Modular X-ray emission spectrograph Design for the ALS

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Abstract: We are in the process of designing and building a modular spectrometer with the goal of being portable for use at a diverse group of endstations at the ALS, LCLS and TLS. The basic design is based upon experience from several years of use with similar designs at the ALS. For detector positions of less than 1.3 m, the design incorporates a composite cantilevered swing arm. Two optical elements are used in the X-ray emission spectrograph (the Hettrick-Underwood design): a spherical mirror for focusing the X-rays onto an in-vacuum CCD detector and a variable line spacing (VLS) plane grating for energy monochromatization. The grating will be operated in the constant incident angle mode, thus variation in the detection photon energy is accomplished by moving the detector along the focal plane. Relatively large source-size resolution allows the spectrograph to be used at the ALS and LCLS beamlines where tightly focused beam won't be available, while small detector-pixel-size resolution gives a good resolving power over the operating photon energy range (~500 up to 1,000 eV). Large acceptance angles enhance the detection efficiency for RIXS measurements, which often have a very small cross-section. The momentum-resolved capability, available through the combination of mounting spectrographs at different scattering ports and rotating the entire qRIXS endstation relative to incident photon beam offers the opportunity to perform truly momentum-resolved RIXS in the soft X-ray regime. The modular design of X-ray emission spectrograph gives the flexibility to tailor for specific applications that may require either high throughput or high resolution. We present the status of our current design.

Project Description

Although there are several very high energy resolution soft x-ray RIXS systems currently being developed at light sources around the world, none of them can perform the truly momentum-resolved RIXS spectroscopy to study the elementary excitations in three-dimensional correlated materials. Furthermore, the project serves to demonstrate the first femtosecond time-resolved qRIXS at the LCLS to establish the scientific cases for the FEL-based light sources. Thus, the qRIXS spectrometer at LBNL is designed to be compact, modular and flexible, instead of trying to achieve the highest energy resolution. The qRIXS spectrometer will cover a large energy range from 100 eV to 1.2 keV, and its compact size allows us to incorporate several of them (three units in the current plan, but the endstation can accommodate up to five units) to cover a large horizontal angular range simultaneously. The modular design also provides flexibility for the spectrograph to be operated either in the inside or outside order, and can be tailored for specific classes of science by making minimal modifications on up and downstream components.

Scientific Justification

Resonant inelastic x-ray scattering spectroscopy (RIXS) is a measurement technique which uses photons with energies tuned to elemental absorption edges to create the direct electronic orbital transitions, and reveal the electron dynamics in femtosecond time and nanometer length scales. With the capability to vary the momentum transfer (Δ**q**) between incident and emitted photons in the scattering plane (Δ**q**=**k**$_f$-**k**$_i$), as well as to analyze the energy loss (ΔE) in the process (ΔE=ω_f-ω_i), the momentum-resolved RIXS (or qRIXS) has been used to measure the dispersion relations of low energy collective modes, such as phonons, magnons and orbitons, that are critically linked to the emergent material properties like high temperature superconductivity, colossal magnetoresistance and multiferroicity [1-7].

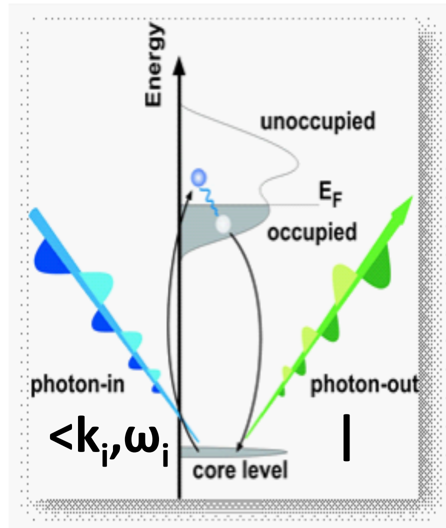

Figure 1: Schematic illustration of the RIXS process. An incident photon excites a core electron into unoccupied state (x-ray absorption, XAS) and the resulting core-hole is quickly filled by another electron in the occupied state, leading to the emission of photon with distinct energy and momentum (x-ray emission, XES). Under the resonance condition, the net process is the creation of particle-hole excitation.

