Figure 1.2  Experimental (left) and calculated (right) O-K edges fine structures in various vanadium oxides. The calculations was performed with the WIEN2k code. Spectra are shifted vertically for better visibility, starting with VO (bottom) and ending with V$_2$O$_5$ (top).
**Figure 1.13** Series of energy filtered diffraction patterns obtained at energy losses corresponding to the C K edge in graphite as indicated in the figure: 270 eV (pre C K edge), 284 eV (corresponding to the $\pi^*$ peak), 296 eV (corresponding to the $\sigma^*$ peak) and 310 eV (the continuum after the edge near edge structures).

**Figure 1.14** Inelastic scattering distribution after background subtraction of the pre-edge intensity at 270 eV. The small circle at the centre of the figure corresponds to the forward scattering direction (i.e. corresponds to $q_{||}$). Left: the $\pi^*$ energy loss; Right: the $\sigma^*$ energy loss.
Figure 2.1 Synchrotron radiation emitted from a bending magnet. Inset right: intensity distribution and polarization characteristics. As a result of the filling of the electron storage ring with electron packages this synchrotron radiation has a defined and adjustable time structure in the picosecond range. Inset left: Magnet structure of a helical undulator. The polarization can be varied by a horizontal shift of the arrangement of the permanent magnets [Bahrdt et al. (2001)].

Figure 2.7 (a) Transition probabilities from the different $m_i = \pm 1/2$ configurations (energetically identical) of the $p_{1/2}$ spin-orbit coupled level separated into the two possible $(m_l,m_s)$ configurations to a final d-state. (b) Percent spin and orbital polarization of the photoelectron after absorption of a right handed photon in an initial $2p_{1/2}$ and $2p_{3/2}$-atomic level corresponding to $L_2$ and $L_3$ absorption.
Figure 2.9  $L_2$-absorption of a left and a right circularly polarized photon and the transfer of the spin-polarized photo electron assumed to have a photoelectron spin polarization of $\langle \sigma_z \rangle = -1$.

Figure 2.10  Fe$_{2.3}$ XAS and XMCD spectra and the analysis via the sum rules on the basis of the theoretical contributions to the XMCD by the orbital, spin and magnetic dipole moment.
Figure 2.11 XAS (upper row) and Co $L_{2,3}$ XMCD spectra of bulk Co, an atomic monolayer on Pt (111), monoatomic Co chains decorated at the steps of vicinal Pt (997) and Co, dimers and trimers on Pt (111). The XMCD spectra in a.u. are normalized to the strengths of the $L_2$ XMCD signal. The corresponding $\langle L_z \rangle$ -values determined via the sum-rules are given as inserts [Gambardella et al. (2003)].

Figure 3.1 Analogy between (a) photon absorption and (b) electron scattering. The target electron is symbolized by a blue diffuse cloud circling the nucleus. By symmetry with respect to the point of closest approach the mean electric field $E$ from the Coulomb interaction between probe and target is parallel to the momentum transfer $\hbar \mathbf{q}$. That makes the electron–electron interaction longitudinal, with the consequence that a screening cloud (red) shields the interaction, contrary to the transverse photon field.
Figure 3.2  The Fourier component of $E$ that gives rise to an electronic transition is parallel to the momentum transfer $\hbar \mathbf{q}$. It can be interpreted as an absorbed effective photon with polarisation $\mathbf{\varepsilon}||\mathbf{q}$.

Figure 3.3  Left: Principle of realising a helical effective photon in EELS, by selecting two perpendicular scattering vectors and a relative phase shift of $\pi/2$. This creates a helical electric wave in space travelling along the direction of $\mathbf{q} \times \mathbf{q}'$. The electric field is drawn in red. The field at the atom rotates counterclockwise when viewed along $\mathbf{q} \times \mathbf{q}'$. Right: Principle of detection in EELS by coherently combining the signals at $\mathbf{q}$ and $\mathbf{q}'$ and inserting a delay line in channel $q$. 
Figure 3.7  The scattering geometry equivalent to the absorption of an effective photon with helicity +1. (a) is reproduced from Fig. 3.3: the detector must in some way combine the wave functions from positions $q$ and $q'$, e.g. by a lens or a biprism. (b) The same effect can be achieved with two coherent incident waves and a single detector. In both cases the phase shift between the perturbing fields must be tuned to $\pi/2$.

