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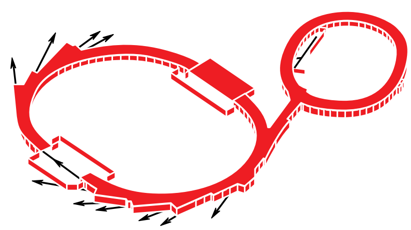
MOLECULAR ENVIRONMENTAL SCIENCE AND SYNCHROTRON RADIATION FACILITIES

An Update of the 1995 DOE-Airlie Report on Molecular Environmental Science

Workshop held at the Stanford Synchrotron Radiation Laboratory
Stanford, CA

January 17-18, 1997



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I. Introduction

This workshop was requested by Dr. Robert Marianelli, Director of the DOE-BES Chemical Sciences Division, to update the findings of the Workshop on Molecular Environmental Sciences (MES) held at Airlie, VA, in July 1995. The Airlie Workshop Report defined the new interdisciplinary field referred to as *Molecular Environmental Science* (MES), reviewed the synchrotron radiation methods used in MES research, assessed the adequacy of synchrotron radiation facilities for research in this field, and summarized the beam time requirements of MES users based on a national MES user survey.

The objectives of MES research are to provide information on the chemical and physical forms (speciation), spatial distribution, and reactivity of contaminants in natural materials and man-made waste forms, and to develop a fundamental understanding of the complex molecular-scale environmental processes, both chemical and biological, that affect the stability, transformations, mobility, and toxicity of contaminant species. These objectives require parallel studies of "real" environmental samples, which are complicated multi-phase mixtures with chemical and physical heterogeneities, and of simplified model systems in which variables can be controlled and fundamental processes can be examined. Only by this combination of approaches can a basic understanding of environmental processes at the molecular-scale be achieved.

Because chemical reactions at the surfaces of natural solids play dominant roles in many environmental processes, molecular-scale studies of contaminant reactions at interfaces (solid-liquid, solid-gas, liquid-gas) have become an important focus of MES research. Most environmental processes involve aqueous solutions, which complicate experimental studies at the molecular scale, especially those using ultra-high vacuum methods. In addition, contaminants are often present at low concentrations (which precludes the use of nuclear magnetic resonance spectroscopy), and mixtures of contaminant elements in environmental samples are common. Because of these complicating factors, high intensity, tunable synchrotron light sources are often uniquely suited for molecular-scale studies of environmental materials and processes.

During the past two years, new synchrotron radiation facilities for MES research have been planned, are under construction, or are in the commissioning stage. Also, the MES user base has continued to grow, with scientists who are new to synchrotron radiation research entering the field and other scientists who are familiar with synchrotron radiation sources redirecting their research to MES. These changes have raised several very important ES&H and user support issues, as well as issues about the adequacy of synchrotron radiation facilities required for MES research. With these issues in mind, the SSRL workshop was organized with the following objectives: (1) to evaluate the adequacy of existing or planned facilities for MES research, (2) to review MES user bases at US-DOE synchrotron radiation facilities (are they shrinking, at a steady state, or growing?), and (3) to recommend needed facilities and operations/user support after a careful assessment of existing facilities and those under construction.

II. Workshop Organization

The workshop was held at SSRL and was convened by Gordon Brown (Stanford University and SSRL). The directors and/or deputy directors of the ALS, APS, NSLS, and SSRL were consulted about appropriate workshop representatives from their facilities, and these representatives were invited. Also invited were scientists experienced in the each of the synchrotron methods that are currently being used or are likely to be used in MES research in the near future. The letter of invitation, including the charge to workshop participants, is included in Appendix A. The synchrotron methods considered at the workshop included (1) x-ray absorption fine structure (XAFS) spectroscopy; (2) hard x-ray microprobe analysis, microspectroscopy, and imaging; (3) soft x-ray/VUV/IR spectromicroscopy; and (4) surface-sensitive methods, including x-ray standing wave (XSW), surface x-ray scattering, photoelectron diffraction (PED), and photoemission spectroscopy (PES). The need for ES&H and operations support was also considered by a separate working group. The workshop was organized around the following five working groups, with participants listed in brackets:

(1) Hard X-ray XAFS Spectroscopy and X-ray Scattering Working Group [John Bargar (SSRL), Gordon Brown (Stanford University & SSRL), Steven Conradson (LANL), Britt Hedman (SSRL), Dale Sayers (North Carolina State University)]

(2) Hard X-ray Microprobe Analysis, Microspectroscopy, and Imaging Working Group [Paul Bertsch (Savannah River Ecology Laboratory), Mark Rivers (Consortium for Advanced Radiation Sources, University of Chicago), Tetsu Tokunaga (LBNL)]

(3) Soft X-ray/IR Microscopy-Spectroscopy Working Group [Larry Carr (NSLS), Erik Johnson (NSLS), Satish Myneni (LBNL), David Shuh (LBNL)]

(4) Surface-Sensitive Methods Working Group [Gordon Brown (Stanford University & SSRL), Tom Rabedeau (SSRL), Neville Smith (ALS)]

(5) ES&H/Operations Working Group [David Clark (LANL), Ian Evans (SSRL), Lynda Soderholm (ANL), Ray Stults (PNNL)]

The workshop began with a review of findings of the 1995 Airlie Workshop (see Appendix B) and the charge to participants, followed by short presentations by each workshop participant. The first group of presentations focused on facilities at each of the four synchrotron radiation sources. The second group of presentations was on research results representative of each of the synchrotron radiation methods useful in MES research. The third group of presentations focused on ES&H and operations issues. These presentations were followed by breakout sessions in which each working group discussed facilities, user bases, and operations/ES&H support and began writing a summary of findings. Each group was asked to include the following information in their reports:

1. Activity level of the science
2. Assessment of user bases (including numbers and types of users)
3. Inventory of existing facilities in each synchrotron radiation method area
4. Inventory of planned facilities, the new capabilities they will provide, and their funding sources
5. Recommendations for new facilities in each methods area (justification was based on scientific need and anticipated or proven user demand)
6. Assessment of operations/user support needs for each existing, planned, and recommended beamline facility.

The second day of the workshop began with presentations of findings and recommendations by each working group followed by a discussion in which all workshop participants took part. The workshop agenda and the names and addresses of all workshop participants are included as Appendices C and D.