The core of soft x-rays qRIXS instrumentation is the grating-based x-ray emission spectrograph. The physical dimension of spectrograph is often determined by the trade-off between resolving power

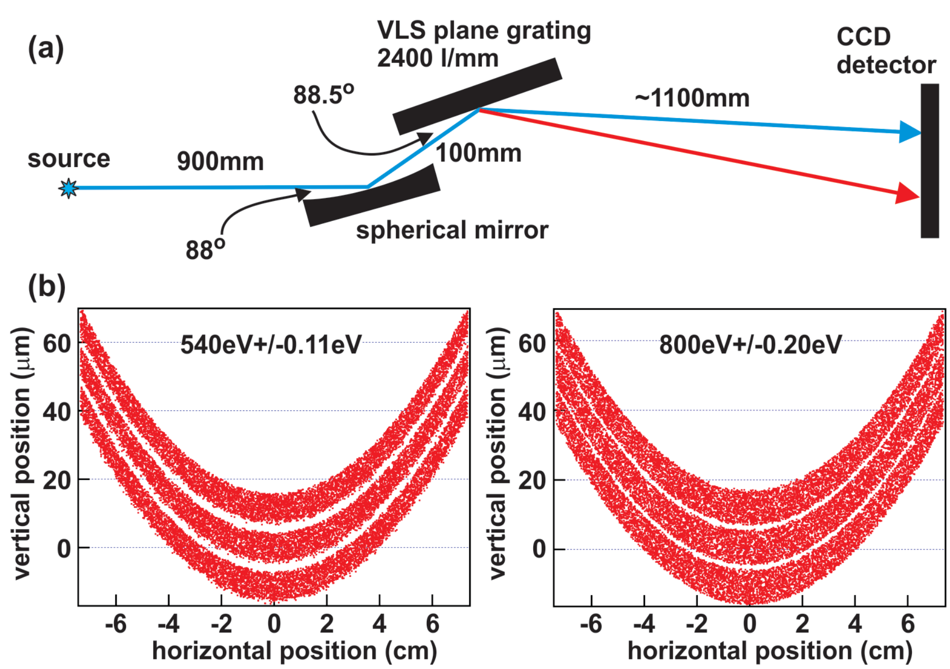

Figure 2: (a) Optical layout of the VLS spectrograph, with 2400 lines/mm grating. (b) SHADOW simulation showing the resolving power at 540eV (left panel) and 800eV (right panel).

and throughput. The resolving power usually scales with the length and the throughput scales inversely with the length squared. In addition, to utilize the newly developed free electron laser (FEL) to perform time-resolved qRIXS in the pump-probe scheme, modularization and motorization of the spectrograph become important factors as well. Although the commercially available x-ray emission spectrograph uses spherical gratings under Rowland circle condition and the microchannel plate detector at grazing incident geometry, the mechanical design becomes increasingly complex with larger spectrograph size. Furthermore, lower detector efficiency and strong coma make it less ideal compared to the variable line-spacing (VLS) plane grating where focal plane can be erected normal to the x-ray beam to utilize CCD detector for direct x-ray imaging. In that regard, we have designed a compact and modular VLS spectrograph for the qRIXS endstation. The advantage of this design is the universal optical chamber that can be used in both inside and outside order of the grating, as well as different modules to suit various optical layouts.