Figure 3.9  EMCD $x$-$z$ map for hcp-Co for sample thicknesses of (a) 20 nm, (b) 50 nm, (c) 70 nm. An incident 3-beam/outgoing 2-beam case was used with the $(1 1 0)$ principal Bragg reflex. The incident plane is located at $z = 0$. The coordinate systems’ $x$-axes are aligned with the crystal’s $[1 1 0]$ direction while the $z$-axes are aligned with the crystal’s $[0 0 1]$ direction. Below each map, the integral relative dichroic signal is plotted. The disks indicate the positions of Co atoms in an ideal crystal. Colour coding by rainbow chart: blue is low, red is high value.
Figure 5.1 Left: Theoretical (solid line) and experimental (gray area) XMCD spectra for Fe (top), Co (middle) and Ni (bottom). Right: Left (blue) and Right (red) polarized XAS. The black lines and the gray are as represent the total theoretical and experimental XAS. The theoretical spectra have been normalized to the $L_3$ experimental edge and shifted by about $+20 \text{ eV}$ in order to allow a direct comparison in the same energy window. Theoretical spectra have been broadened by a Lorentzian of 0.6 eV (0.4 eV) width on the $L_3$ edge and 1.8 eV (0.8 eV) on the $L_2$ edge, and by a Gaussian of 0.2 eV (0.4 eV) width for Fe and Co (Ni). The experimental spectra for nickel have been taken from [Chen et al. (1994)], and for iron and cobalt from [Chen et al. (1990)].
Figure 6.1 Experimental X-ray absorption coefficient at the $L_3$, $L_2$ and $L_1$ edges of a Gd single crystal for right $\mu^+(E)$ and left $\mu^-(E)$ circularly polarized X-rays (top) [Wende (2004)]. The dichroic signal $\mu_M(E) = \mu^+(E) - \mu^-(E)$ is given at the bottom. Both, in the X-ray absorption data (top) as well as in the dichroic signal (bottom) a clear oscillatory fine structure can be detected in the extended energy range. This is the EXAFS and the MEXAFS, respectively.
Figure 6.2  Comparison of experimental (solid line) and theoretical XMCD spectra (FEFF) at Tb $L_3$ (left) and $L_2$ (right) edges: electric dipolar (dashed line) and quadrupolar (dotted line) contributions [Wende (2004)].

Figure 6.3  Density of states for spin-up (solid line) and spin-down (dashed line) electrons in Tb using the FEFF8 code [Ankudinov et al. (2004)]. The asymmetry parameter $a$ (doted line) characterizes the difference from unity of the ratio between spin-up and spin-down matrix elements Eq. (6.14). The zero of the energy is the Fermi level $E_F$. 
**Figure 6.4** Experimental Tb EXAFS (top) and MEXAFS (bottom) oscillations $k \cdot \chi (k)$ and $k \cdot \chi_M (k)$ (left) and the corresponding Fourier transforms (right) in comparison to *ab initio* calculations (FEFF8.2) [Wende *et al.* (2005)].

**Figure 6.5** Theoretical separation of multiple and single-scattering contributions in the Tb MEXAFS (FEFF8.2) [Wende *et al.* (2005)]. (b) Depiction of the dominant multiple-scattering paths.
Figure 7.1  $\mathbf{q}$ and $\mathbf{q}^*$ are shown for different orientations of $\mathbf{q}$ with respect to the incident wave vector $\mathbf{k}$.

Figure 7.5  Longitudinal weighting factor considered as a function of the collection and incidence angles, in the case where the electron beam energy is 200 keV. This factor is $1/3$ if $\beta_{\text{m}}/\theta_{\text{E}} \approx 1.47$ or $\chi_0 \approx 54.74^\circ$.
Figure 8.1 Asymmetry of the two-beam case geometry. (a) Thales circle construction with transmitted beam 0 and Bragg-reflected beam G. The “Thales circle positions” are denoted by A and B, respectively. (b) Setting the two beam case by tilting the sample from zone axis orientation. A tilt by $\alpha \sim 10^\circ$ leads to an asymmetric row condition and tilt by $\beta = G/2$ (few milliradians) leads to a two beam case. (c) Side view of the sample tilt with schematics of the underlying crystal (or reciprocal) lattice and the Thales circle construction in the diffraction plane. The Ewald spheres corresponding to the two outgoing beam directions have different relative orientations to the reciprocal lattice. Therefore the outgoing Bloch fields differ and this causes the asymmetry in dynamical diffraction effects. The x axis of the coordinate system is parallel with the systematic row of reflections and the z axis is parallel to the zone axis. Reproduced from [Rusz et al. (2010)] with permission from publisher.
Figure 8.2  Variation of the apparent $m_l/m_s$ ratio due to asymmetry in the two-beam case. Values below or beyond the range from $-0.5$ to 0.5 are coloured black or white, respectively. The sample is bcc iron, $G = (110)$, acceleration voltage 300 keV, tilt $10^\circ$. The systematic row is indicated as a horizontal line and Bragg spots by small circles. The transmitted beam is in the middle.

