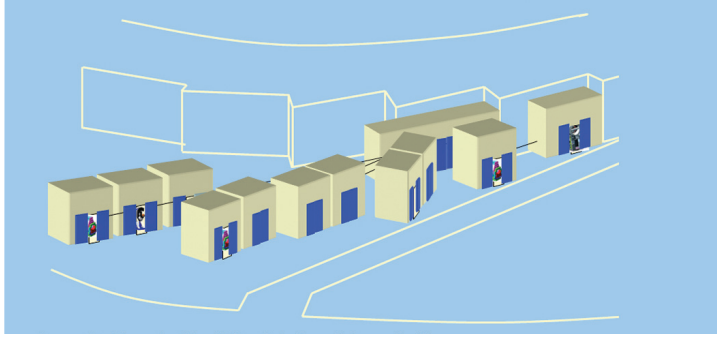
4.4 BEAMLINES FOR INTERFACES IN COMPLEX SYSTEMS

X-RAY INTERFACIAL SCIENCE FACILITY

Interfacial science by its very nature brings together a diverse community with interests in catalysis, biomembranes, oxide film growth, semiconductors, geochemistry, surface physics, corrosion, nano-science, tribology, and electrochemistry. With close involvement of external users (through a Collaborative Development Team) we plan to build an innovative, dedicated X-ray Interfacial Science (XIS) facility (fig. 4.4.1) at a sector of the APS that will fully exploit the unique capabilities of the APS to advance our understanding of interfacial science. The XIS facility will provide state-of-the-art X-ray scattering, spectroscopy, and microscopy tools for multi-length-scale (from angstroms to microns), element-specific studies of vacuum/solid, gas/solid, liquid/solid, solid/solid interfaces and supported nanostructures. The proposed facility has two optimized, canted undulators producing four separate x-ray beams: one with variable-energy and three with selectable fixed energies. In addition, the bend magnet port will be developed to support those measurements that do not require the brightness of the ID beam lines. The tandem experimental hutch arrangement includes both general-purpose diffractometers and custom-designed spectrometers to provide an *in-situ* controlled environment accomodating growth chambers for various advanced materials synthesis activities involving molecular-beam epitaxy (MBE), metal-organic chemical vapor deposition (MOCVD), atomic-layer deposition (ALD), and pulsed-laser deposition (PLD), as well as a dedicated state-of-the-art interfacial X-ray microscopy spectrometer. Laboratory preparation and advanced off-line characterization facilities such as scanning tunneling microscopy (STM) and atomic force microscopy (AFM) are recognized as an important component of the XIS facility.