III. Major Findings of the SSRL Workshop

1. The use of synchrotron radiation methods in MES research has led to significant scientific contributions and improved understanding of environmental processes at the molecular level, and new constraints on remediation technologies, including the following:

- ***XAFS studies of the speciation of contaminant ions at low concentrations in heterogeneous solids*** - have revealed that surface-bound species are very important in natural samples and that multiple elemental species are often present in environmental samples. XAFS spectroscopy, in combination with other analytical methods, is providing the first direct speciation information on many contaminants (including the actinides) in environmentally relevant solutions, solids, and multi-phase mixtures, as well as the scientific basis for improved remediation technologies.
- ***XAFS characterization of uranyl species in tank wastes and contaminated soils*** - has led to the discovery of an insoluble uranyl phosphate phase in tank wastes and in contaminated soils from Fernald, Ohio, that is not removed by standard carbonate washing methods. This discovery could potentially result in substantial cost savings in the clean-up effort at DOE U-processing and temporary waste storage facilities.
- ***Hard x-ray microspectroscopy studies of heterogeneous environmental samples*** - are providing the first detailed information on the spatial distribution (at a few micron resolution) of different species of a given element in environmental samples. Such information is important in designing remediation technologies and in defining the distribution of important contaminant reactions and concentrations in heterogeneous soils, plants, and animals.
- ***Conventional and grazing-incidence XAFS studies of chemical interactions of aqueous metal ions at metal oxide surfaces in situ (i.e., with an aqueous solution in contact with the surface)*** - have provided the first detailed structural and chemical information on chemisorption reaction products, including the reaction rates of sorbed species and their mode of bonding at solid-aqueous solution interfaces. They have also provided some of the first information on reactive sites on metal-oxide surfaces.

- ***XAFS studies of contaminant speciation in living materials (plant and animal tissue)*** - have revealed that transformations of highly toxic chromate and selenate ions occur in the cytoplasm and nuclei, respectively, of certain plants. These types of studies are providing some of the first molecular-scale information on phytoremediation processes, which are becoming increasingly important in removing toxic elements from contaminated waters.
- ***Characterization studies of contaminant ions in waste forms (glasses, ceramics, and cements)*** - have shown that Tc can be reduced from the toxic and mobile Tc(VII) species to the less toxic and less mobile Tc(IV) species by adding iron- and sodium-sulfides to cement waste forms. These types of studies, which have used XAFS and several other complementary synchrotron radiation methods, are providing the fundamental speciation information necessary to evaluate the suitability of particular waste forms and to improve waste-form processing. The potential cost savings are enormous.
- ***Hard-x-ray x-ray standing wave (XSW) studies of the diffuse double layer above metal oxide surfaces*** - have provided the first direct information about the distribution of metal ions in solution above the α-Al_2O_3 surface as a function of solution pH and ionic strength. These results provide the first experimental check of the Gouy-Chapman model of the diffuse double layer, which is the basis for most models of surface complexation used in predicting the transport of contaminant species in soil-sediment-water systems.
- ***Crystal truncation rod x-ray scattering studies of contaminant ions on metal carbonate surfaces*** - have shown that cations like Pb(II) substitute for Ca(II) in the surface layer of carbonates, which are very common phases in the environment.
- ***Imaging of humic substances using soft x-ray/VUV spectromicroscopy*** - has provided the first detailed images (at 30 nm resolution) of the shape and changes in shape of these high molecular weight materials as a function of solution conditions. C K-edge microscopy is also revealing some of the first detailed information on surface functional groups on these very common environmental organic substances that sorb metal-ion contaminants.
- ***Photoemission studies of model metal-oxide surfaces and adsorbate interactions*** - has led to a deeper understanding of the reactions of water and aqueous metal-ion species with oxide surfaces, which are among the most important reactions in natural systems.
- ***Metal ion speciation at high spatial resolution using L-edges of first-row transition elements and K-edges of second-row elements*** - has revealed changes in Mn speciation on Mn-oxide surfaces caused by Mn-reducing bacteria. This finding has important implications for changes in the redox capacity of natural Mn-oxides, which are ubiquitous and can oxidize or reduce important contaminant species in soils.
- ***Soft x-ray/VUV x-ray standing wave (XSW) studies of metal oxide surfaces*** - have provided element-specific information on relaxation/reconstruction of metal oxide surfaces before and after reactions with water and other adsorbates. Few other surface-sensitive methods can provide element-specific structural information on surfaces.
- ***Soft x-ray/VUV photoelectron diffraction studies of metal oxide surfaces*** - have shown that surface reconstruction of epitaxially grown α-Fe_2O_3 (0001) is insignificant. The surfaces of iron oxides are very important in adsorption reactions in soils and sediments and their structures have been difficult to determine by other methods.
- ***Synchrotron infrared spectromicroscopy studies of organic and metal ion adsorbates on environmental particles*** - have the potential of providing structural and speciation information on adsorbates at much lower concentration levels than is possible in laboratory-based FTIR studies.

2. Growth of MES user demand for synchrotron beam time has doubled at NSLS and SSRL and has almost tripled at the ALS during the past 1.5 years, based on the number of proposals submitted for beamtime. The rate of growth in MES demand is roughly twice that estimated from the 1995 MES user survey (see 1995 Airlie Workshop Report). MES research is one of the two fastest growing areas at U.S. synchrotron radiation laboratories, the other being structural molecular biology.

3. Because of the complexity of environmental processes, studies of "real" environmental samples should be coupled with studies of simplified model systems in which variables can be controlled.

4. XAFS spectroscopy continues to be the main synchrotron-based method used by MES researchers to determine the molecular-scale speciation of metal-ion contaminants in environmental samples and to characterize reaction products at solid-aqueous solution interfaces.

5. Synchrotron beamlines with higher fluxes are needed to extend XAFS studies of contaminant speciation and interface reaction products down to the low concentration ranges (parts per billion) found in natural samples.

6. Because of the spatial (micron-level) and species heterogeneity of metal-ion contaminants in environmental samples, micro-XAFS spectroscopy has become an increasingly important technique in MES research during the past two years. Higher brightness is the limiting factor in these studies.

7. When new hard x-ray beamlines at the APS (BESSRC-CAT, GSECARS-CAT, MR-CAT, PNC-CAT) and SSRL (BL-11) become available to general users in 1998 and 1999, the number of such beamlines available for MES research, including existing beamlines at NSLS and SSRL, should satisfy the hard x-ray demand by MES users through 2002, which is estimated to be on the order of 1600 station days/year in 1999 on the basis of a national user survey that estimated the growth in demand of MES synchrotron users (see 1995 Airlie Report). There will be a continuing need for new experimental equipment on these beamlines, however, as new technologies become available (*e.g.*, new detectors).

