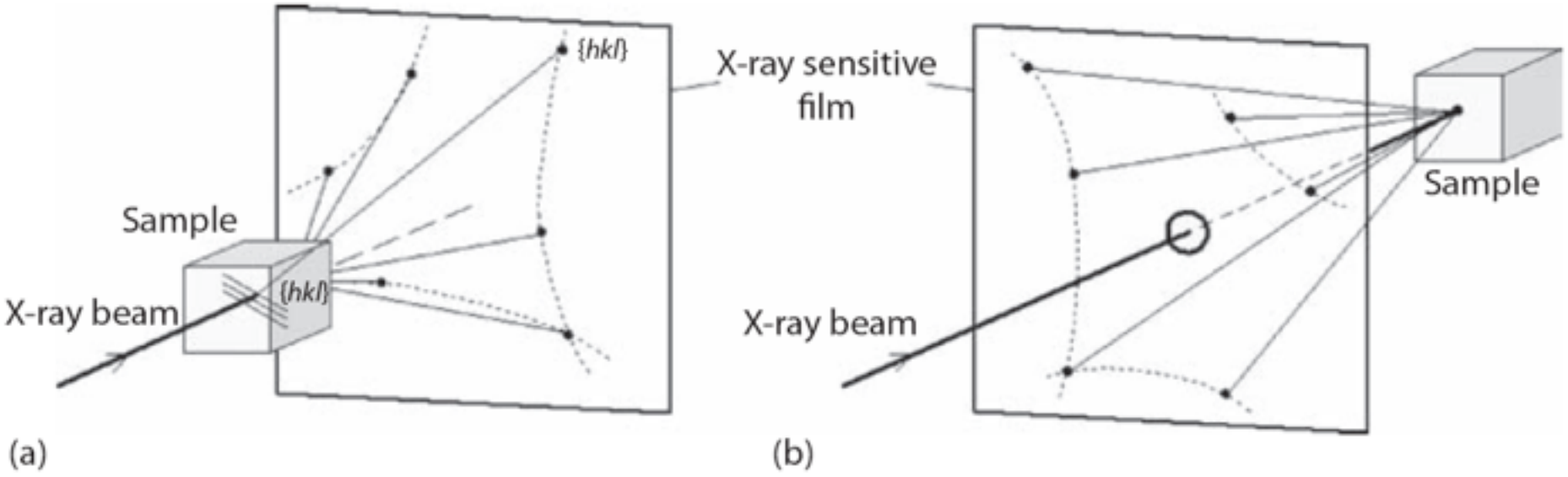
FIGURE 3.8
θ/2θ diffraction spectrum of ordered Ni_3Al ($L1_2$ structure) showing superstructure peaks (x-ray CoKα radiation).

Measurement of orientations

- At constant θ , the wavelength λ is varied (Laue method)

- At constant λ , (i.e., monochromatic radiation), θ is varied (rotating crystal method/ Debye-Scherrer method)

Laue method for orientation determination



Transmission

Reflection

FIGURE 3.10
Measurement of individual orientations according to the Laue technique. (a) Transmission technique, (b) reflection technique.