Figure 8.3  Variation of the apparent $m_l/m_s$ ratio due to asymmetry in a slightly tilted three-beam case (Laue circle centre set to 0.02$G$), taking the EMCD signal as a difference between upper and lower half-plane. See caption of Fig. 8.2 for details.

Figure 8.4  Same as Fig. 8.3, but taking the EMCD signal as a difference between left and right half-plane.
Figure 8.5  Same as Fig. 8.3, but taking the EMCD signal as a double difference.

Figure 9.6  Thickness profile of the EMCD at the Co $L_3$ edge, obtained with the detector shift method in a cobalt [001] hcp single crystal specimen, tilted to the $G = (100)$ systematic row and with LCC = $(\frac{1}{2}00)$. The illuminated area is 200 nm in diameter. The experiment (blue asterisks) is compared with DFT based band structure calculations for the same dynamical diffraction conditions. The blue and green solid curves are DDSCSs calculated for opposite helicities, the dashed black curve is the DFF part of the DDSCS (which does not depend on the helicity). The red line with circles is the relative dichroism defined as difference of DDSCSs divided by their sum, the red solid curve is the absolute dichroism. When the specimen is very thin, the measured values are smaller than predicted. This is because as the thickness becomes smaller, the relative effect of surface oxide layers and contaminations, both non-magnetic, becomes bigger; moreover, the shape anisotropy becomes stronger and increases the tendency for the magnetization to lie in the specimen plane, with the consequence that it becomes more difficult to saturate the magnetization in a direction parallel the optic axis (out of plane).
Figure 9.10 CBED configuration. The Co crystal is tilted in the (−110) direction from the [001] zone axis to a three-beam case i.e. where, besides the transmitted beam, only two Bragg spots are excited with the same intensity, namely \( \mathbf{G} = (110) \) and \( -\mathbf{G} \). The red dots indicate the Bragg spots which appear in the energy filtered image of the diffraction pattern taken at the \( L_{2,3} \) edge. The black dots show the positions where the other Bragg spots would appear if they were not so weakly excited. The detector shift technique is used without SAA to record spectra from the positions A and B, indicated by grey disks. The spatial resolution is given by the size of the focused spot, in this case \( \approx 3 \text{ nm} \). Figure adapted from [Rubino (2007)].

Figure 9.12 Left: Energy filtered diffraction pattern at 784 eV energy loss using a slit width of 20 eV. The sample was oriented in the two-beam case, capturing both reflections with in the SEA. When the spectrometer is switched to spectroscopy mode, a \( q\)-\( E \) diagram is obtained. Right: EMCD spectra obtained as line traces from the \( q\)-\( E \) diagram for values of \( q_y \) corresponding to the positions A and B on the Thales circle.
Figure 9.13 Dichroic signal at the cobalt $L_3$ edge as function of the scattering angle $q$ (in units of $G$) in the direction perpendicular to the Bragg scattering vector $\vec{G}$. Positions $A$ and $B$ (see Fig. 9.12) correspond to points $q/G = 0.5$ and $-0.5$ respectively.

Left: 3D spectral plot of the dichroic signal, calculated as difference from the average spectrum. Right: Comparison between ab initio simulation (line) and experimental data (crosses), obtained as line trace along the $L_3$ edge in the $q$-$E$ diagram. In both cases the values shown are obtained by first integrating the signal at $L_3$ over an range of 5.1 eV and the $q_x$ determined by the SEA (virtual in the case of the simulations) and then subtracting the corresponding value for $-q_y$.

The plot results to be antisymmetric by construction (i.e. the origin is an inversion centre). The error bars correspond to simulated Poissonian noise (2σ). Adapted from [Schattschneider et al. (2007b)].
Figure 9.14 ESD: a series of energy filtered images (left) of the diffraction pattern of bcc Fe in two-beam case is acquired with an energy window of 2 eV and energy step of 1 eV. By placing two virtual apertures (squares of 0.5G × 0.5G) on the Thales circle positions, EMCD spectra can be extracted from the data cube (top right). Dichroic maps can be obtained (experiment, bottom left and simulation, bottom right) by using the horizontal mirror axis to subtract, pixel by pixel, the signal in the upper half plane from the signal in the lower half plane and integrating the energy slices corresponding to the $L_3$ or $L_2$ edge. Alternatively, the spectrum in each pixel can be fitted to obtain the area under each relevant edge (see Chapter 10). A Tecnai F30 operated at 300 keV was used for this experiment, figure adapted from [Lidbaum et al. (2009)].
**Figure 9.15** Scheme of ESI measurements: the OA is placed at the A position on the Thales circle, the TEM is switched to image mode and an EFS is acquired scanning the \( L_{2,3} \) edge of the element of interest. The OA is then shifted to the B position and another EFS is taken over the same energy range. For every point in real space (i.e. for the same \((x, y)\) pixel in each energy slice), two spectra are obtained (blue for position A, red for position B). Under certain assumptions (see text) the difference between the integrated spectral intensity at \( L_3 \) should be the opposite than at \( L_2 \). An example is shown in [Lidbaum et al. (2010)].