8. There is a significant shortage, relative to demand, of soft x-ray/VUV beamlines optimized for MES research at the four DOE synchrotron radiation laboratories.

9. Soft x-ray/VUV spectromicroscopy is emerging as one of the primary means of characterizing environmental samples, including the types and distributions of functional groups on humic and fulvic substances, which play very important roles in environmental chemistry. Soft x-ray microscopy is also providing unique information on the macromolecular structures of these high molecular weight materials and on the distribution of contaminant species in plant and animal tissues. We view soft x-ray/VUV spectromicroscopy as a major growth area for MES research.

10. Surface-sensitive synchrotron methods, including photoemission spectroscopy, x-ray emission spectroscopy, x-ray standing wave methods, surface scattering, and photoelectron diffraction, are important soft x-ray/VUV methods that are beginning to provide a fundamental understanding of chemical reactions at environmental interfaces involving solids and aqueous solutions. The use of differential pumping will allow novel soft x-ray/VUV studies of "wet" environmental samples as well as more fundamental studies of simplified model systems. This combination of soft x-ray/VUV synchrotron methods applied to environmental interfaces is another important growth area for MES synchrotron research.

11. We strongly recommend the construction of a new soft x-ray/VUV branch beamline for MES research at the ALS with two undulator insertion devices arranged in chicane fashion, which will allow independent operation. One source should be optimized for spectromicroscopy studies of environmental samples, and one for x-ray emission spectroscopy studies of chemisorption reactions on model metal oxide and sulfide surfaces. A strong case can also be made for a 1-3 keV beamline for soft x-ray spectroscopy studies of environmental samples. This energy region contains the K-edges of the second-row elements, which are of great importance in the environmental and/or life sciences. These recommendations were developed at a separate MES workshop at the ALS held in March 1997 and are described in more detail in the attached white paper on MES research opportunities at the ALS (see Appendix E). There are many opportunities for cutting-edge MES research in the soft x-ray/VUV energy region (50 eV to 4 keV). However, existing soft x-ray/VUV beamlines at the ALS are heavily subscribed by other scientific communities and are poorly optimized for MES studies. In addition, existing soft x-ray/VUV beamlines at the NSLS and SSRL have lower brightness, thus are not optimized for high spatial resolution, element-specific spectromicroscopy studies of environmental samples.

12. Following the completion of five IR spectroscopy/microscopy beamlines at the NSLS and one IR beamline at the ALS in 1998, no additional IR beamlines are likely to be needed within the next five years for MES research. We strongly recommend that one or more user workshops be held on IR spectromicroscopy at the NSLS and/or the ALS to introduce new users to this method and to assess the interest level of MES users.

13. User support was identified as one of the major needs at MES beamline facilities. Many of the new MES users have little or no experience in synchrotron radiation methods. More experienced MES synchrotron radiation users typically have relatively small research groups and have limited technical knowledge about detectors and beam line optics, so they cannot operate independently at synchrotron sources. Thus technical support is essential if the existing, new, and planned beamline facilities are to be used efficiently by MES users. Efficient use of synchrotron beamtime is considered to be a significant problem at the four DOE synchrotron radiation laboratories. This situation could be improved by implementing this recommendation.

14. Because environmental samples are often toxic or contain radioactive elements, there are special ES&H issues associated with studies of these samples at synchrotron radiation facilities. Specially trained ES&H specialists and sample containment facilities are needed at each of the synchrotron laboratories that study significant numbers of environmental samples.

IV. SYNCHROTRON FACILITIES REPORTS

A. Advanced Light Source (LBNL)

The ALS is a 1.5-1.9 GeV third-generation source optimized for extremely high brightness in the soft x-ray/VUV region (50 eV- 4 keV). This energy range contains the K-edges of the first- and second-row elements, K, Ca, and the L-edges of the first-row transition elements, which includes most of the elements important in the life sciences and those that make up the majority of environmental materials. There are 11 operating beamlines and 8 under construction at the ALS. At the time of the Airlie Workshop, there was about 0.2 of a full time beamline in use for MES-related work distributed over BL 10.3.1 (x-ray microprobe), BL 6.1.2 (zone-plate microscope), and BL 7.0.1 (spectromicroscopy of actinides). This activity has since expanded to about 0.43 of a full time beamline distributed over six beamlines. Of the most recent batch of independent-investigator proposals, 13 out of 78 proposals (17%) are MES-related, with 5 requesting time on BL 10.3.1 and 8 requesting time on soft x-ray/VUV beamlines and roughly an even distribution over the techniques of zone-plate microscopy, photoemission spectroscopy, NEXAFS (Near-Edge

XAFS) spectroscopy, and photoelectron diffraction. Table 1 presents data on ALS beamlines that are currently being used in MES research, including estimates of MES user time, independent investigator (II) time, and general availability of each beamline. Table 2 contains the same information on ALS beamlines that could be used for MES research but are not currently being used for this purpose, and Table 3 provides information on new or planned beamlines at the ALS.

Table 1. Operating ALS Beamlines with Active MES Programs

ALS Beamline	II%	MES%	Availability*
BL 6.1.2	25%	10%	fully-subscribed
BL 6.3.2	25%	5%	over-subscribed
BL 7.0.1 & 7.0.2	40%	10%	very over-subscribed
BL 9.0.1, 9.0.2.1., & 9.0.2.2	6%	0%	very over-subscribed
BL 9.3.1	25%	2.5%	fully-subscribed
BL 9.3.2	25%	5%	very over-subscribed
BL 10.3.1	25%	10%	fully-subscribed

*fully-subscribed = 100% usage; over-subscribed = equivalent of 100-150% usage; very over-subscribed = equivalent of 150-200% usage; subscription rates are determined by the number of proposals received divided by the number that are awarded beamtime

Techniques having high spatial resolution represent a mainstream development activity at the ALS, and can be categorized into microprobes, imaging microscopes, and scanning microscopes. The existing x-ray microprobes have relatively modest spatial resolution of one micron to a few tens of microns. The next generation of microscopes should eventually be able to reach 20 nm or better. Since the Airlie Workshop, the blood-cell work by McGowan et al. on BL 6.1.2 has become much more detailed, demonstrating the power of this microscopy beamline for looking at biological samples in their natural aqueous environment.

Table 2. Operating ALS Beamlines That Could Be Used For MES Research

ALS Beamline	II%	MES%	Availability
BL7.3.1.1 & 7.3.1.2	0%	0%	under commissioning, full PRT usage (Intel)
BL 8.0*	25%	10%	fully-subscribed

* 25% independent investigator beamtime will become available in June '98, with 10% of the BL slated for MES research. Over-subscription is anticipated.

