Midterm Upgrade Proposal for 30-ID XOR/IXS Beamline

1. Executive Summary

We propose (i) to perform R&D and build two novel inelastic x-ray scattering (IXS) spectrometers **ANGIX** and **UHRIX**. These new spectrometers would both significantly broaden the scope of research, allowing IXS to enter unexplored territories, and would increase the throughput of experiments by more than an order of magnitude. We also propose (ii) to extend the straight section, install a third undulator, (iii) to develop state of the art scientific IXS software, and (iv) to make improvements to the existing spectrometers.

ANGIX (**A** **N**ext **G**eneration **IX**S) will offer the following capabilities, as compared to the existing HERIX:

	ANGIX	HERIX
Number of analyzers	130-180	9
Scattering angle 2Θ	$-40^{\circ} < 2\Theta < 120^{\circ}$	$2\Theta < 35^{\circ}$
Max. momentum transfer Q	190 nm^{-1} (@ 22 keV)	67 nm^{-1}
	90 nm^{-1} (@ 10 keV)	-
Energy resolution ΔE	1.5 meV (@ 22 keV)	1.5 meV
	20 meV (@ 10 keV)	-
Analyzer arm radius	2 m	9 m
Scattering geometry	vertical	horizontal

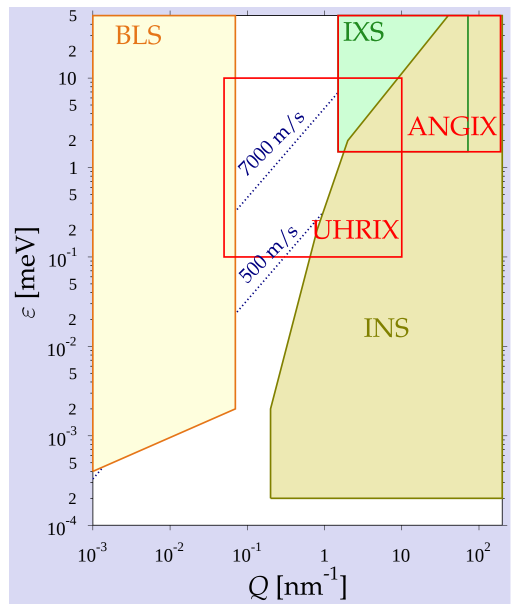

Figure 1: Existing techniques and proposed spectrometers mapped onto the energy ε and momentum transfer Q space.

Snapshots of the vibrational dynamics will be taken in glassy and disordered systems in the whole momentum and energy space. ANGIX will eventually supersede HERIX.

UHRIX (**U**ltra **H**igh **R**esolution **IX**S) will add the following unprecedented capabilities:

	UHRIX
Energy resolution ΔE	$0.1 - 0.3$ meV
Momentum resolution ΔQ	$0.01 - 0.1$ nm^{-1}
Momentum transfer Q	$\simeq 10 - 20$ nm^{-1}
Spectral function	extremely steep wings

It will allow IXS to enter an absolutely new dynamic region inaccessible today to IXS, inelastic neutron scattering (INS), and Brillouin light scattering (BLS). Studies of the visco-elastic crossover and other phenomena in glassy and disordered systems would become possible.

2. Scientific Case

Progress on many of the key problems in condensed matter physics is held back because current excitation probes are limited in both energy resolution and dynamic range. Instruments filling the gap between high and low frequency hypersonic techniques would allow critical experiments on a wide variety of important systems. Recent developments in IXS techniques allow a remarkable extension of the explored dynamic range to almost cover with a single spectrometer the whole transition from the collective, hydrodynamic regime to the single particle regime (Scopigno et al., 2000). However, presently such results cannot be achieved in a straightforward way. In fact existing spectrometers either do not cover the whole Q region of interest or they require rather lengthy changes in scattering geometry, incident energy and instrumental resolution. Another major limitation is their rather broad energy resolution ($\simeq 1.5$ meV) (Masciovecchio et al., 1996) which is particularly limiting at the lowest Q's. A decisive step forward requires the development of next generation spectrometers both covering a much wider angular range and having a higher resolution.