**Figure 10.4** Illustration of the two ways used to extract the dichroic signal: (a) spectra are extracted from apertures at positions 1 and 2 in Fig. 10.3 and (b) is the difference spectrum of these two spectra; (c–e) dichroic maps, i.e. difference between the top half and the bottom half of the energy slice calculated for each pixel in the diffraction plane, (c) in the pre-edge region, (d) at the \( L_3 \) edge, (e) at the \( L_2 \) edge. The colour coding is identical for the three maps.
Figure 10.8 Simulation of the displacement position of the Fe (200) reflection at the $L_2$ edge caused by the presence of the dichroic signal as a function of sample thickness. The simulations were carried out as described in Rusz et al. orienting the sample on a 2-beam case. To demonstrate the displacement effect, simulation is shown in the vicinity of the $g = (200)$ reflection.
Figure 10.13 Reciprocal space maps of the EMCD signal for Fe oriented 3BC geometry [Lidbaum et al. (2009a)]. Theoretically simulated relative EMCD maps at the $L_3$ edge are shown in (a). The inset shows the simulated diffraction pattern. In (b) and (c) 3BC maps of experimentally obtained relative EMCD signal at $L_3$ and $L_2$ edges are shown. The black lines indicate the applied mirror axes and blue spots the positions of the transmitted and Bragg scattered $G = (200)$ and $-G = (-200)$ beams. The insets in (b) and (f) show the diffraction patterns averaged over an energy interval from 695 eV to 740 eV.
**Figure 10.14** Map of the $m_1/m_5$ ratio of bcc iron evaluated pixel-by-pixel using the double difference procedure.

**Figure 11.3** EMCD map showing the relative EMCD signal on the $L_3$ edge of bcc Fe for different thicknesses at 300 kV in 100 zone axis orientation. Note the strong effect of channelling on the EMCD pattern, which makes it far from trivial where to choose the collection aperture so as to obtain the maximum signal. The thicker the crystal, the more the channelling destroys the EMCD signal.
Figure 11.4 EMCD map showing the relative EMCD signal on the $L_3$ edge of bcc Fe for different thicknesses at 300 kV in 100 zone axis orientation with a beam tilt of 14 mrad. The signal gets more asymmetric and stronger with respect to exact zone axis orientation. Also the thickness dependence changes.

Figure 11.5 EMCD map showing the relative EMCD signal on the $L_3$ edge of bcc Fe for different thicknesses at 300 kV in 100 zone axis orientation with a beam tilt of −14 mrad. Note the symmetry with respect to +14 mrad tilt.
Figure 11.6 Two beam simulation showing the relative EMCD signal on the $L_3$ edge of bcc Fe for 300 kV and different thicknesses.

Figure 11.7 Three beamsimualtion showing the relative EMCD signal on the $L_3$ edge of bcc Fe for 300 kV and different thicknesses. A slight mistilt is introduced by shifting the Laue circle centre to $LCC = (0.02, 0.02, 0)$. 
Figure 12.4 (A) Fe-$L_{2,3}$ edge after background subtraction of the scan at the position with positive chirality. (B) Spectra from the middle of the 3 nm Fe layer. The difference is the dichroic signal. (C) Dichroic signal of the $L_3$ edge of the whole scan. (D) Intensity profiles integrated over 6 eV of the dichroic signals in the Fe-$L_{2,3}$ edges, the intensity profile of the iron edge and the fitted curve.
Figure 14.1 Electron probe in the lateral plane, Eq. (14.2) caused by the 3 transition channels. Real part of the wave function (left column), imaginary part of the wave function (middle) and intensity (right). The initial and final state magnetic quantum numbers of the atom are indicated as \( m, m' \). Incident plane wave and perfect lens assumed. See text for details. Colour coding by rainbow chart shown as insert in the left upper panel (blue: low, red: high).

Figure 14.2 Real and imaginary parts of the Fourier transformed functions \( \psi \pm 1 (q) \) (left and middle columns), and phase with superimposed aperture function (third column; colour coding from \(-\pi\) to \(+\pi\)). The fourth column shows the resulting intensities in the high resolution image. In a real experiment, they would correspond to up/down magnetic moments.
Figure 14.6 Diagonal element of the density matrix $\rho_f(x, x, q_y, q_y, k_0 - q_e, k_0 - q_e)$ after excitation of a chiral transition with $\Delta m = -1$. Colour coding by rainbow chart (blue: low, red: high).