In figure 2, we show the optical layout of the spectrograph and SHADOW simulations at incident photon energies around 540eV (figure 2(b), left panel) and 800eV (figure 2(b), right panel). The spectrograph consists of two optical elements, a spherical mirror focusing the x-rays onto an in-vacuum CCD detector and a 2,400 lines/mm VLS plane grating for energy monochromatization. The grating operates in the inside order (incident angle is larger than the emission angle), and in constant incident angle mode. Varying the detection energy is done by moving the detector along the nearly vertical focal plane (~5^{o} away from vertical). The overall length of the spectrograph is around 2.1m, and the acceptance angle is roughly 2.6mrad (v) by 60mrad (h). As shown by the simulation, the resolving power of this design can achieve >5,000 and drops down to ~3,300 at 1,000eV.

Spectrometer Endstation Layout

The optical design of this qRIXS spectrograph is similar to several spectrometers designed (Hettrick-Underwood design) and in operation at the ALS. The design incorporates a spherical pre-mirror and a VLS plane grating. To facilitate alignment and serviceability, all position sensitive component are mounted on a common vacuum chamber lid. Both optics are mounted on a common cradle with the pivot point locations machined to achieve the required tolerance of .0005” for the relative placement of the optics.

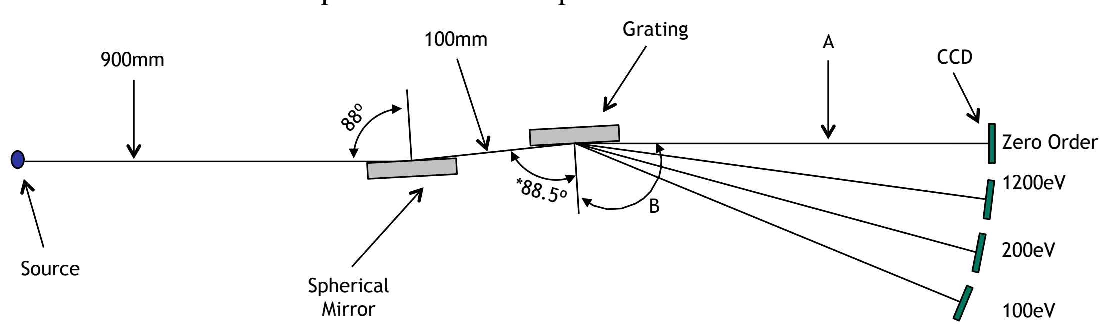

Figure 3: Optical layout and range of motion

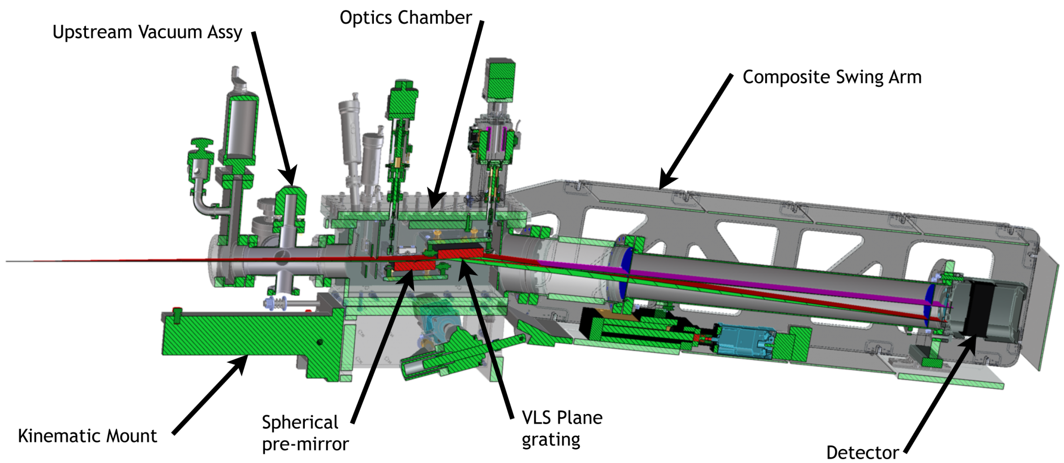

Figure 4: Spectrometer Layout

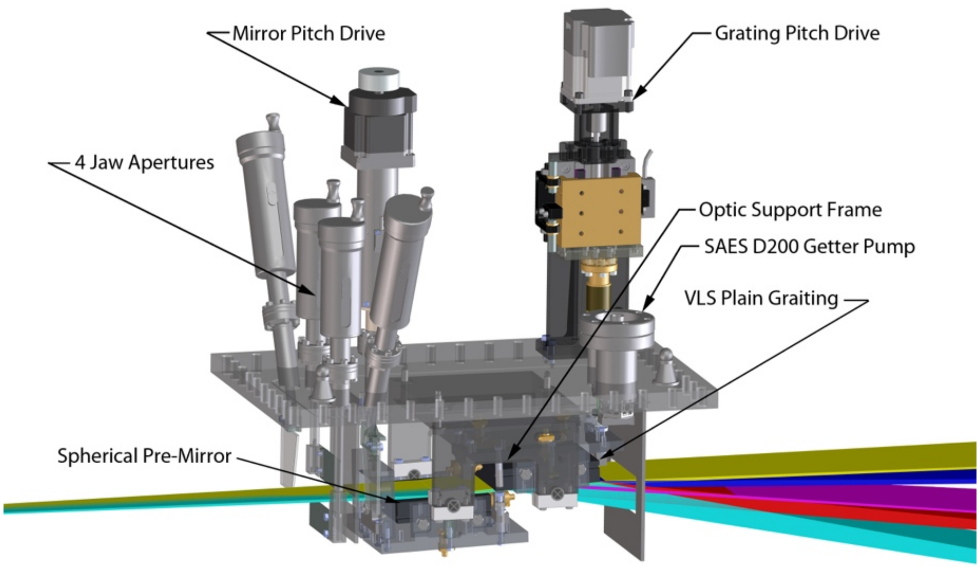

Figure 5: Optical Hardware Vacuum Components

The wire seal design for the qRIXS spectrometer optics chamber is adopted from Cornell. The team at Cornell has established a procedure in conjunction with chamber design rules that consistently produces a UHV seal. Although this wire seal design was optimized on large vacuum vessels and the qRIXS vacuum chamber is a