ANGIX would ideally allow measurement of the transition from *hydrodynamics* to *single particle* regimes within a single acquisition, while UHRIX would extend the probed Q range to bridge the gap existing with low Q spectroscopic techniques. In the following subsections we mention relevant examples of hot scientific topics which will considerably benefit from these improvements.

2.1 The high frequency dynamics of liquids and glasses

2.1.1 Low Q's

The relaxation dynamics in liquids and glass formers. The study of relaxation phenomena in simple fluids (Scopigno et al., 2002; Sinn et al., 2003) and glass-formers (Masciovecchio et al., 1998) is one of the outstanding topics in condensed matter physics. However, the high viscosity of glass formers and associated fluids makes relaxation processes rather slow. The Q region of structural relaxations in these systems ($0.1 - 1$ nm^{-1}) falls far beyond the window covered by existing spectrometers. This window will be ideally matched by the novel UHRIX spectrometer.

The origin of acoustic attenuation in glasses. One of the long-lasting and still open controversies on the dynamics of glasses is the physical origin of acoustic damping (Pilla et al., 2004). The key experiments to elucidate these phenomena are studies of the Q dependence of glasses spectra in a Q region bridging the gap between visible light and existing INS or IXS spectrometers. Moreover, the needed accuracy in the lineshape determination is extremely high and cannot be achieved by the present 1.5 meV resolution. Therefore, a spectrometer with $0.1 - 0.3$ meV resolution is required. The UHRIX spectrometer will be suited to fulfill these constraints.

2.1.2 Intermediate and high Q's

The onset of quantum deviations in the dynamics of simple fluids. The study of the transition between classical and quantum dynamical regimes in moderately quantum fluids still represents a challenge for spectroscopy (Cunsolo et al., 2003). At low Q, quantum effects are hardly discernible and show up only when Q become comparable with the inverse of the de Broglie wavelength, i.e. in the nm^{-1} range. A study of the whole Q-transition from the classical to the fully quantum regimes would be of prominent scientific interest, but is presently unfeasible since it would require a large dynamic range. This limitation will be overcame by the ANGIX spectrometer.

2.2 Phonons in crystals

The multi-analyzer ANGIX will allow concurrent measurements in a very broad Q range. This will make feasible measurements both, of the longitudinal phonon branches along main high symmetry directions in single crystals and of the transverse branches (acoustic and optical), due to a vast quantity of the off axis data available in "random" points of the Brillouin zone. Very accurate measurements of the phonon density of state in polycrystalline systems will be possible, as demonstrated by (Bosak and Krisch, 2003), with the best results achievable at very high Q's. An extension of the probed Q range is advantageous also due to the fact that phonon intensities increase as Q^2. Studies under extreme thermodynamic conditions, e.g., temperature and pressure, limited to samples and thus scattering volumes of small size, will also benefit from the high-throuput ANGIX.

2.3 Electronic excitations

Most current spectrometers probe either very low energy excitations ($\simeq 1$ meV) or the ones belonging to the $100 - 500$ meV range, but a gap still exists in the intermediate range. Many interesting questions exist in this energy range concerning strongly correlated electron systems, e.g. high temperature superconductors, which require the ability to probe the superconducting gap as a function of Q. However, the small scattering rate of most of the related excitations makes existing spectrometers inadequate. The high-throuput multi-analyzer ANGIX will solve this problem. The energy gap of the superconductors is $E \simeq 2\Delta$ or $0 < E < 80$ meV, which will be fully covered. In addition, a number of excitons (for example those in CdS, BaO, AgBr, AgCl) have binding energies of tens of meV, and therefore could be ideally investigated by this novel instrument. Further, charge density waves will also be detectable; they have energies in the $10 - 100$ meV window. In general since 10 meV $\simeq 100$ K, many physical topics involving electronic energies corresponding to hundreds of Kelvin can be investigated by ANGIX.

