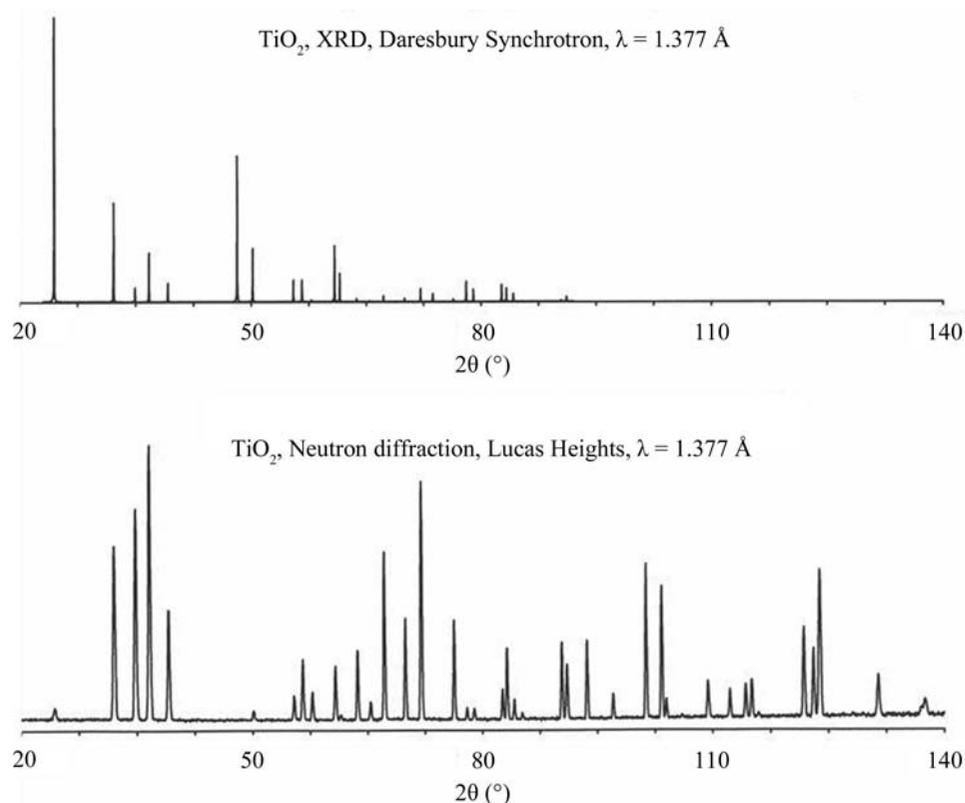
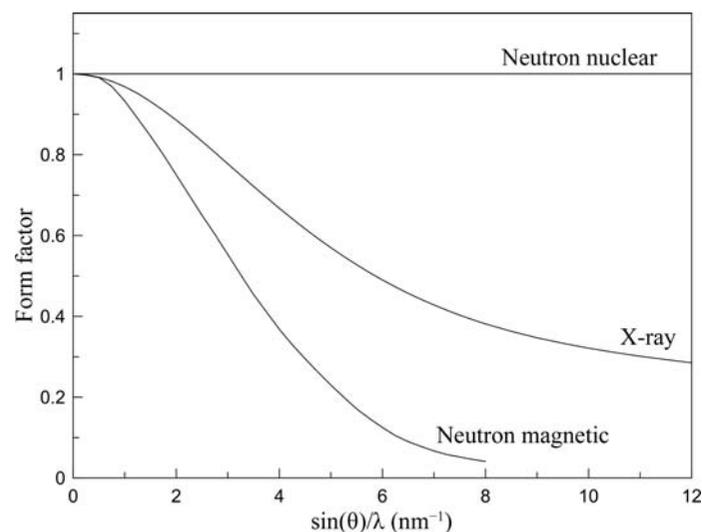


## 2.3. NEUTRON POWDER DIFFRACTION



**Figure 2.3.2**

Comparison of X-ray and neutron powder-diffraction patterns from rutile,  $\text{TiO}_2$ . The patterns were recorded at the same wavelength, 1.377 Å. The differences between form factors and scattering lengths give rise to large differences in the relative intensities of the different peaks; note also that the fall off in the form factor evident in the X-ray case does not occur for neutrons.



**Figure 2.3.3**

The magnetic form factor for  $\text{Mn}^{2+}$  compared with the normalized X-ray form factor and the normalized neutron nuclear scattering length.

of nuclear moments in metallic copper ( $^{65}\text{Cu}$ ) at temperatures below 60 nK (Hakonen *et al.*, 1991).<sup>3</sup>

- (c) *Low attenuation*: The combination of the small scattering cross sections and generally low cross sections for absorption (notable exceptions are B, Cd and Gd) gives thermal neutrons the ability to penetrate quite deeply into most materials. Indeed, the linear attenuation coefficient for thermal (25 meV) neutrons in Fe is  $110 \text{ m}^{-1}$ , and for neutrons in Al it is only about  $9.8 \text{ m}^{-1}$ ; the implication is

that it takes about 10 cm of Al to reduce the intensity by a factor  $1/e$ . The fact that neutrons are so little attenuated by these materials makes it easier to design large and complex sample-environment chambers which may be used for *in situ* studies at high temperature, under pressure or stress, in magnetic fields, and in reaction cells (Chapters 2.6–2.9; Chapter 3 in Kisi & Howard, 2008). Neutron powder diffraction is well suited to quantitative phase analysis (QPA, see Chapter 3.9 and Chapter 8 in Kisi & Howard, 2008); as pointed out in Chapter 8, Section 8 of Kisi & Howard (2008), neutron QPA provides a better sampling ability and is less prone to micro-absorption errors than the X-ray technique; indeed, neutron diffraction was the method employed in one of the earliest and most convincing demonstrations of the Rietveld method in QPA (Hill & Howard, 1987). Another advantage conferred by the deep penetration of neutrons is the ability to probe below the surface of samples to measure such aspects as structure, phase composition and stress; a particular example is the application to the analysis of

zirconia ceramics (Kisi *et al.*, 1989) where the surface composition (as would be measured by X-rays) is unrepresentative of the bulk. A downside of the small scattering cross sections (along with neutron sources of limited ‘brightness’) is that relatively large samples may be required.

- (d) *Low energy*: We note from equation (2.3.1) that, for a specified wavelength, the energy of the neutron is much less than that for lighter probes, such as electrons or photons. This is critically important for studying inelastic processes (*e.g.* measurement of phonon dispersion curves), but is usually not a factor in neutron powder diffraction.<sup>4</sup>

Neutron sources, in common with synchrotrons, are large national or international facilities, set up to cater for scientists from external laboratories. There are usually well defined access procedures, involving the submission and peer review of research proposals. Visiting users are usually assisted in their experiments by in-house staff. In some cases external users can mail in their samples for collection of diffraction data by the resident staff.

### 2.3.2. Neutrons and neutron diffraction – pertinent details

#### 2.3.2.1. Properties of the neutron

The basic properties of the neutron are summarized in Table 2.3.1.

<sup>4</sup> However, if the incident beam is monochromatic, a crystal monochromator placed in the diffracted beam can be used to exclude inelastic scattering from the ‘background’.

<sup>3</sup> This study depends on the spin-dependent scattering lengths rather than magnetic scattering *per se*.