Laue pattern

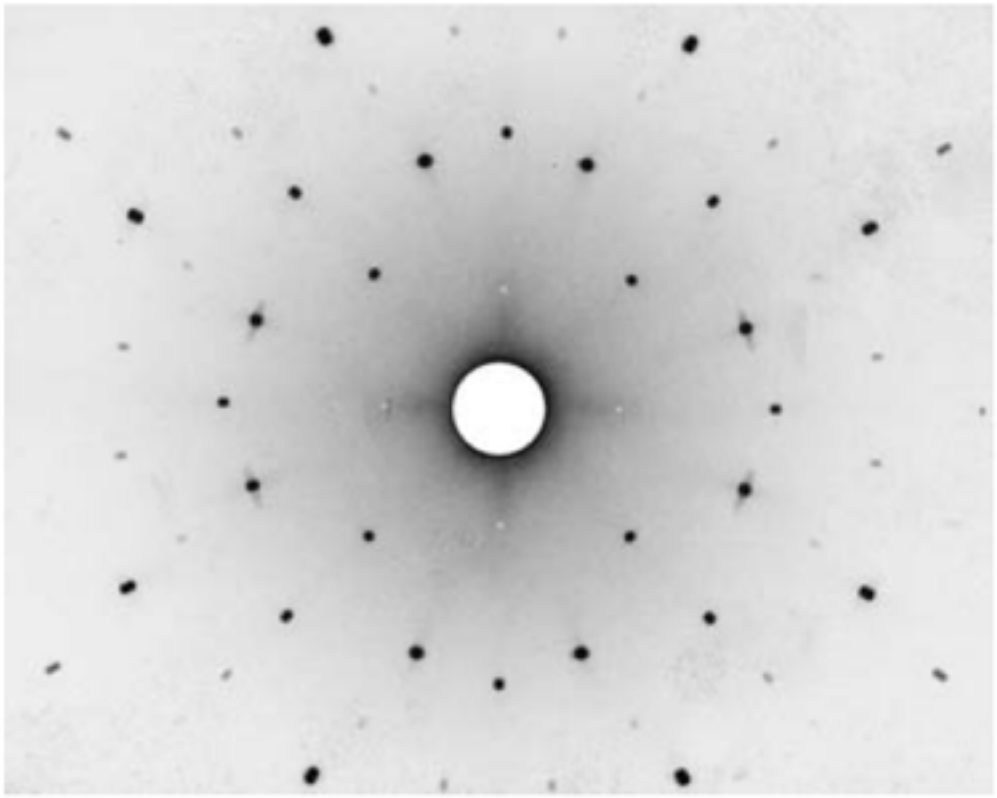


FIGURE 3.9
Laue diagram of a silicon single crystal (reflection technique).

