International Tables for Crystallography (2006). Vol. C, Figure 4.2.3.5, p. 219.

Table 4.2.3.1. *Some synchrotron-radiation facilities providing XAFS databases and analysis utilities*

Country	Synchrotron source	Address
France	LURE	Université Paris-Sud, LURE, 91405 Orsay, France
Italy	Frascati	Laboratori Nationali di Frascati, CP 13, 00044 Frascati, Italy
Japan	Photon Factory	Photon Factory, National Laboratory for High Energy Physics, 1-1 Oho, Tsukuba-gun, Ibaraki 305, Japan
Germany	DESY	DESY, Notkestrasse 85, 2000 Hamburg 52, Germany
United Kingdom	SRC/ Daresbury	Daresbury Laboratory, Daresbury, Warrington WA4 4AD, England
USA	CHESS	CHESS, Cornell University, Ithaca, New York 14853, USA
	NSLS	NSLS, Brookhaven National Laboratory, Upton, New York 11973, USA
	SPEAR	SSRL, Stanford University, Bin 69, PO Box 4349, Stanford, California 94305, USA

thin films. More recently, Oyanagi *et al.* (1987) have applied the technique to the study of short-range order in high-temperature superconductors. Oyanagi, Martini, Saito & Haga (1995) have studied in detail the performance of a 19-element high-purity Ge solid-state detector array for fluorescence X-ray absorption fine structure studies.

A less-sensitive technique, but one that can be usefully employed for thin-film studies, is that in which XAFS modulations are detected in the beam reflected from a sample surface. This technique, *ReflEXAFS*, has been used by Martens & Rabe (1980) to investigate superficial regions of copper oxide films by means of reflection of the X-rays close to the critical angle for total reflection.

If a thin film is examined in a transmission electron microscope, the electron beam loses some of its kinetic energy in interactions between the electron beam and the electrons within the film. If the resultant energy loss is analysed using a magnetic analyser, XAFS-like modulations are observed in the electron energy spectrum. These modulations, electron-energy-loss fine structure (*EELS*), which were first observed in a conventional transmission electron microscope by Leapman & Cosslet (1976), are now used extensively for microanalyses of light elements incorporated into heavy-element matrices. Most major manufacturers of transmission electron microscopes supply electron-energy-loss spectrometers for their machines. There are more problems in analysing electron-energy-loss spectra than there are for XAFS spectra. Some of the difficulties encountered in producing reliable techniques for the routine analysis of EELS have been outlined by Joy & Maher (1985). This matter is discussed more fully in §4.3.4.4.2.

A more recent development has been the observation of *topographic XAFS* (Bowen, Stock, Davies, Pantos, Birnbaum & Chen, 1984). This fine structure is observed in white-beam topographs taken using synchrotron-radiation sources. The technique provides the means of simultaneously determining spatially resolved microstructural and spectroscopic information for the specimen under investigation.

In all the preceeding discussion, however, the electron was assumed to undergo only single-scattering processes. If multiple scattering occurs, then the theory has to be changed somewhat. §4.2.3.4.2 discusses the effect of multiple scattering.

4.2.3.4.2. *X-ray absorption near edge structure (XANES)*

In Fig. 4.2.3.2(*c*), there appears to be one cycle of strong oscillation in the neighbourhood of the absorption edge before the quasi-periodic variation of the XAFS commences. The electrons that cause this strong modulation of the photoelectric scattering cross section have low k values, and the electron is strongly scattered by neighbouring atoms. It was mentioned in §4.2.3.4.1 that conventional XAFS theory assumes a weak, single-scattering interaction between the ejected photoelectron and its environment. A schematic diagram illustrating the difference between single- and multiple-scattering processes is given in Fig. 4.2.3.5. Evidently, the multiple-scattering process is very complicated and a discussion of the theory of XANES is too complex to be given here. The reader is directed to papers by Pendry (1983), Lee (1981), and Durham (1983). A more recent review of the study of fine structure in ionization cross sections and their use in surface science has been given by Woodruff (1986).

The data from XANES experiments can be analysed to determine structural information such as coordination geometry, the symmetry of unoccupied valence electronic states, and the effective charge on the absorbing atom (Natoli, Misemer, Doniach & Kutzler, 1980; Kutzler, Natoli, Misemer, Doniach & Hodgson, 1981). XANES experiments have been performed to resolve many problems, *inter alia*: the origin of white lines (Lengeler, Materlik & Müller, 1983); absorption of gases on metal surfaces (Norman, Durham & Pendry, 1983); the effect of local symmetry in $3d$ elements (Petiau & Calas, 1983); and the determination of valence states in materials (Lereboures, Dürr, d'Huysser, Bonelle & Lenglet, 1980).

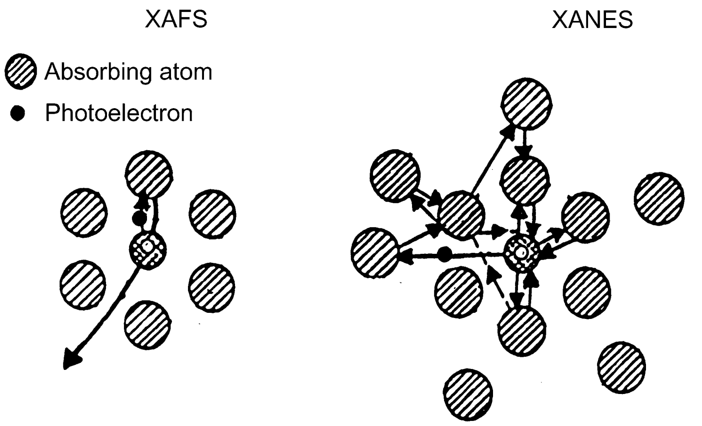

Fig. 4.2.3.5. Schematic representations of the scattering processes undergone by the ejected photoelectron in the single-scattering (XAFS) case and the full multiple-scattering regime (XANES).