Table 3. New/Planned ALS Beamlines That Could Be Used For MES Research

ALS Beamline	II%	MES%	Availability
BL 1.4*	100%	?%	subscription unknown completed FY98
BL 4.0.1, 4.0.2**	0%	0%	over-subscribed completed FY99
BL 4.0.3, 4.0.4	0%	0%	over-subscribed completed FY98
BL 7.3.3***	25%	0%	under construction completed FY97

* Infra-red independent investigator user facility, funded by ALS.
** Magnetic microscopy/spectroscopy beamline. No MES usage envisioned due to over-demand by magnetics community.
*** Microdiffraction beamline (4-12 keV); significant potential use by MES community.

Preliminary studies of Mn-reducing bacteria by Tonner and Nealson on BL 6.1.2 and BL 7.0.1 demonstrate the power of "spectromicroscopy" (i.e., the combination of microscopy with spectroscopy); the Mn L-edge fingerprint spectra are particularly rich in structure. These instruments have drawbacks, however. BL 6.1.2 is on a bend magnet, thus does not enjoy the power of an undulator. BL 7.0.1 is on an undulator, but the monochromator has been designed for very high energy resolution, far beyond that needed in spectromicroscopy, which reduces usable flux. There is, therefore, a pressing need for a dedicated spectromicroscopy beamline that does not make these compromises. Such a line would be ideal for MES work.

A summary of ALS beamlines in operation, under construction, or planned and their current or anticipated uses is given below. Because an important issue addressed in this report is the need for additional high-brightness beamlines devoted to MES research in the soft x-ray/VUV energy region, more details are provided on ALS beamline facilities than for other SR facilities.

Operating ALS beamlines:

BL 5.0.2: Wiggler beamline for multiple-wavelength (MAD) protein crystallography. The energy range is 3.5-14 keV.

BL 6.1.2: Bend-magnet line for biomicroscopy using a zone-plate full-field imaging soft x-ray/VUV transmission microscope. The energy range is 250-600 eV using wavelength dependence of the zone-plate focal length. It has no other monochromator, so the x-ray spectroscopy capability is limited. Approximately 10% of the time on this beamline is used for MES research.

BL 6.3.2: Bend-magnet beamline equipped with a spherical grating monochromator. The energy range is 50-1000 eV, and it is used for softx-ray/VUV XAFS spectroscopy, XPS, and PED. Approximately 5% of the time on this beamline is used for MES research.

BL 7.0.1 & 7.0.2: Undulator branch beamline equipped with a spherical grating monochromator. The energy range is 60-1000 eV. It is used for spectromicroscopy, zone-plate scanning transmission x-ray microscope (STXM), zone-plate scanning photoemission microscope (SPEM), full-field imaging photoelectron emission microscope (PEEM), XPS, micro-XPS, PED, and soft x-ray emission spectroscopy (SXES). Approximately 10% of the time on this beamline is used for MES research.

BL 7.3.1.1 & 7.3.1.2: Bend-magnet branch beamline for materials/surface science with micro-x-ray photoelectron spectroscopy (Intel Corp.) and XAFS applications. The energy range is 260-1500 eV.

BL 8.0: Undulator beamline with a spherical grating monochromator. The energy range is 60-1000 eV. This beamline is used for soft x-ray emission spectroscopy, XAFS spectroscopy, XPS, and PED. This is a PRT beamline with no time available for independent investigators until 1998.

BL 9.0.1, 9.0.2.1, & 9.0.2.2: Undulator branch beamline with a spherical grating monochromator. The energy range is 20-310 eV. PRT usage is dominated by chemical dynamics studies on BL 9.0.2.1 and by gas-phase photoemission and absorption studies on BL 9.0.1. No time is available for MES research except within existing PRT efforts.

BL 9.3.1: Bend-magnet beamline with a double-crystal monochromator. The energy range is 700 eV to 6 keV. This beamline is used for SEXAFS, XAFS, and x-ray standing wave measurements. 2.5% of this beamline is available for MES research.

BL 9.3.2: Bend-magnet beamline equipped with a spherical grating monochromator. The energy range is 30-1500 eV. It is used for XPS, PED, soft x-ray/VUV XAFS spectroscopy. Used approximately 5% for MES.

BL 10.3.1 & 10.3.2: Bend-magnet branch beamline with the bandpass centered at 10 keV. They are used for hard x-ray fluorescence microprobe studies (10.3.1) and micro-machining (LIGA) (10.3.2). Approximately 10% of the time on BL 10.3.1 is used for MES research.

BL 12.0: Undulator beamline with an energy range of 30-300 eV. It is used for extended UV studies (lithography, surface and materials science applications, and optics development). No time is available for MES research.

ALS beamlines under construction:

BL 1.4: Bend-magnet beamline for infrared spectromicroscopy; completion in 1998. Energy range is 0.05 to 1.0 eV.

BL 4.0.1 & 4.0.2: Elliptically polarizing undulator (EPU) beamline with an energy range of 20-1800 eV. Anticipated uses are spectroscopies needing circularly polarized soft x-rays. Usage will focus on magnetic spectroscopy.

BL 4.0.3 & 4.0.4: Elliptically polarizing undulator (EPU) beamline with an energy range of 20-1800 eV. Anticipated uses are microscopies needing circularly polarized soft x-rays. Usage will focus on magnetic microscopy.

BL 5.0.1: Wiggler beamline for monochromatic protein crystallography. The energy range is 7-14 keV.

BL 6.3.1: Bend-magnet beamline for calibration, standards, EUV/soft x-ray optics testing, and solid state chemistry. The energy range is 500-2000 eV. Intel will be a major user of this BL.

BL 7.3.3: Bend-magnet beamline under construction. The energy range will be 3-12 keV and is optimized for 6 keV. Its primary use will be for microdiffraction. Usage will be dominated by the microelectronics industry.

BL 10.0.1: Undulator beamline for high energy resolution atomic, molecular, and optical physics, and photoemission studies of highly correlated materials. No time available for MES research. The energy range is 20-310 eV.

BL 11.3: Bend-magnet beamline for deep-etch lithography (LIGA), covering an energy range of 3-12 keV, and for scanning transmission x-ray microscopy (STXM) over the energy range 260-750 eV.

B. Advanced Photon Source (ANL)

The APS is now in operation. The storage ring is providing user beam approximately 50% of the time, with operations periods of 3-4 weeks, separated by shutdowns of about the same length. The ring is operating at its design current and lifetime. The vertical emittance of the ring has been reduced by a factor of 4 from the values in Table 7.1 of the Airlie Report, by reducing the value of the coupling from 10% to about 2.5%. This has increased the brilliance of the source by a factor of 4 over that shown in Figure 7.2 of the Airlie Workshop Report.

