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Concept of a one-shot RIXS spectrometer for XFELs

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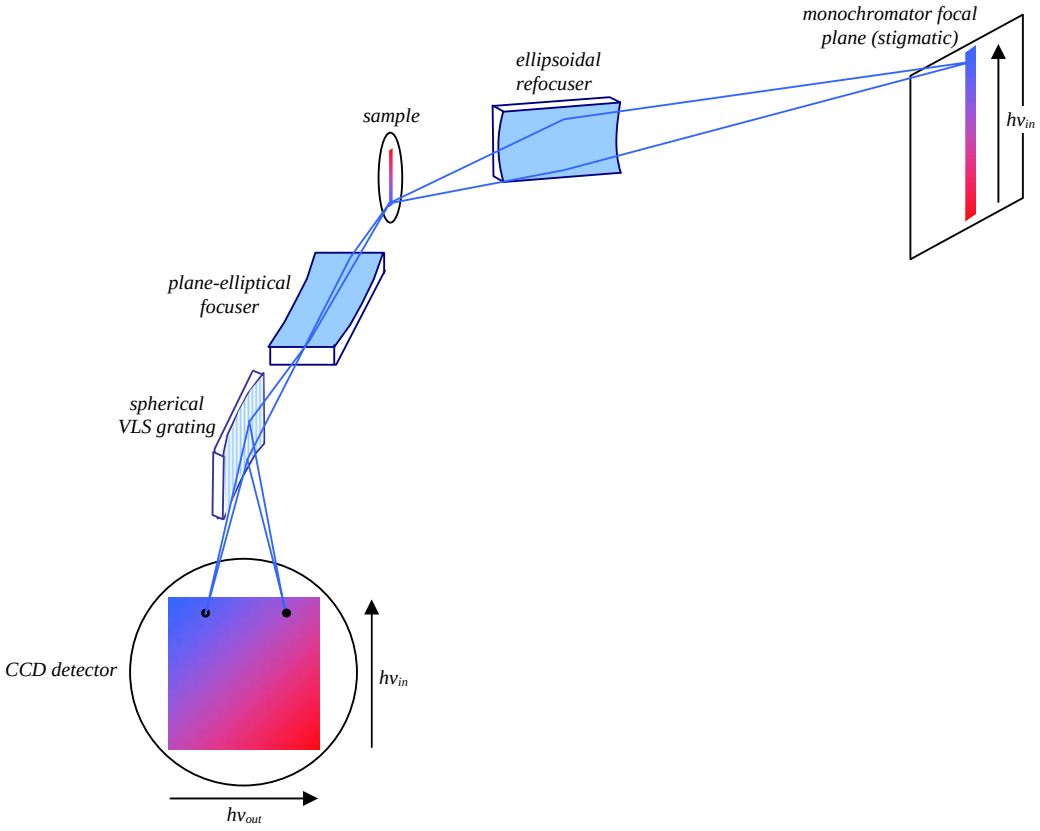
High-resolution RIXS (Resonant Inelastic X-ray Scattering) is a powerful experimental technique giving information about the spectrum of low-energy excitations of correlated electron systems in solids, liquids and gases. Presently, one acquires the RIXS data – X-ray fluorescence intensity depending on the incoming and outgoing photon energies $I(h\nu_{in},h\nu_{out})$ – by measuring single $I(h\nu_{out})$ spectra for a series of incoming photon energies $h\nu_{in}$ delivered by the monochromator. Here, a concept of RIXS spectrometer is proposed to enable acquisition of the whole array $I(h\nu_{in},h\nu_{out})$ of the RIXS data in one shot. The concept relies on the ability of XFELs to deliver a round spot profile.

Optical scheme of such a one-shot RIXS spectrometer – nicknamed $h\nu^2$ for simultaneous detection in $h\nu_{in}$ and $h\nu_{out}$ – is shown in the sketch. The monochromator produces in its focal plane an image of light dispersed in energy $h\nu_{in}$. The ellipsoidal refocuser demagnifies the image onto the sample. The vertical demagnification is important for inhomogeneous samples, and horizontal demagnification to achieve high energy resolution of the spectrometer operated slitless. The first element of the spectrometer is a plane-elliptical mirror, which produces on the CCD an image of fluorescence magnified and dispersed in the vertical direction in $h\nu_{in}$. The spherical VLS grating disperses the fluorescence in $h\nu_{out}$ and focuses in onto the CCD in the horizontal plane. In this way the *full two-dimensional image* of RIXS intensity $I(h\nu_{in},h\nu_{out})$ is formed on the CCD.



Further notes:

• The $h\nu^2$ spectrometer includes for free an option for *one-shot XAS* data acquisition in total fluorescence yield (TFY). This measurement mode is realized by setting the grating to zero diffraction order. The vertical line formed in this case on the CCD is the XAS spectrum as a function of $h\nu_{in}$. Note: The spherical aberrations from the grating may affect only the horizontal image profile and thus have no influence on the XAS spectrum.

• Prerequisite for the $h\nu^2$ spectrometer to achieve high energy resolution in $h\nu_{out}$ is that the monochromator produces small horizontal focus. This can only be achieved with XFELs delivering a *round* spot profile.

• The use of the *ellipsoidal refocuser* requires that the focal plane of the monochromator is stigmatic. If not, a KB optics with two plane-elliptical mirrors shall be used for refocusing.

• Normally, the VLS grating spectromeres have the exit arm variable as a function of energy. In the present scheme the *exit arm is fixed* in order to stay focused in the $h\nu_{in}$ direction, and the focalization is performed only by pitch of the grating. Prerequisite for high energy resolution, cancellation of the coma aberrations [1] can be achieved in this case for any energy by variation of the entrance arm through the grating translation.

• Typical PGMs are characterized by dispersion in their focal plane ~5 eV/mm for photon energies near 1 keV. The vertical image size for a typical RIXS experiment will then be ~1 mm. A demagnification onto the sample about a factor of 10 can routinely be achieved with ellipsoidal mirrors. This produces the *vertical spot size* ~100 μm, which is acceptable even for small samples.

• The plane-elliptical focuser magnifies the vertical size of the image on the CCD by a factor about 10 up to ~1 mm. With a realistic spatial resolution of the CCD being ~20 μm, the *resolution in* $h\nu_{in}$ appears about 100 meV, matching the state-of-art resolution in $h\nu_{out}$.

• For every single $h\nu_{in}$, the $h\nu^2$ spectrometer is fully equivalent to a normal RIXS spectrometer with spherical VLS grating, where the focuser mirror acts to focus the beam on the CCD in the vertical direction. Therefore, the one-shot concept adds simultaneous detection in $h\nu_{in}$ as a 'free lunch' *without compromising the detection efficiency* in $h\nu_{out}$. Moreover, the focuser mirror further increases the spectrometer acceptance by a factor of ~3 compared to the single-grating design used at the ADRESS beamline of SLS.

References:

V.N. Strocov, Th. Schmitt and L. Patthey, PSI Technical Report No. SLS-SPC-TA-2008-309, 2008