Debye-Sherrer technique

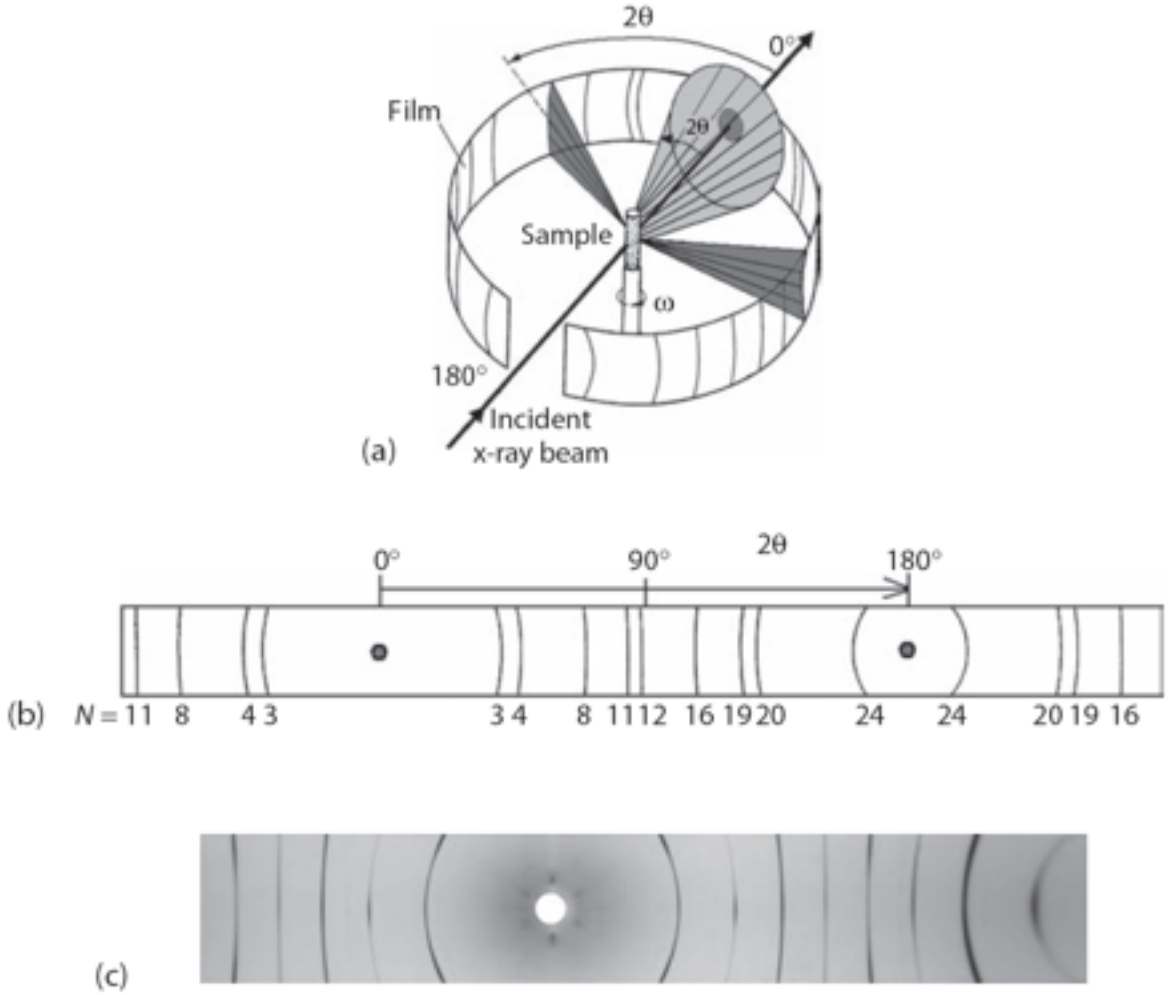


FIGURE 3.11
(a) Debye–Scherrer technique to determine the crystal structure and texture of a polycrystalline sample. Diffraction cones from two lattice planes are shown intersecting the film. (b) Schematic diffraction pattern of an fcc crystal on an unrolled film. (c) An example of a Debye–Scherrer diagram of bcc tungsten. (Courtesy of J. Ihringer.)

Absorption and depth of penetration

Mass Absorption Coefficients (μ/ρ) for X-Rays and Neutrons for Different Wavelengths

	X-Ray			Neutrons
Material (Atomic Number, Z)	**$\lambda = 0.07107$ nm (MoKα)**	**$\lambda = 0.15418$ nm (CuKα)**	**$\lambda = 0.17902$ nm (CoKα)**	**$\lambda = 0.108$ nm**
Be (4)	0.3	1.5	2.3	0.0003
Mg (12)	4.1	38.6	59.5	0.001
Al (13)	5.16	48.6	74.8	0.003
Ti (22)	24.2	208	308	0.044
Mn (25)	34.7	285	*414*	0.083
Fe (26)	38.5	308	52.8	0.015
Co (27)	42.5	*313*	61.1	0.21
Ni (28)	46.6	45.7	70.5	0.028
Cu (29)	50.9	52.9	81.6	0.021
Zn (30)	*55.4*	60.3	93.0	0.0055
Mo (42)	18.4	162	243	0.009
Ag (47)	25.8	218	321	0.2
Cd (48)	27.5	231	338	14
W (74)	99.1	172	253	0.035
Au (79)	115	208	302	0.17
Pb (82)	120	232	334	0.0003

Note: Examples of absorption edges are italic. (Section 3.6.1).

Source: X-rays—Data for x-rays taken from Barrett, C.S. and Massalski, T.B., *Structure of Metals: Crystallographic Methods, Principles and Data*, McGraw-Hill, New York, NY, 1980; data for neutrons taken from Bacon, G.E., in *Neutron Diffraction* (3rd edition), Clarendon Press, Oxford, 1975.

