Inelastic Soft X-ray Scattering Beamline System

The soft X-ray photon-in-photon-out experiment is a powerful technique for probing the electronic structure of highly correlated electron systems, polymers, biological samples, artificially structured and interfacial materials. The wavelength of soft X-ray is ideal for probing materials on the nanoscale, and the long penetration depth of soft X-ray photons reveals true bulk properties. Photons are free from the interference of external electric and magnetic field, so photon-in-photon-out experiments are well suited for the study of materials under external fields. Combined with other unique properties of synchrotron radiation, the synchrotron-based photon-in-photon-out experiment offers a wide range of new possibilities in materials research.

The Inelastic X-ray Scattering (IXS) Spectroscopy is one type of photon-in-photon-out technique that studies the dynamics of scattering and electronic structure of materials. Since the signal of IXS is usually very low, high-intensity and high-resolution excitation sources together with a high-efficiency spectrometer are required. To meet these two stringent requirements for IXS in the soft X-ray region, we have designed an elliptically polarized undulator - active grating monochromator - active grating spectrometer (EPU-AGM-AGS) beamline system that will increase the signal collection efficiency by two orders of magnitude. The engineering design of the AGM-AGS beamline system is shown in Fig. 1. This beamline system consists of two major sub-systems, the AGM monochromator and the AGS spectrometer, as described in the following.

The AGM takes the output from the EPU photon source. The combination of EPU and AGM can deliver high-intensity and high-resolution photon beams with any degree of circular polarization. Its design is similar to that of the EPU-SGM beamline, except that it uses an variable-line-space (VLS) active grating rather than the spherical grating in the SGM beamline. The radius of the active grating is continuously adjustable during energy scanning to keep the selected photon beam focused at the sample position at all energies. With a grating of 1,200 *l*/mm groove density and entrance slit opening of 10 μm, the EPU-AGM delivers an average photon flux of 1×10^{12} photons/(sec.0.01%BW.200 mA).

The design of EPU-AGM-AGS beamline system is based on the energy compensation principle of grating dispersion, as shown in Fig. 2. Two

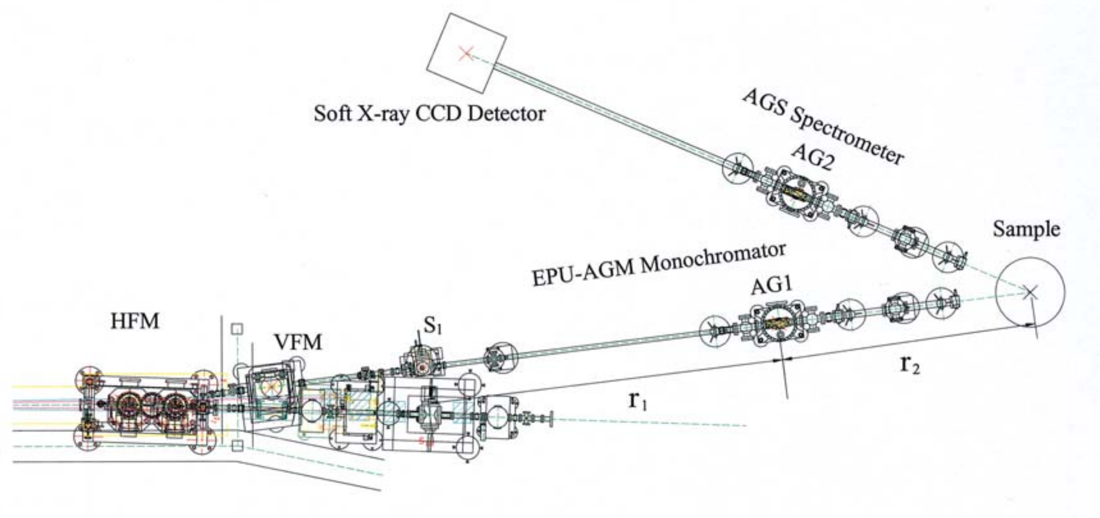

Fig. 1: The engineering design of the AGM-AGS beamline system.