3. Technical Details of the Proposed Instruments

3.1 ANGIX: A Next Generation IXS Spectrometer

Multiplication of the analyzers by an order of magnitude or more is an evident way of increasing significantly the throughput of the IXS spectrometers and adding qualitatively new capabilities. However, it is not a trivial task in many respects. Integration of the position sensitive detectors (PSD) into IXS spectrometers solves many existing problems and opens up a path to the compact, mutianalyzer, wide scattering angle, high-resolution IXS spectrometers (Huotari et al., 2005). Application of the PSDs makes the spectrometer compact without worsening the energy resolution, makes possible the use of the vertical scattering geometry thus extending the Q-range, simplifies analyzer production, etc. The schematic of the proposed ANGIX spectrometer, with a static analyzer assembly covering a big scattering angle on an arc of a radius of 2 m and a strip detectors array on an arc of 15 cm, is shown in Fig. 2. The spectrometer will be placed either in the rebuilt C-station, or in a new D-station. The major R&D task is to build an array of $\simeq 150-180$ low noise, cryogenically cooled, Ge strip detectors with low crosstalks between the analyzers. However, addressing some more practical questions like analyzer alignment, handling the data stream, would also be crucial.

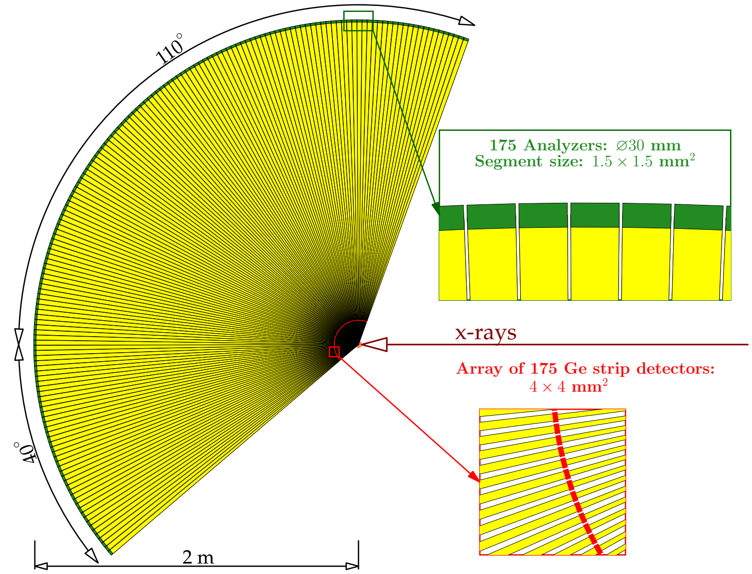

Figure 2: Schematic layout of ANGIX.

3.2 UHRIX: Ultra-High-Resolution IXS Spectrometer

To achieve sub-meV energy resolution (0.1 meV resolution seems to be feasible) and simultaneously to achieve very high Q-resolution ($0.01-0.1$ nm^{-1}), a new x-ray optics concept will be implemented with the UHRIX spectrometer. It is based on the principle of monochromatization and spectral analysis, which exploits the effect of angular dispersion in asymmetric Bragg diffraction (Shvyd'ko, 2004). One of its beneficial features is the use of x-rays with intermediate photon energy $E = 9$ keV, i.e. the energy where the existing undulators perform best. The spectrometer uses the angular-dispersive (CDW-type) monochromators and analyzers (Shvyd'ko, 2004; Shvyd'ko et al., 2006, 2007).

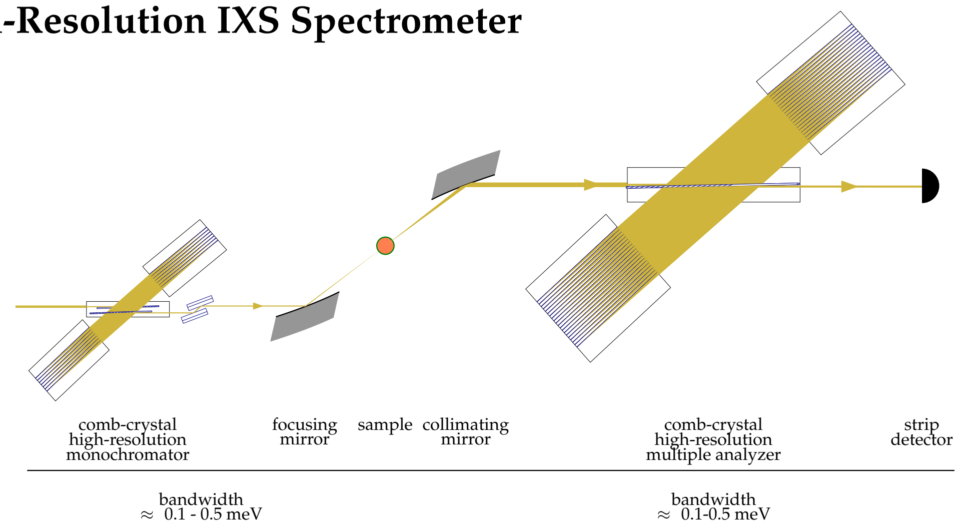

Figure 3: Optical scheme of UHRIX.

