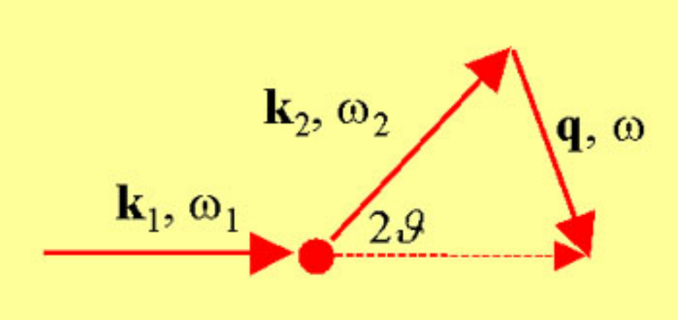
ID16 - Inelastic Scattering I



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Synopsis

ID16 is an undulator beamline dedicated to high and very high resolution inelastic X-ray scattering (IXS). This technique allows both the energy and the momentum transfer to be controlled in rather wide regions, which makes possible the study of quite distinct physical (and chemical) problems in condensed matter, including phonon-like excitations as well as electron spectroscopies at valance and core level.

Three spectrometers have been developed on the beamline; two of them (the so called *horizontal* and *vertical* spectrometers) were designed to study the dispersion relations of phonons, with very high energy resolution. The key elements of these are a backscattering monochromator, utilizing a Si(*nnn*) reflection, which can provide an X-ray beam with sub-meV energy resolution, and the several thousands analyser crystallites, arranged on spherical surfaces, which use the same reflection as the monochromator.
These set-ups allow to cover a **q**, *E*-range not accessible to related techniques, like inelastic neutron scattering. This has opened up the possibility of high frequency dynamics studies in disordered systems, e.g. liquids and glasses. Moreover, the intense and focussed X-ray beam makes possible to study samples only available in very small quantities or submitted to high pressures.

The third, high-resolution IXS set-up provides an energy-resolution and energy transfers suitable for the exploitation of inelastic scattering from electron valence excitations, Raman and resonant Raman scattering. Besides, core level high resolution X-ray absorption and emission spectroscopies are also available for many elements. Raman scattering, or better *non-resonant IXS* is complementary to electron energy loss spectroscopy (EELS) as it is bulk sensitive and practically free of problems arising from multiple scattering.

The beamline characteristics are as follows:

Horizontal and vertical spectrometers

- Incident photon energy: 13840, 15817, 17794 and 21747 eV.
- Total energy resolution of 7.0, 5.5, 3.0 and 1.5 meV.
- Energy transfer: 0 - 500 meV
- Momentum resolution: typically 0.4 mm^{-1}
- Momentum transfers
    - 1 - 35 nm^{-1} for the horizontal spectrometer
    - 1 - 160 nm^{-1} for the vertical spectrometer
- Recording of five momentum transfers simultaneously (horizontal spectrometer)

Spectrometer for electronic excitations

- Incident photon energy: 5 - 15 keV
- Energy resolution: 0.1 - 1.5 eV
- Spectrometer arm: 1 m (can be extended to 1.5 m or 2 m)

- Angular range: 0-170 degree
- Beam focus: 100 micron (H) x 50 micron (V) or 100 micron (H) x 1 mm (V)
- Monocromator: Si(111), but several channelcuts can be inserted for higher resolution
- Analyser crystals: a great choice (for 1 m Rowland-circle)

Scientific Applications

High frequency dynamics

The determination of the phonon dispersion, or more generally, of the high-frequency (THz) collective dynamics, allows to access various material properties such as sound velocities, elastic constants, interatomic force constants, phonon-phonon interactions, phonon-electron coupling, dynamical instabilities, relaxation phenomena etc. Applications of inelastic X-ray scattering from phonons on ID28 can be roughly divided into three categories:

- Phonon dispersion under extreme conditions of very high pressure (up to 100 GPa): (geophysically relevant materials, metals, liquids)
- Determination of the high-frequency collective dynamics in disordered systems: (Hydrogen-bonded liquids, liquid metals, molten salts, glass formers, quantum liquids, biological materials)
- Phonon dispersion in crystalline materials, only available in very small quantity, or otherwise incompatible with inelastic neutron scattering techniques: (High-temperature superconductors, large bandgap semiconductors , actinides)
- Study of the empulse approximation regime on quantum fluids.

Electronic excitations

The experimental method can be classified as *resonant IXS*, if the incoming photons energy is close to an absorption edge, or as *non-resonant IXS*, if it is far from any absorption edge. In contrast to electron spectroscopies, both of them are sensitive to bulk properties. Methods based on resonant IXS are element (and in fortunate cases even spin or site) selective probes of unoccupied and occupied electronic states, as well as local magnetism. Non-resonant IXS based methods, besides bringing information on atomic ground state properties, are probes of local and collective electronic excitations, similarly to electron spectroscopies.

The main applications of these methods (with links to recent examples):

Non-resonant IXS

- electron-hole pair creation -- valance excitations, gaps
- plasmons -- energy spectra and dispersion
- inner core excitations -- K-edges of light elements
- Compton scattering -- ground state electronic properties

Resonant IXS

- Charge-transfer excitations -- metal-insulator transitions
- Resonant X-ray Emission -- valance state transitions
- Partial Fluorescence Yield X-ray Absorption -- unoccupied electronic DOS, local geometry
- X-ray Emission Spectroscopy -- local /atomic/ magnetism

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