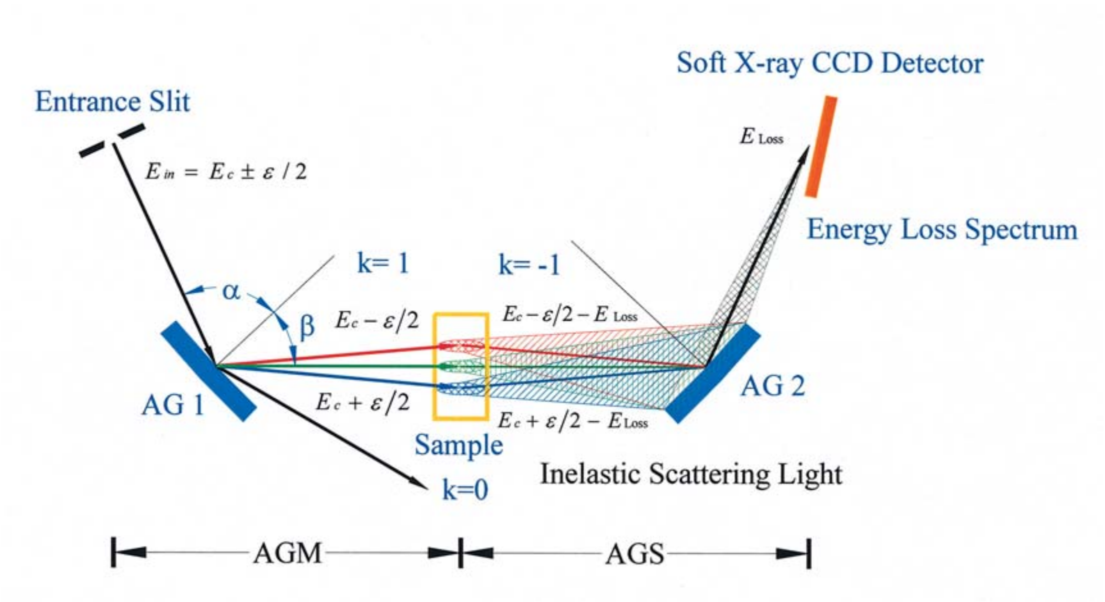

Fig. 2: The energy compensation principle applied in the AGM-AGS system.

identical gratings are employed in the system, one in the AGM labeled as AG1 and the other in the AGS labeled as AG2. The AGM and AGS are arranged in a reverse configuration to satisfy the energy compensation condition and hence provide very high signal collection efficiency in the inelastic scattering, i.e. energy loss, spectra.

Based on the energy compensation principle, the photon beam with central energy E_c and energy spread ε, after passing the entrance slit, is dispersed and focused onto the sample by AG1. By using the k = +1 diffraction order for the AGM, the incident excitation photons with energies from $E_{in} = E_c - \varepsilon/2$ to $E_c + \varepsilon/2$ are focused on the sample from low to high energies sequentially in a well-defined pattern. For an energy loss spectrum, the inelastically scattered photons will have energies $E_{out} = E_{in} - E_{loss}$. The inelastically scattered photons will have a nearly identical energy spread on the sample as the incident excitation photons, and thus can be collected, diffracted and refocused by AG2, with k = −1, onto the soft X-ray CCD detector located at the exit slit. Consequently, the signal collection efficiency is greatly increased as compared to conventional designs that do not employ the energy compensation principle.

In order to simulate the performance of the AGM-AGS IXS beamline system, we have developed a special ray-tracing program that can handle multiple-energy, multiple-source-point photon beams simultaneously. After a series of simulations, we found that a VLS grating can greatly improve the performance of the AGM-AGS system. By setting the entrance slit opening at 10 μm, the optical footprint on both gratings at 100 mm, the grating center ruling density at 1,200 *l*/mm, the entrance arm length at 3.5 m, and the exit arm length at 2.5 m, the spectral resolving power in full-width-root-mean-square (FWRMS) of the energy loss spectra excited by incident photon beams with energy spread (ε/E_c) of 1% is calculated to be between 3,000 and 8,000 for center excitation energy (E_c) ranging from 400 eV to 1,400 eV when using constant-line-space (CLS) gratings (see Fig. 3).

In this calculation, the scanning angle of the AGS grating is set at 1.5 eV lower than the central excitation energy, i.e. an energy loss of 1.5 eV. Although this resolving power is sufficient for most IXS experiments, the grating radius, 33 m to 55 m, required for the entire excitation energy range from 400 eV to 1,400 eV, is far beyond the bending range of the active grating we have developed.

To solve this problem and to further increase the spectral resolution, we have also studied the performance of the AGM-AGS system when using VLS gratings. For a VLS grating, by choosing $n_1 = 0.8\ l/\mathrm{mm}^2$ to optimize the system performance in energies from 500 eV to 1,200 eV, the grating radius is between 75 m and 155 m for photon energy 400 eV to 1,400 eV, which is well within