The users now have complete control of undulators during operations, including changing the gap and taper under computer control at any time. This has important implications for XAFS techniques which are very important in MES research. It is now possible to either taper the gap to broaden the undulator peaks sufficiently to perform XAFS (with reduced brilliance), or to scan the undulator in synchrony with the monochromator to perform XAFS at the full brilliance of the undulator. It is clear that high quality XAFS research can be performed in either mode.

There are now 4 CATS whose scientific plans include MES research, with MR-CAT having been added to this list since the Airlie Report. The plans and funding of these CATS for MES research have in several cases changed significantly since the Airlie Report. In addition, the DOE Scientific Facilities Initiative has funded a facility to assist users with handling radioactive materials through the ANL Chemistry Division.

GeoSoilEnviroCARS (GSECARS-CAT)

The GSECARS sector (#13) began running early experiments on the bending magnet in December, 1996, and on the undulator in February, 1997. These experiments are being conducted in the first-optics enclosures, pending commissioning of the beamline transport and shielding verification on the experimental stations. The first two-week run on the undulator has proven that undulator tapering and scanning will work well for XAFS spectroscopy. The first microspectroscopy studies with the undulator, a water-cooled monochromator, and Kirkpatrick-Baez mirrors were begun in April, 1997.

Since the Airlie Workshop, GSECARS has received funding from DOE's Scientific Facilities Initiative for a dedicated microspectroscopy instrument on the undulator beamline. This microspectroscopy facility will be equipped with Kirkpatrick-Baez mirrors capable of 1-2 micron beam sizes, a multi-element Ge detector, and a wavelength dispersive spectrometer. This facility will be a very important part of the GSECARS instrumentation for MES research.

In addition to the microspectroscopy facility, GSECARS facilities for MES research will include an XRF microprobe (usable on both the bending magnet and undulator beamlines) and microtomography instrumentation on the bending magnet beamline. It will also include facilities for powder and single crystal diffraction on both the bending magnet and undulator beamlines. There will be two stations on the bending magnet, each capable of operating 100% of the time. The two stations on the undulator can run simultaneously when a fixed-energy diffraction experiment is being done in the upstream station and the high-pressure users don't need to change the undulator gap. For other types of experiments on the undulator, the two stations will share beam time.

GSECARS will be operated as a national user facility for scientists in the earth, soil, and environmental sciences. In the mature phase of the sector, more than 65% of the beam time will be available to this community on a peer-reviewed proposal basis. There will be no specific set-aside proportion of this time for MES research. However, approximately 25-30% of the proposed science on each beamline is expected to be MES research, including imaging, bulk sample XAFS on the bending magnet, micro-XAFS on the undulator, microtomography, and diffraction. There will thus be a total of approximately one full-time station equivalent for MES research on the GSECARS-CAT sector.

Pacific Northwest CAT (PNC-CAT)

The PNC-CAT is building an insertion device (ID) and bending magnet (BM) beamline at sector 20 at the APS. Both lines will have microfocusing, XAFS spectroscopy, and diffraction capabilities which can be applied to MES studies. Since the Airlie Report, significant funding has been received from DOE through the EMSP initiative which will permit construction of the bending magnet beamline and surface-science facilities.

Focusing will be provided by toroidal mirrors (to 200 microns), Kirkpatrick-Baez mirrors (5-10 microns), and tapered capillary x-ray concentrators (sub-micron on the ID line and 1-3 microns on the BM line). The ID line will also include a dedicated UHV surface science chamber capable of surface XAFS, diffraction, and standing wave studies. A smaller UHV surface XAFS chamber will be available on the bending magnet line. It is planned to couple these facilities with state-of-the-art detectors such as multi-element Si or Ge fluorescent detectors and high speed avalanche photodiodes. PNC-CAT is working with programs at ANL and PNNL to facilitate the measurement of radioactive samples. Currently it is expected that at least 30-40% of the PNC-CAT member research will involve MES studies. This will include imaging, micro-XAFS and diffraction, and surface studies both on UHV and *in-situ* samples. In addition, 25% of the time will be available to outside users, and could be used for MES studies. Most of the equipment needed for MES studies is fully funded, including the beamlines, microfocusing optics, spectroscopy setups, and UHV facilities. PNC-CAT requires further funding for additional diffraction capabilities, time resolved capabilities, and advanced detector development. A rough estimate is that 0.75 full-time station equivalent will be available for MES research on the PNC-CAT sector.

Basic Energy Sciences Research CAT (BESSRC-CAT)

The BESSRC-CAT has made significant progress since the Airlie Report, and has recently conducted its first monochromatic experiments in the experimental enclosures. The techniques being developed by BESSRC-CAT which are applicable to MES research include XAFS (on the bending magnet beamline), surface scattering and x-ray standing waves, small-angle scattering and time-resolved diffraction. The fraction of time on the BESSRC-CAT sector for MES research is estimated at 1.0 full-time station equivalent.

Materials Research CAT (MR-CAT)

The MR-CAT is currently developing its insertion device beamline to allow the use of a wide variety of techniques. The general capabilities will include an eight-circle Huber for diffraction and reflectivity studies and the standard detectors for XAFS spectroscopy experiments. Although the beamline will initially be limited to the use of a monochromatic, unfocused undulator beam, microfocusing capabilities for both diffraction and spectroscopy experiments should be available in the next 1-1.5 years. Advanced detectors for the study of extremely dilute samples are also expected on this timescale. Funding for most of these capabilities is currently available, though additional funding may be required for multielement detectors and different types of wavelength dispersive detectors. There is no funding to develop the bending magnet beamline at the present time. This is an area where additional funding would be useful for MES research.

The best estimate at this time is that 10% of the total MR-CAT beamtime will be devoted to MES, representing 0.1 full-time station equivalents at present.

The ANL Chemical Technology Division (CMT, an MR-CAT member) has a significant interest in radionuclides, and that division is pursuing funding for the development of radioactive capabilities (a "rad hutch") on the bending magnet beamline. At this point, however, there is no funding to build such a facility.

