به نام ِ خدا

دانش‌گاه ِ صنعتی‌ی ِ اصفهان ـ دانش‌کده‌ی ِ فیزیک

تصاویر فصل ۱۴

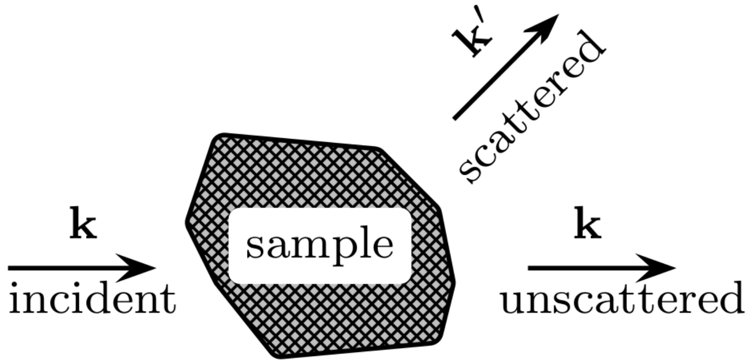

Fig. 14.1 A generic scattering experiment.

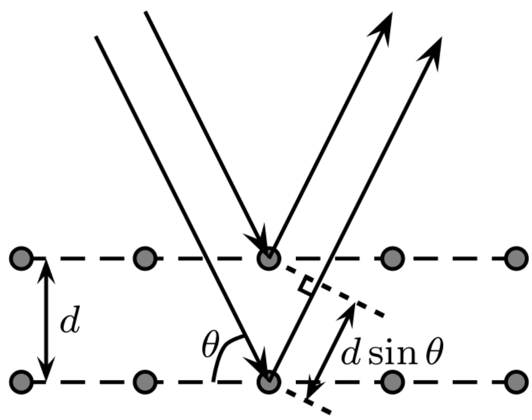

Fig. 14.2 Bragg scattering off of a plane of atoms in a crystal. The excess distance traveled by the wave striking the lower plane is $2d\sin\theta$.

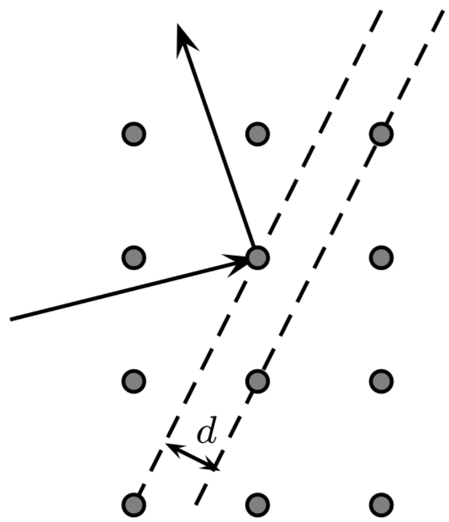

Fig. 14.3 Scattering off of the $(2\bar{1}0)$ plane of atoms.

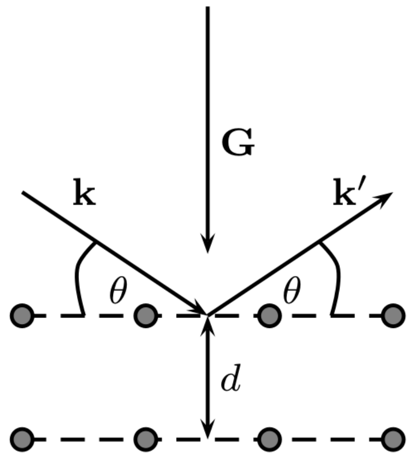

Fig. 14.4 Geometry of scattering.

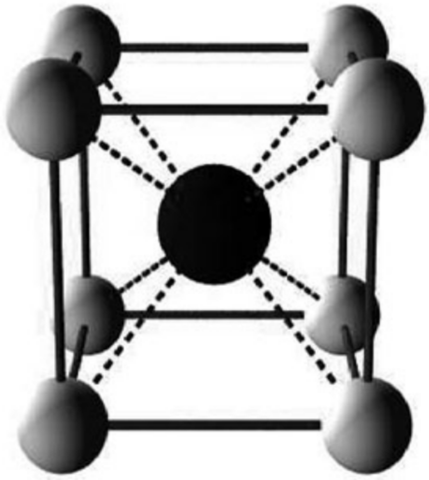

Fig. 14.5 Caesium chloride unit cell. Cs is the white corner atoms, Cl is the darker central atom. This is simple cubic with a basis. Note that bcc Cs can be thought of as just replacing the Cl with another Cs atom.