Figure 3 shows an optical scheme of UHRIX. The main components are the angular-dispersive CDDW in-line monochromator, the focusing mirror, the CDW backscattering segmented analyzer with a paraboloidal collimating mirror, and the position sensitive detector. The spectrometer is shown integrated into the IXS beamline together with other main beamline components: undulator, high-heat-load monochromator, etc. The spectrometer will be installed in station B, and will make use of the available space in the MERIX monochromator vacuum tank and focusing mirror.

The main technical challenges, which have to be addressed in R&D, are comb crystals, paraboloidal graded multilayer mirror, etc. The use of comb crystals will allow the spectrometer to be compact.

3.3 Extended Straight Section

We propose to extend the straight section to integrate a third 2.4 m long undulator. If available, we would like to have a 1.6 cm period superconducting undulator covering $17-25$ keV range in the first harmonic. The flux on the sample would increase by a factor of 2.5. If it would be not possible, we propose to install conventional 3.0 cm or shorter period device.

3.4 Other Improvements, Software

We propose to buy two MAR-6 CCDs cameras (each $\simeq$ \$300K) and relevant software for crystal orientation, which would be used with MERIX and HERIX/ANGIXS. CCD will also allow snapshots of $S(Q)$ for liquids and disordered systems especially under high pressure. Handling enormous data stream from the multi-analyzer ANGIX would require a major effort in software development. We propose to develop scientific IXS software, that would allow users to evaluate, interpret and predict spectra, including the spectra from random positions in the Brillouin zone.

4. Partnership and User Interest

The proposal was discussed with the beamline advisory group (BAG) members

Burns, Clement	Professor of Physics	Western Michigan University
Cai, Yong	Group Leader	Brookhaven National Laboratory
Hill, John (chair)	Division Director	Brookhaven National Laboratory
Farber, Daniel	Group Leader	Lawrence Livermore National Laboratory
Larson, Bennett	Corporate Fellow	Oak Ridge National Laboratory
Sinn, Harald	Group Leader	DESY/XFEL

who are simultaneously the core beamline users. The BAG members have endorsed the proposal.

5. Estimated Budget and Effort

ANGIX						
	Year 1	Year 2	Year 3	Year 4	Year 5	Total
M&S	$150K	$100K	$100K	$100K	$50K	$500K
Capital	$700K	$800K	$1100K	$600K	$100K	$3300
Total	**$850K**	**$900K**	**$1200K**	**$700K**	**$150K**	**$3800K**
UHRIX						
	Year 1	Year 2	Year 3	Year 4	Year 5	Total
M&S	$150K	$100K	$100K	$50K	$50K	$450K
Capital	$450K	$900K	$700K	$250K	$50K	$2350
Total	**$600K**	**$1000K**	**$800K**	**$300K**	**$100K**	**$2800K**
SCU and other beamline improvements						
	Year 1	Year 2	Year 3	Year 4	Year 5	Total
M&S	$50K	$50K	$50K	$50K	$50K	$250K
Capital	$300K	$700K	$2000K	$50K	$50K	$3100
Total	**$350K**	**$750K**	**$2050K**	**$100K**	**$100K**	**$3350K**
All Projects Total	**$1800K**	**$2650K**	**$4050K**	**$1100K**	**$350K**	**$9950K**

Effort: R&D, commissioning, and operation of ANGIX and UHRIX would require at least one additional scientist position per instrument For ANGIX to be fully realized a position for the development of the scientific IXS software would be required. **Total:** 3 scientist positions are required, which could be partly post-doc positions initially.

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With contributions of: *Clement Burns, Yong Cai, Alessandro Cunsolo, Roger Dejus, John Hill, Daniel Farber, Yury Ivanyushenkov, Ben Larson, Ayman Said, Yuri Shvyd'ko, Harald Sinn, Mary Upton*

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