Other Sectors at the APS

In addition to the CATs whose scientific programs specifically include MES research, each CAT at the APS is required to make available 25% of the beamtime to "Independent Investigators" from any field. Thus, time will be available at the APS for MES research on other sectors besides those described above. Some of these other CATs are developing capabilities that are ideal for MES research. For example, the Synchrotron Radiation Instrumentation (SRI)-CAT is developing microprobe/ microspectroscopy capabilities, the Dupont-Northwestern-Dow CAT is developing XAFS facilities, and the University of Illinois CAT is developing scattering facilities. The amount of time that is actually available on these sectors for MES research will depend upon the quality and number of Independent Investigator proposals that are received in this area. The reasoning used to estimate the availability of beamtime for MES research on other sectors at the APS is as follows:

- There are 15 sectors in addition to the ones belonging to the 4 CATS described above.
- Of these, about 10 are capable of MES research (others are specialized for protein crystallography, magnetic scattering, etc.)
- These 10 sectors will have about 16 stations capable of simultaneous operation.
- Each station will be available 25% of the time for Independent Investigators. This represents about 4 full-time station equivalents.
- If the fraction of successful MES proposals is between 10 and 25% of the total proposals, then 0.4-1.0 full-time station equivalents could be available via this route for MES research.

Summary

The total beamtime available for hard x-ray MES research at the APS, including XAFS, micro-XAFS, and other techniques, is estimated to be:

Sector	Full-time station equivalents
GSECARS-CAT	1.00
PNC-CAT	0.75
BESSRC-CAT	1.00
MR-CAT	0.10
Other	0.50 (0.4-1.0)
TOTAL	**3.35** beam stations

This number is subject to considerable error, since there is no way of knowing in advance how MES proposals will fare in the peer-review process. However, it is about one station more than the estimate in the Airlie Workshop Report. This is due to the new funding that GSECARS-CAT, PNC-CAT, and MR-CAT have received, and also to the inclusion of Independent Investigator time on other sectors.

The Airlie Workshop Report estimated that the demand for beam time at the APS in 1997 would be 495 station days, and that the APS would run 220 days in 1997. The latter estimate was quite optimistic from the point of view of user time, and the actual number is considerably smaller (for example, we estimate that only about 40 days will be available for XAFS and micro-XAFS work in 1997), but it is clearly growing. Furthermore, most of the APS sectors doing MES research will not begin user operations until late 1997 or early 1998, which is borne out by experience at the APS through May 1997. As a result, we have revised the estimates of available beamtime for XAFS and micro-XAFS research at the APS in the Airlie Workshop Report (see Table 6) from 495 to 40 station days. With the APS will running ≈ 190 days in 1998, there should be ≈ 640 station days available for MES research of all types that year, based on 3.35 beam stations that should be available for MES research. This is 35% more than the estimated demand for MES beam time at the APS in 1997 (based on the national user survey reported in the 1995 Airlie Report), which is the approximate annual growth rate in demand for MES beam time in previous years. We thus conclude that the APS capability for MES research should be sufficient for the short-term. However, if the past rate of growth of MES beam time demand continues, the MES facilities at the APS will be significantly oversubscribed after 1998. This is consistent with the estimates that were made in the Airlie Workshop Report. Given that very few MES experiments have yet been done at the APS, it is premature to begin funding and constructing additional facilities. However, we recommend that the DOE continue to keep in mind that there may be a significant demand for more facilities at the APS, based on the experience at existing beamlines at other sources.

C. National Synchrotron Light Source (BNL)

The NSLS provides synchrotron light ranging from hard x-rays to IR. Beam time at the NSLS is allocated in the following way: 75% to the membership of Participating Research Teams (PRT's) and 25% to scientists through general user proposals. The total number of users, representing people with guest appointments who conducted research at the NSLS in FY'96, was 2,268. Geographically, the NSLS user base is heavily weighted to the northeast corridor, although there are a substantial number of users centered in the midwest and California. NSLS also has a significant international user community, accounting for roughly 10% of the users and 4% of the available beam time.

The PRT composition also represents a broad range of institutions, consisting of roughly 25% industry, 20% universities, 34% government labs, and 21% held by the NSLS. Collectively, these institutions are responsible for the construction and operation of 80 beamlines which in FY' 96 represented a resource of nearly 400,000 station hours.

The response of BNL to the recommendations of the 1995 Airlie Workshop Report was primarily in detector development (the 128 element detector project in particular), some new technique and resource development (IR and x-ray tomography beamlines, expanded NSLS capability in XAFS spectroscopy), and an effort to integrate capabilities across departments at the laboratory. The Department of Applied Science is creating a Center for Environmental Science and Technology, with the support of the Lab Director and the DOE. They have recently started advertising for a senior person to head the center.

Due to the organization of the NSLS (independent management of the beamlines) and of the DOE reporting categories (MES has not as yet become an independent category), statistics are rather difficult to extract regarding beam usage and allocation in the MES area. Some portion of the PRT-sponsored work often goes unreported to the NSLS. The NSLS user data base was examined, however, to obtain some idea about the MES community at the NSLS. By looking for active appointments in Geological and Environmental Sciences, 137 MES users were identified, 113 or 83% of which actually ran experiments at NSLS in FY'96. This number represented 5% of the total number of NSLS users in 1996. This sorting is suspect since some investigators who are active in the MES field did not show up in the survey, because they had categorized themselves in other fields when they applied for guest appointments (*e.g.*, solid state physics). It is also suspect because only about half of the geoscience users at synchrotron sources do research that can be classified as MES. Given these caveats, examination of the base of 137 users indicates that MES users represented 53 institutions (11 government labs, 35 universities, 7 industrial labs). 18 beamlines were used for MES research, but 6 beamlines accounted for 86% of MES users.

A review of the publication lists submitted by the users to the NSLS FY'96 Activity Report identified 7 publications from the UV ring and 50 on the x-ray ring that are classified as MES research. A search of user names in *Current Contents* is also underway to try to identify MES users. It is likely that the number of MES users at the NSLS is under-reported by as much as a factor of two.

A review of titles of general user proposals and the beam time allocated to the proposals with titles relevant to MES research leads to a 1996 estimate of about 280 station days for MES work by general users, who can apply for only 25% of our available beam time. Some work may have been associated with review categories that were not searched, or were not recognized as being relevant to MES. This number should be compared with the beamtime requirement anticipated by the Airlie Report which would have been approximately 350 to 400 station days *for all users*. Since the hours reported above are only for general NSLS users, it is likely that the overall usage estimate of the Airlie Workshop Report has been exceeded, as suggested by Table 4.

There has been a steady increase in Geoscience and Ecology use (except for FY'91) during this period. It is estimated that the equivalent of 2.0 station years on imaging beamlines and 1.5 station years on spectroscopy beamlines were used in FY'96 for MES-related activities. The huge growth in Life Sciences is largely driven by macromolecular crystallography, but it has some MES component to it, as do most of the other categories.