relatively small vessel this process is anticipated to work well for our system. Fundamental to the wire seal design is the concept of controlling the wire compression and elongation to enable a consistent seal. This is accomplished by exploiting the inherent flexibility in stainless steel lids while employing spring tension to accommodate any elongation resulting from the sealing process. During the sealing procedure, the chamber lid is forced to flex at each end of the chamber via two set screws. Working from the center towards the outer edge of each flange surface a light tightening of bolts creates a consistent compression of the sealing wire. The final tightening of the bolts is accomplished after the set screws are removed. On the qRIXS optics chamber, all wire seal surfaces have a 16 surface finish and flatness of 0.02" with no more than 0.004" over a 7.5" length. The lid flange is 0.75" thick with a bolt spacing of 1.1". It is anticipated that a 0.032" diameter aluminum will be used for the wire seal. To reduce bolt torquing requirements, cutouts for the aluminum wire after the wire crossovers were included in the optics chamber flange at all four corners. Clearance holes were designed into the chamber flange to avoid chamber rework for damaged threads or seized bolts.

Kinematic mount

The qRIXS endstation requires that each spectrometer has the ability to be interchangeably located at each of five mounting locations. Each spectrometer must be able to be reproducibly replaced and placed on any of its mounts to a tolerance of X = 500 µm or 0.020", Y = 1,000 µm or 0.040", Z = 50 µm or 0.002". We looked at several options for kinematic or semi-kinematic mounts and chose a six point 3-2-1 design that is independently adjustable at each of its contact points. The mount is oriented with the 3 points in the vertical direction such that the cantilevered mass of if the spectrometer keeps the mount engaged. The two remaining directions are loaded with springs.