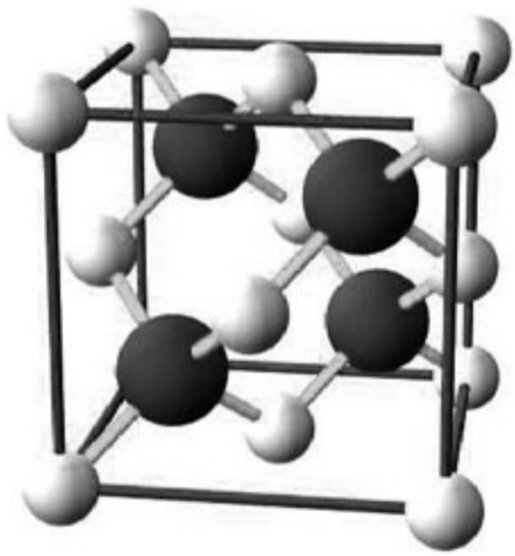

Fig. 14.6 Zinc sulfide (zincblende) conventional unit cell. This is fcc with a basis given by a Zn atom (light) at $[0, 0, 0]$ and a S atom (dark) at $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$.

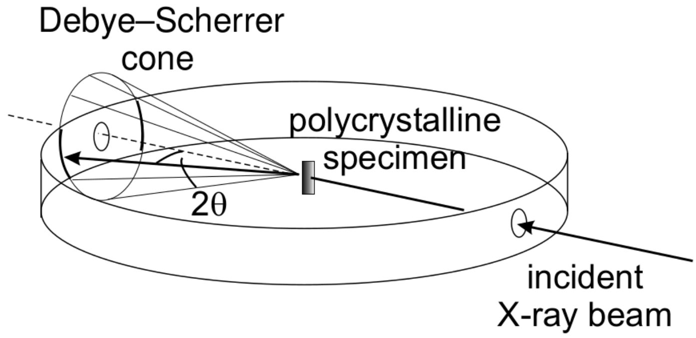

Fig. 14.7 Schematic of a Debye–Scherrer powder diffraction experiment.

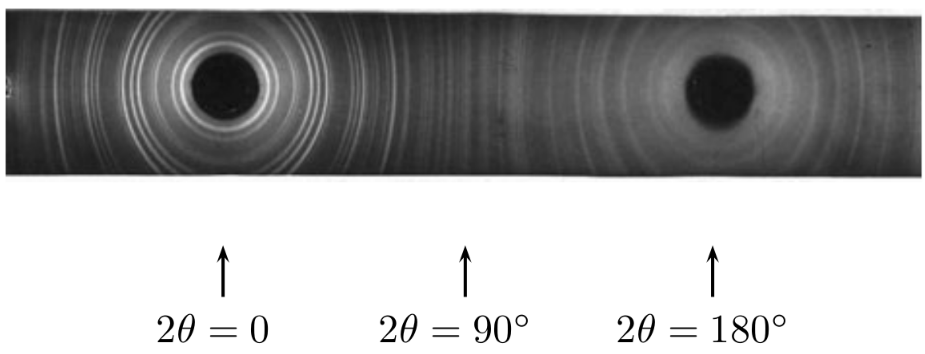

Fig. 14.8 Debye–Scherrer powder diffraction data exposed on photographic film. In modern experiments digital detectors are used.

Table 14.1 Selection rules for cubic, bcc, and fcc lattices.

$\{hkl\}$	$N = h^2 + k^2 + l^2$	multiplicity	cubic	bcc	fcc
100	1	6	✓		
110	2	12	✓	✓	
111	3	8	✓		✓
200	4	6	✓	✓	✓
210	5	24	✓		
211	6	24	✓	✓	
220	8	12	✓	✓	✓
221	9	24	✓		
300	9	6	✓		
310	10	24	✓	✓	
311	11	24	✓		✓
222	12	8	✓	✓	✓
⋮	⋮	⋮	⋮		

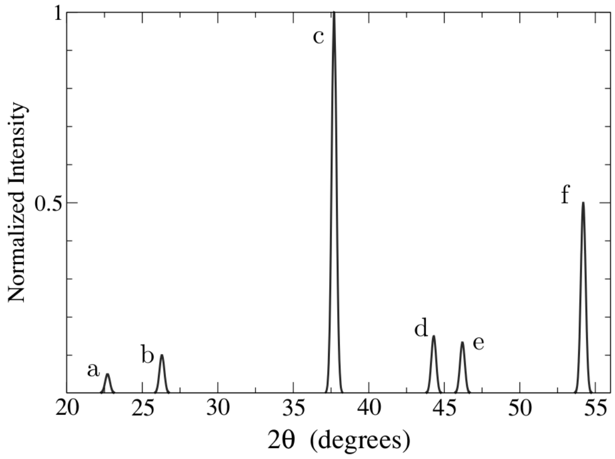

Fig. 14.9 Powder diffraction of neutrons from PrO_2. The wavelength of the neutron beam is $\lambda = .123$ nm. (One should assume that Lorentz corrections have been removed from the displayed intensities.)

peak	2θ	$d = \lambda/(2\sin\theta)$	d_a^2/d^2	$3d_a^2/d^2$	$N = h^2+k^2+l^2$	$\{hkl\}$	$a = d\sqrt{h^2+k^2+l^2}$
a	22.7°	0.313 nm	1	3	3	111	.542 nm
b	26.3°	0.270 nm	1.33	3.99	4	200	.540 nm
c	37.7°	0.190 nm	2.69	8.07	8	220	.537 nm
d	44.3°	0.163 nm	3.67	11.01	11	311	.541 nm
e	46.2°	0.157 nm	3.97	11.91	12	222	.544 nm
f	54.2°	0.135 nm	5.35	16.05	16	400	.540 nm

Table 14.2 Analysis of data shown in Fig. 14.9.