Table 4. Station days for all users at the NSLS for the past seven years

	FY'90	FY'91	FY'92	FY'93	FY'94	FY'95	FY'96
Chemical Sciences	264	304	303	318	321	281	291
Materials Sciences	837	993	882	1105	929	952	916
Life Sciences	62	167	286	354	503	548	642
Geosciences and Ecology	62	26	75	80	113	106	123
Applied Science and Engineering	155	106	167	186	177	147	138
Optical/Nuclear/General Physics	170	129	183	151	129	128	117
Not specified	0	0	0	0	56	44	34

D. Stanford Synchrotron Radiation Laboratory (SLAC)

Since the 1995 Airlie Report, both the number of experimental stations and the number of days of user beam delivered per year have grown at SSRL. SSRL is now producing user beam approximately 9 months per year as a result of the DOE Scientific Facilities Initiative funding increase.

With the completion of beamline 9, SSRL will have 9 VUV/soft x-ray and 20 hard x-ray experimental stations, of which 24 can operate simultaneously. Of the 29 total stations, 14 of the hard x-ray and three of the VUV stations are illuminated by insertion devices. Two additional insertion device stations are currently under development. One of these is a new branch line featuring a 10-40 eV, normal-incidence, grating monochromator for VUV research on the beamline 5 undulator. The other station is the BL-11 wiggler end station optimized for hard x-ray MES-XAFS studies. This station features a 26 pole, 1.9T hybrid insertion device with optics designed for 5-23 keV operations. The experimental hutch includes special sample- and air-handling capabilities that insure the containment of any spills of toxic or radioactive materials during XAFS or x-ray scattering studies of such materials. Both the sample containment facility and high speed detectors/hutch electronics have been funded since the 1995 Airlie Workshop by the DOE Scientific Facilities Initiative. Inclusion of a microprobe/microspectrometer capability on BL-11 to probe areas of approximately 50 μm^2 on environmental samples is currently under investigation. The intensity of a microprobe beam would be significantly enhanced and the spot size reduced to about 6 μm^2 should the SPEAR storage ring be upgraded to 18 nm rad emittance as proposed by Helmut Weidemann of SSRL. First light from BL-11 is anticipated early in 1999.

The MES program at SSRL has grown steadily from approximately 13 station days in 1990 to 358 station days in 1996 (see Table 6). Last year, the MES program consumed the equivalent of about two SSRL station years, as was predicted in the 1995 Airlie Report. Most of the MES program at SSRL concentrates on hard x-ray XAFS studies, although significant growth has recently been observed in soft x-ray/VUV spectroscopy and x-ray standing wave studies of metal oxide surfaces. The continuing growth of the MES program at SSRL has stimulated the hiring of a new staff scientist, Dr. John Bargar, to assist with MES user support and to help coordinate MES research at SSRL. Staff scientists at SSRL are also expected to havew active research programs.

In addition to providing staff for general user support, SSRL maintains a loaner equipment pool consisting of multi-element detectors and associated electronics, sample cryostats, and a grazing-incidence XAFS apparatus. Two of the 13 element Ge detectors have been upgraded for higher throughput since the Airlie Report. Shortly, SSRL will add a multi-element Ge hard x-ray detector, a UHV compatible multi-element Ge detector, a sample cryostat, a second grazing-incidence XAFS apparatus, and other equipment devoted to the MES program. This new equipment was funded through the DOE Scientific Facilities Initiative. Since the Airlie Report, SSRL, in collaboration with scientists at LANL and LBNL, has also established an actinide handling protocol based on triple containment of samples. Until the containment facilities associated with BL-11 are commissioned, this protocol involves the temporary installation of radiation monitoring and survey instrumentation at the appropriate experimental station for the duration of actinide measurements.

V. Reports from Working Groups

A. XAFS Spectroscopy and X-ray Scattering Working Group

Summary of Findings

1. Activity level of the science

XAFS spectroscopy in the hard x-ray region (> 4 keV) is and will continue to be one of the most effective methods for determining the chemical speciation of metal ions in many environmentally important materials including crystalline, amorphous, and heterogeneous solids, organic substances, aqueous solutions, and at solid-liquid interfaces (*e.g.*, metal ions sorbed on soil particles). This was one of the major findings of the 1995 Airlie Workshop which was reconfirmed by the data presented at the 1997 SSRL Workshop. XAFS spectroscopy has also proven to be very useful for characterizing the fundamental surface chemical properties of reactive environmental solids, such as the reactivities and densities of metal-ion binding sites on mineral surfaces and the compositions and structures of reactive coatings on soil particles. This is accomplished by using XAFS methods to probe the second and more distant neighbors of metal ions sorbed on solid surfaces. Information on the chemical speciation of environmental contaminants and the surface properties of environmental solids is crucial to the development of effective high-level waste remediation technologies such as reactive barriers, chemical separations methods, accurate metal-ion reactive transport models, and risk assessment models. XAFS spectroscopy will continue to be very important to MES research in the foreseeable future.

This working group also considered x-ray scattering methods, which have not been used widely in MES research to date, but which are certain to have an increasing impact in this research area over the next five years. For example, powder x-ray diffraction is an essential method for identification of fine-grained crystalline phases such as clays, which are common constituents of environmental samples. Synchrotron beamlines devoted to powder diffraction at the APS, NSLS, and SSRL will lower the detection limits of this method for environmental samples and will permit high accuracy Rietveld analysis of the structures of fine-grained samples because of the superior signal-to-noise levels and flater backgrounds of synchrotron powder diffraction patterns relative to laboratory powder diffraction patterns. Routine use of synchrotron x-ray powder diffraction for characterizing fine-grained environmental samples will undoubtedly increase. In addition, wide angle x-ray scattering (WAXS) is beginning to be used for studies of fine-grained and poorly crystalline environmental samples. For example, WAXS studies of fine-grained ferric hydroxide phases, which are abundant in the environment and which provide surfaces on which environmental contaminants commonly adsorb, have helped define the local structural arrangement in these materials. Differential anomalous X-ray scattering (DAXS) and differential anomalous fine structure (DAFS) spectroscopy are two methods that can also provide important structural information on amorphous materials and, in the case of DAFS, mixtures of amorphous and crystalline phases. Neither has yet been applied in MES research. On the other hand, crystal truncation rod (CTR) scattering measurements on mineral surfaces are beginning to shed light on important adsorption reactions on carbonate minerals, which are very common environmental phases. CTR methods are also certain to become more commonly used in studies of important model systems in which complex processes at environmental interfaces can be studied.