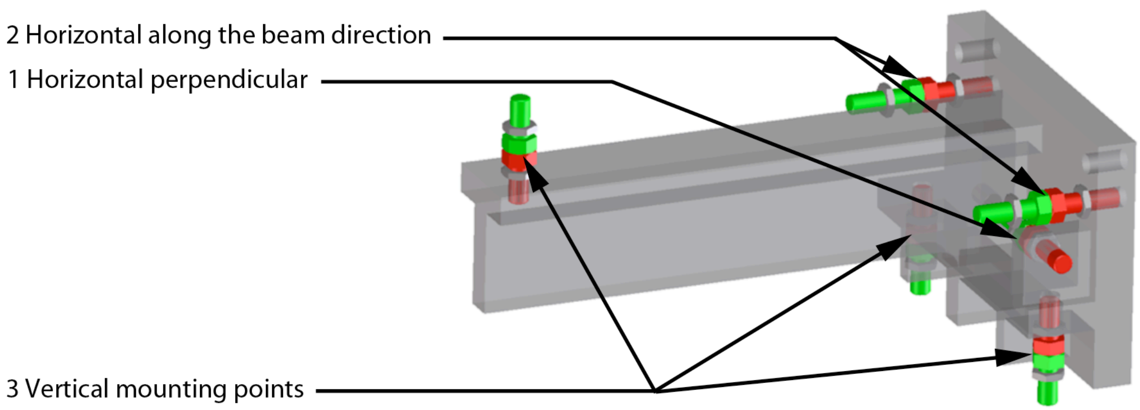

Figure 6: Kinematic Mount Assembly

Detector Positioning

The swing arm design has often been used at the ALS to allow precise encoding of the detector position around the grating pivot point. This is typically driven vertically at the detector location. In this case we are trying to take advantage of the increase in stiffness and lighter weight of the composite swing arm assembly to cantilever the arm from the chamber support. The pivot utilizes preloaded angular contact bearings and also provides the mounting for the encoder.

Composite Swing Arm Design

The swing arm design was developed with the LBNL Composite group and produced a 60% savings in structural mass with increased damping relative to aluminum. The first vibrational mode of the swing arm is is 47 Hz in the vertical direction and 29.6 Hz in the horizontal direction. The lay up consists of two 1.25mm fiber section on either side of a 1/2" aluminum honeycomb core. The laminations are made up of five plies of CN60 in an orientation of 0,45,90,-45,0 with 32% resin.

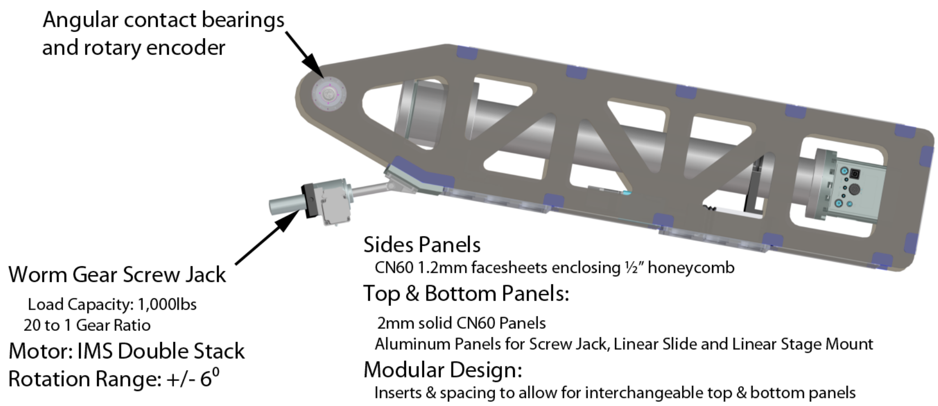

Figure 7: Swing Arm Design

Detector Design

The initial plans for the spectrometer include the use of commercial detectors but the system is ultimately designed to take advantage of a detector design being produced at LBNL. The detector provides a spatial resolution of 5 microns in the energy dispersive direction, which is expected to result a resolving power of > 5000 O K edge @ 540eV.

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