$$I = I_0 \exp(-\mu t)$$

$$\frac{\mu}{\rho} = \sum_i w_i \left(\frac{\mu}{\rho}\right)_i$$

X-rays for texture analysis

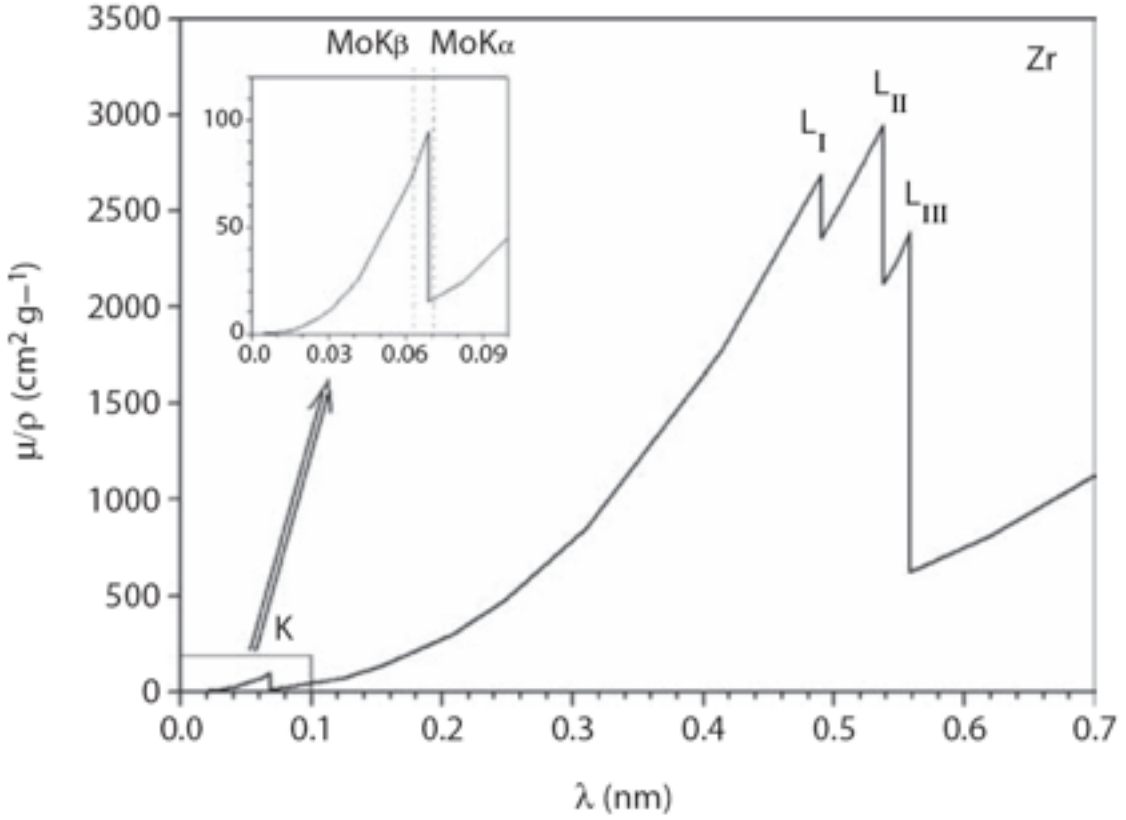


FIGURE 3.12
Variation of the mass absorption coefficient μ/ρ with wavelength λ in zirconium, showing the K- and L-absorption edges. The inlay shows the K_{Zr} absorption edge used to produce (quasi) monochromatic MoKα radiation for x-ray diffraction experiments (see Section 4.3.1).