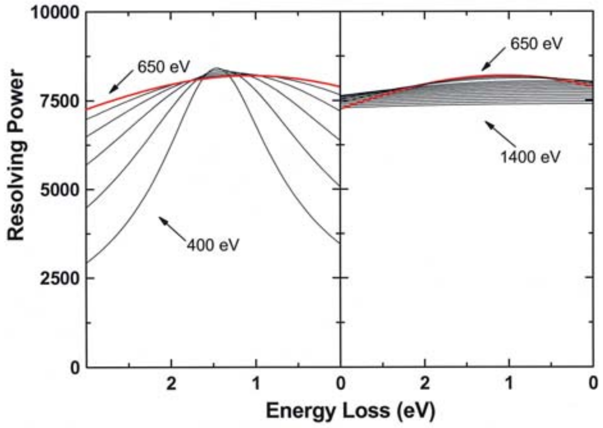

Fig. 3: The resolving power as a function of energy loss for various incident photon energies of the AGM-AGS system. The energy spread (ε/E_c) is set at 1% and the optimal resolution is set at the 1.5 eV energy loss. The beamline optical parameters are: r_1 = 3.5 m, r_2 = 2.5 m, n_0 = 1,200 l/mm, 100 mm optical footprint on both gratings and 10 μm entrance slit opening.

the bending range of the active grating we have developed.

The calculated resolving power of the energy loss spectrum for the AGM-AGS system is between 5,000 and 30,000 when using VLS gratings with n_1 = 0.8 *l*/mm^2 (see Fig. 4). The higher resolving power is due to the fact that the VLS grating focuses the incident photon beams on a nearly vertical plane, rather than on a inclined curved surface, thus matching the sample surface well and satisfying much better the energy compensation condition.

The ray tracing results of the instrumentation lineshape for the energy loss spectra is shown in Fig. 5. In this simulation, the incident excitation photon energy (E_c) and its energy spread (ε) are set at 800 eV and 8 eV, respectively. The optimal resolution is set at loss energy of 1.5 eV and gives the narrowest FWRMS linewidth of 29 meV. Even with the slightly un-compensated optical path at both the 0 eV and 3 eV ends, the spectral linewidths are still as good as 84 meV. By setting the optimal resolution at different loss energies, one can always reach a resolving power greater than 14,000 for any spectral features of interest within the entire range of the incident excitation photons.

In summary, we have designed an AGM-AGS beamline system for inelastic soft X-ray scattering experiments. By applying the energy compensation principle, the energy loss photons emitted from the sample excited by the incident photon beams monochromatized by the AGM are effectively collected, diffracted and focused by the AGS. For IXS experiments, this system has a signal collection efficiency two orders of magnitudes higher than the conventional design while reaching a resolving power greater than 14,000 in the energy loss spectra. The use of VLS gratings in the system relaxes the mechanical specification of the bender and the grating substrate as well as

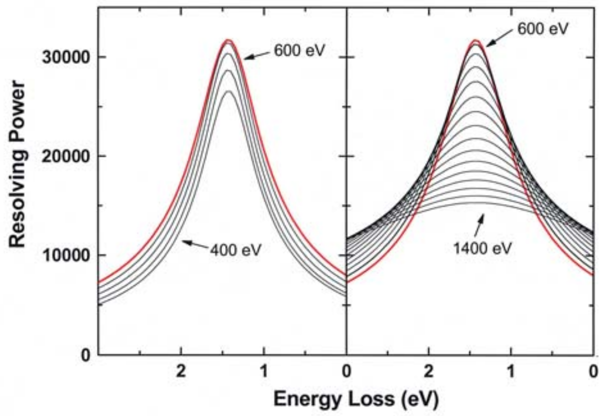

Fig. 4: The resolving power as a function of energy loss for various incident photon energies of the AGM-AGS system. The energy spread (ε/E_c) is set at 1% and the optimal resolution is set at the 1.5 eV energy loss. The beamline optical parameters are: r_1 = 3.5 m, r_2 = 2.5 m, n_0 = 1,200 l/mm, n_1 = 0.8 l/mm^2, 100 mm optical footprint on both gratings and 10 μm entrance slit opening.

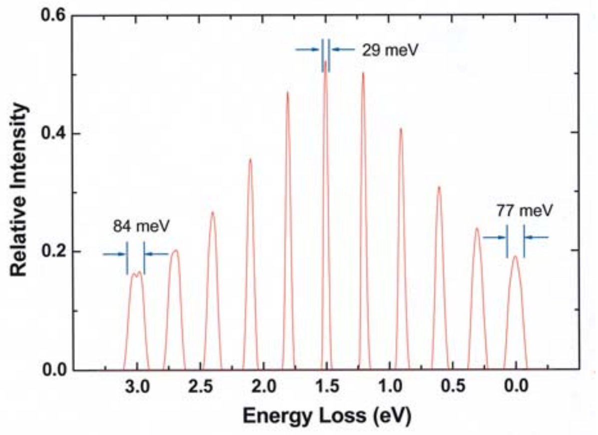

Fig. 5: The AGM-AGS beamline system energy loss instrumentation lineshape as a function of the loss energy. The incident excitation photon energy E_c and its energy spread ε are set at 800 eV and 8 eV, respectively. The beamline optical parameters are identical to those shown in Fig. 4.

improves the overall performance. This IXS beamline system is currently under construction and will be completed for commission in the spring of 2004.

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