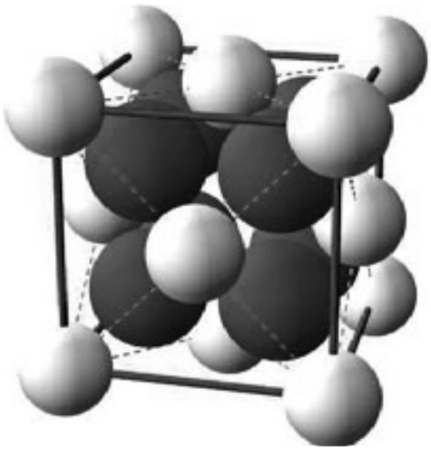

Fig. 14.10 The fluorite structure of PrO_2. This is fcc with a basis given by a white atom (Pr) at $[0, 0, 0]$ and dark atoms (O) at $[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$ and $[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$.

Scattering Intensity

peak	$\{hkl\}$	$I_{\{hkl\}}/C \propto M\|S\|^2$	Measured Intensity
a	111	$8\,b_{Pr}^2$	0.05
b	200	$6\,[b_{Pr} - 2b_O]^2$	0.1
c	220	$12\,[b_{Pr} + 2b_O]^2$	1.0
d	311	$24\,b_{Pr}^2$	0.15
e	222	$8\,[b_{Pr} - 2b_O]^2$	0.13
f	400	$6\,[b_{Pr} + 2b_O]^2$	0.5

Table 14.3 Predicted versus measured scattering intensities. Here the prediction is based purely on the scattering structure factor and the scattering multiplicity (Lorentz factors are not considered).

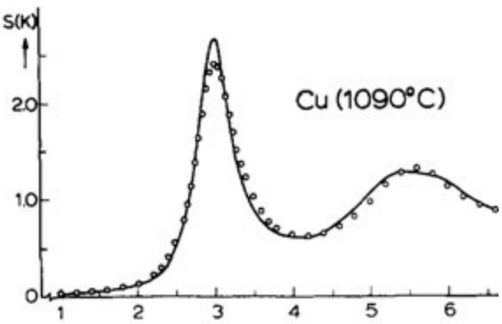

Fig. 14.11 The structure factor of liquid copper. Broad peaks are shown due to the approximately periodic structure of a liquid. Figure from K. S. Vahvaselka, *Physica Scripta,* **18**, 266, 1978. doi:10.1088/0031-8949/18/4/005 Used by permission of IOP Publishing.

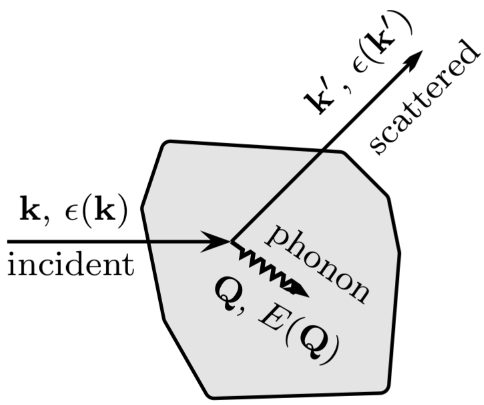

Fig. 14.12 Inelastic scattering. Energy and crystal momentum must be conserved.

Fig. 14.13 The Rutherford Appleton Laboratory in Oxfordshire, UK. (Photo used by permission of STFC). On the right, the large circular building is the DIAMOND synchrotron light source. The building on the left is the ISIS spallation neutron facility. This was the brightest neutron source on earth until August 2007, when it was surpassed by one in Oak Ridge, US. The next generation neutron source is being built in Sweden and is expected to start operating in 2019. The price tag for construction of this device is over 10^9 euros.

- Understand diffraction of waves from crystals in both the Laue and Bragg formulations (equivalent to each other).
- The structure factor (the Fourier transform of the scattering potential) in a periodic crystal has sharp peaks at allowed reciprocal lattice vectors for scattering. The scattering intensity is proportional to the square of the structure factor.
- There are systematic absences of diffraction peaks depending on the crystal structure (fcc, bcc). Know how to figure these out.
- Know how to analyze a powder diffraction pattern (very common exam question!).