Neutrons for texture analysis

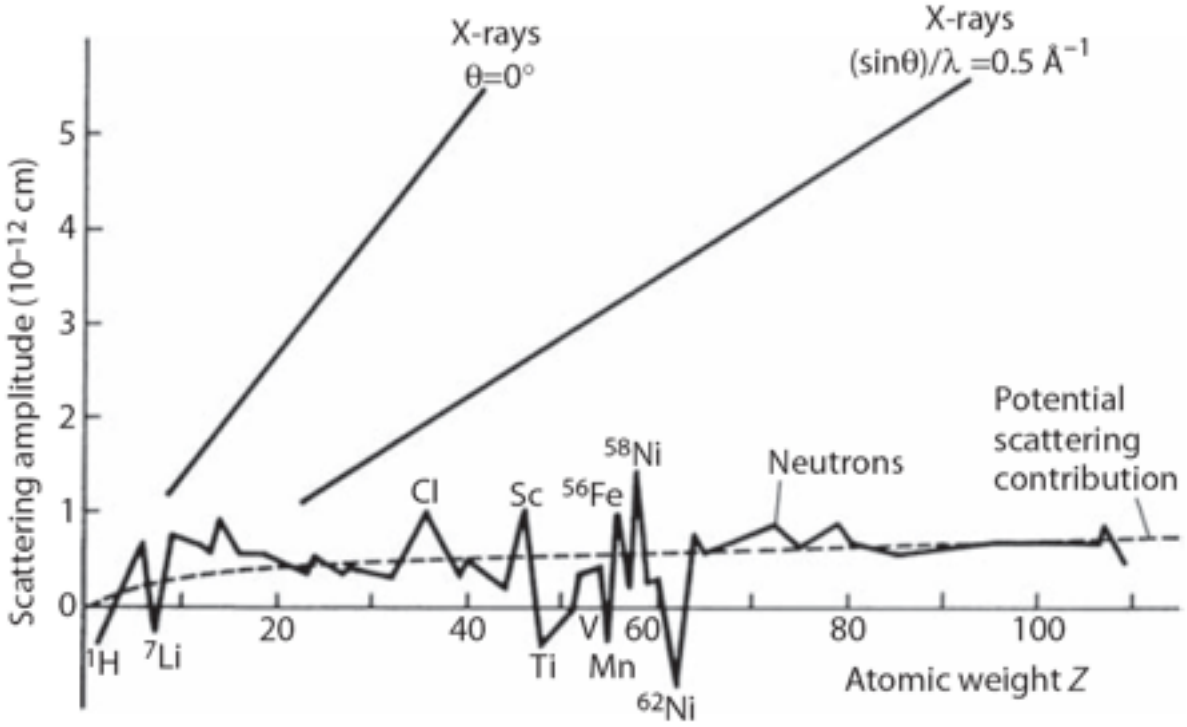


FIGURE 3.13
Variation of the neutron scattering amplitude with atomic number Z due to the superposition of resonance scattering and potential scattering. The regular increase in x-rays is shown for comparison. (Data taken from Bacon, G.E., *Neutron Diffraction*, Clarendon Press, Oxford, 1975.)