Fig. 4.4.1. *Conceptual layout of the X-Ray Interfacial Science facility.*



HIGH-ENERGY BEAMLINES

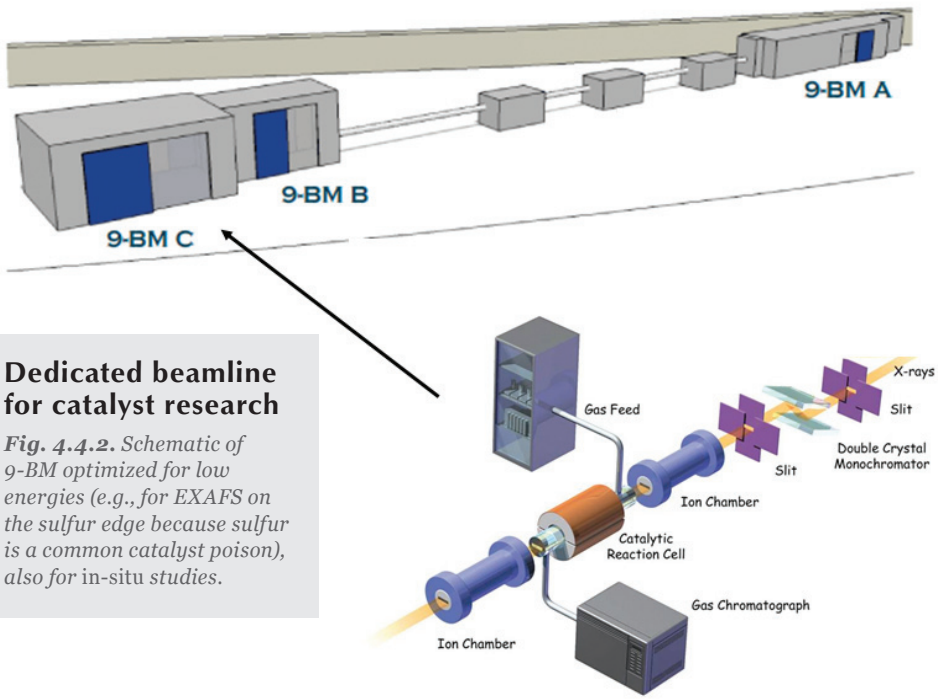
Our existing 1-ID beamline, the only beamline in the western hemisphere with energy tunability and high brilliance for photons in the range of 50-120 keV, is heavily oversubscribed for experiments in the areas of high-energy diffraction microscopy (HEDM), mechanical measurement of aggregate materials (i.e., stress, strain, texture), and microfocusing pair distribution function (PDF) measurements. We plan to replace the current monochromatic station with two larger white-beam capable stations and add a side branch beamline that can be used simultaneously with the main beamline. With this upgrade, the experimental instruments will be given dedicated space and, consequently, be optimized for significantly improved performance. We propose to develop a superconducting undulator (section 6.2) that will increase brilliance over one order of magnitude and to add improved optics and state-of-the-art area detectors. With the planned new configuration, both performance (100x) and capacity will be greatly improved because we obviate the need for moving and aligning key instruments. Upgrades are also planned for the high-resolution diffraction microscopy beamline at 34-ID-C, where a dedicated optimized undulator (at present one versatile undulator A serves two stations at 34-ID) and enhanced optics and detectors will improve the flux in a nano-focused spot and extend the mapping of strains to higher spatial resolution and greater

speed (allowing time-dependent measurements). 34-ID is complementary to 1-ID and has pioneered the technique of polychromatic micro-focusing (now nano-focusing) for mapping phases and the strain tensor at the nano-level. Software and computing infrastructure are recognized as an essential component of the 1-ID and 34ID-C beamline upgrades, because the analysis of complex HEDM data is a major barrier to expansion of the technique.

There is increasing demand for PDF data especially for nanocrystalline samples. PDF's must be taken at high-energies where the Q-range is suitably large. We plan to upgrade PDF capabilities at Sectors 11-ID and 1-ID.

CATALYSIS CAPABILITIES

The recommendations of a major user workshop on catalysis held at APS in 2005 were that we needed to establish a dedicated spectroscopy beamline on a bending magnet for *in-situ* catalysis studies and to make many other beamlines with other techniques available with expert assistance and a suite of mobile experimental equipment. Beamline 9-BM has been chosen as a focal point for catalyst research and will be upgraded for concurrent XAFS and x-ray diffraction on operating catalysts (fig. 4.4.2). XAFS and XANES techniques provide *in-situ* element-specific atomic-level chemical and geometric information on the structure of real working catalysts (both heterogeneous and homogeneous). *In-situ* synchrotron X-ray powder diffraction (SXRPD) is invaluable for structural analysis of catalytic materials. This central facility will complement other unique capabilities at the APS that will be applied to catalyst research, including techniques such as small angle scattering, PDF measurements, and inelastic x-ray scattering. A major component of this activity is to provide the nucleus of expertise and capabilities (such as sample cells) that can be transferred for use at these other beamlines and establish "CatSynch" as a gateway to facilitate this area of research.



Dedicated beamline for catalyst research

Fig. 4.4.2. *Schematic of 9-BM optimized for low energies (e.g., for EXAFS on the sulfur edge because sulfur is a common catalyst poison), also for* in-situ *studies.*