Much low absorption and higher penetration

The scattering amplitude of neutrons is independent of θ

Electrons for texture analysis

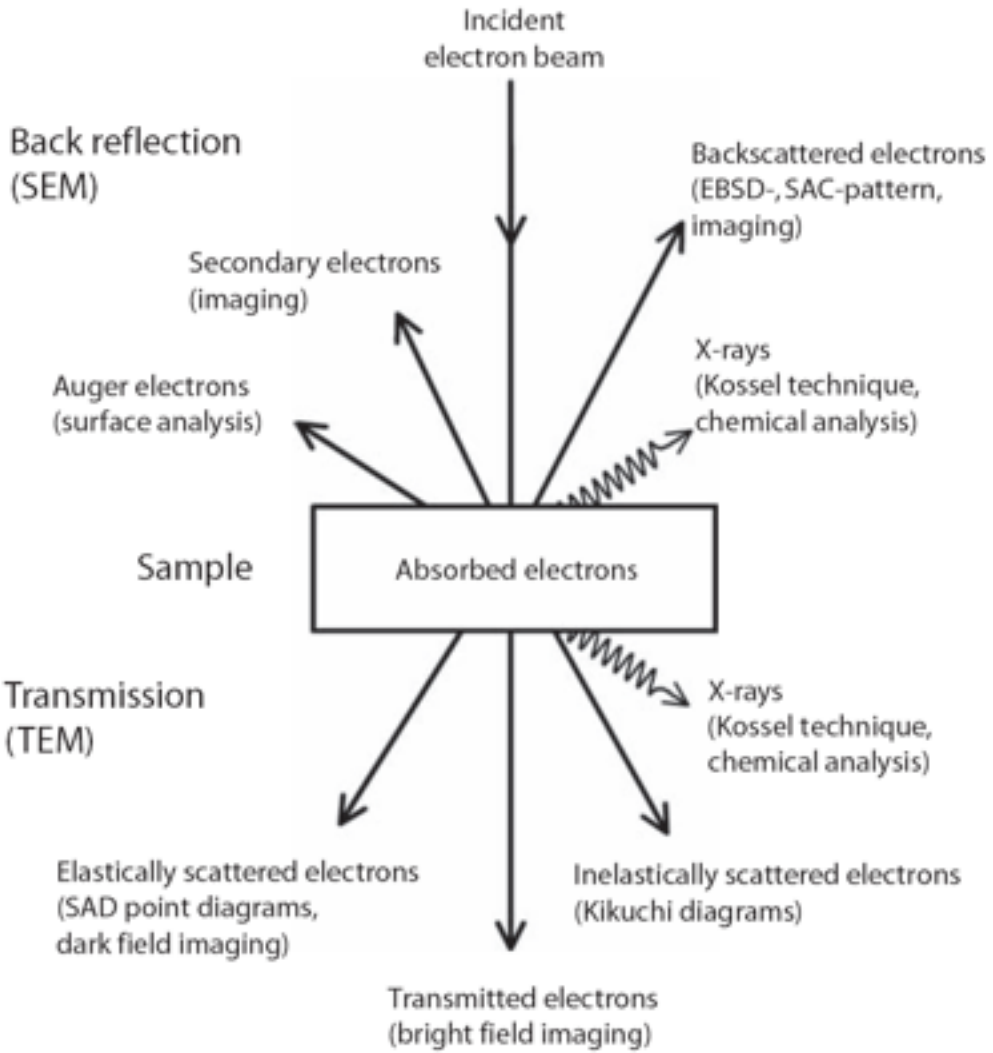


FIGURE 3.14
Summary of the various signals obtained by interaction of electrons with matter in an electron microscope.

Categorization of texture measurements

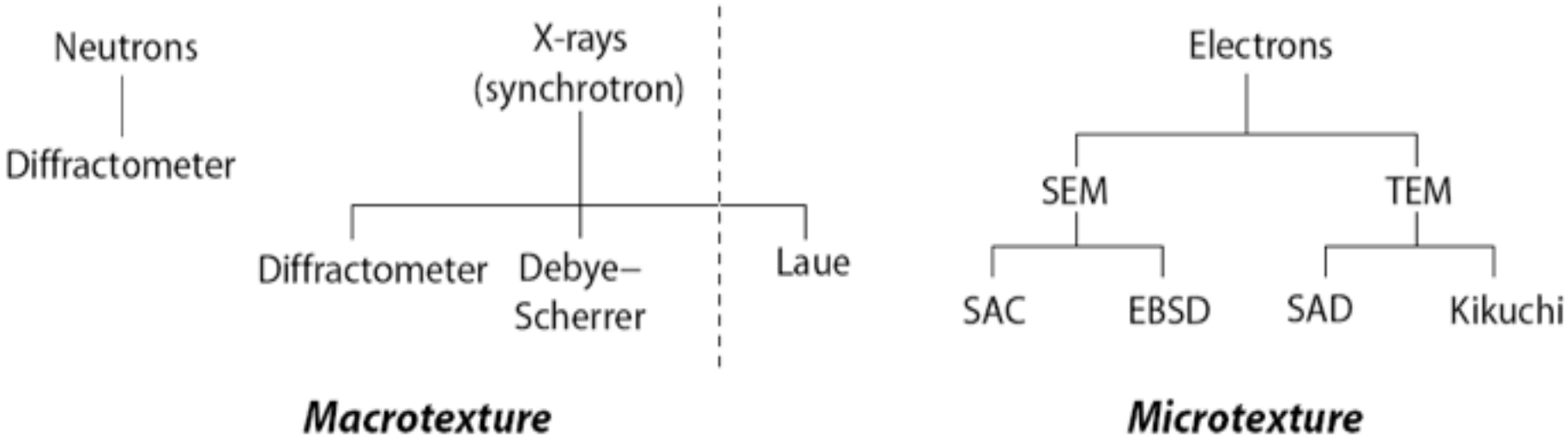


FIGURE 3.15
Categorization of the mainstream techniques for texture determination according to the radiation used as a probe. Macrotexture and microtexture methods are on the left- and right-hand parts of the diagram, respectively.