There are several critical needs of the growing MES synchrotron user community that utilizes hard x-ray XAFS spectroscopy. One is access to adequate beam time. A second is the need for higher flux sources required to detect and characterize low concentrations of environmental contaminants in complex bulk samples. A third is the need for higher brightness sources to characterize the spatial distribution of different species in heterogeneous samples such as soils. A fourth is the need for higher throughput detectors, without which the benefits of higher flux sources cannot be fully realized. These needs are true for standard XAFS studies of bulk samples, for grazing-incidence XAFS studies of surfaces, and for micro-XAFS studies of the spatial distribution of chemical species in heterogeneous samples (See Section V.B). Similar needs are also apparent in x-ray scattering studies of environmental samples which complement XAFS spectroscopy studies.

Current and projected rate of growth of XAFS. Overall, the level of research activity using hard x-ray XAFS spectroscopy is growing at the rate projected at the Airlie Workshop, which, through 1996, predicted a doubling in activity every year from a small base level. This exponential growth rate will most likely progress to an arithmetic one as those scientists already in current MES disciplines who are not familiar with XAFS learn to use this technique on the full range of MES problems. However, two factors currently in flux could result in a resumption of this very rapid growth rate within three to five years if the technology and policy arena driving MES evolves in certain ways. These include:

(1) The extension of MES beyond its origins in chemistry, geochemistry, and soil science into basic research areas where it has not been applied, notably life and environmental materials sciences. For example, recent applications of XAFS to characterizing the effects of metal ion speciation on processes such as phytoremediation and microbially mediated sequestration of actinides, are showing that these areas are also fundamental to MES. As a result of this new activity, a new group of scientists are becoming involved in MES, creating an increased demand for hard x-ray beamtime. Similarly, the applicability of XAFS to the characterization and development of radioactive waste disposal forms and the assessment of aging issues for radioactive materials should result in substantially greater demand for hard x-ray beamtime.

(2) The application of XAFS and other hard x-ray synchrotron techniques to routine characterization of environmental samples. The regulatory community is increasingly recognizing that the speciation of contaminants is very important in determining their impact in the environment, including their toxicity, bioavailability, mobility and fate in groundwaters, and the cost effectiveness of technologies for remediation. Because of the environmental importance of contaminant speciation, its definition is a necessary first step in developing risk assessment models and remediation strategies for contaminated sites. The adoption of this scientific, speciation-based approach promises substantial cost savings by identification of contaminants which may not require remediation due to their chemical state, *e.g.*, they may occur in highly insoluble phases and as a result be immobile. We anticipate that routine XAFS-based determination and monitoring of the chemical speciation of metal ions at contaminated sites could become almost as common as the determination of their concentrations, resulting in a substantial increase in the demand for synchrotron facilities and beamtime.

Table 5: Anticipated Growth Areas for Hard X-ray MES Research

Field	Application	Source
Soils Science	Contaminant speciation characterization	Beamtime requests
& Geosciences	Contaminant distribution characterization	Beamtime requests
Bio-MES	Phytoremediation	Beamtime requests
	Microbial remediation strategies	Beamtime requests
Mat. Sci./Chem.	Waste Characterization	1997 DOE EMSP call
	Spent nuclear fuels characterization and stabilization	1997 DOE EMSP call
	Fissile materials stabilization and remediation	1997 DOE EMSP call
	Waste disposal forms	1997 DOE EMSP call
Analytical Service	Monitoring/sampling	Anticipated demand

Impact on synchrotron facilities and research funding levels. The success and continuing development of XAFS and other synchrotron-based hard x-ray techniques for solving environmental problems have created significant new facilities and support needs necessary to maintain the current level of progress and support future experimenters. These needs include:

(1) MES operations and user support. DOE support for MES to date has emphasized construction of new facilities. These increases, however, have not been accompanied by commensurate increases in funding for operations and user support. If uncorrected, this situation will lead to significant unrealized returns on the DOE's investments in these MES resources. For example, the SSRL BL-11 experimental station and radioactive sample environmental enclosure were funded, but funds requested for necessary EH&S personnel were not committed. In addition, it will be necessary to hire technicians to maintain the beamline in operating condition for users. Funds for these personnel do not currently exist in the SSRL operating budget, and these services cannot be provided by users. Similar imbalances between the number of existing/planned MES facilities and committed MES operations are common at other synchrotron facilities in the US. Therefore, it is necessary that operations and user support be targeted for increased funding in the near future. This action will ensure that MES users can fully utilize the existing and planned facilities. This working group has identified several key areas of operations support, which, when funded, will significantly enhance MES synchrotron facilities:

- *Scientific Staff*. Staff scientists are important resources for user and facilities support programs at synchrotron light sources. The Biotechnology Program at SSRL, which has evolved to serve the needs of biotechnology users and is highly successful, is a useful model for demonstrating the importance of staff scientists. SSRL biotechnology scientists direct a small group of technicians, engineers, and programmers, who maintain beamlines and experimental facilities dedicated to biotechnology research. In addition to developing experimental techniques and conducting basic research, the staff scientists instruct users about how to carry out experiments, conduct user education workshops, trouble-shoot beamline problems for users, and answer many other types of user questions. These services are necessary because even experienced users generally do not have sufficient understanding of x-ray beamline optics, detectors, and electronics to conduct experiments without this support. Currently, the Biotechnology Group at SSRL is also supporting MES and other users in XAFS spectroscopy, although it does not have the resources to continue doing so. Much of the success of MES research at SSRL is directly attributable to support provided by the Biotechnology Program. MES staff scientists at SSRL are providing an important interface between the MES user community and the DOE.

• *Beamline technicians and programmers/computer managers.* As demonstrated by the SSRL biotechnology program, beamline engineers, electrical/mechanical technicians, laboratory technicians, and computer programmers play critical roles in user support.

• *EH&S technicians.* Such personnel are absolutely essential for the safe operation of facilities that will accommodate actinides and other radioactive samples, such as SSRL BL-11, and the APS actinide facility.

• *User education.* MES user education programs are needed for instruction at two levels: (1) There is a need to educate scientists in environmental areas who are not familiar with synchrotron-based techniques about the applications of these techniques to environmental problems. (2) There is a need to educate synchrotron facility users about how to perform XAFS and other hard x-ray experiments and properly analyze the resulting data. This need is particularly significant, since many hard x-ray experiments and data analysis techniques are highly complex. Given this situation, there exists the potential for improper analysis and interpretation of XAFS data, which would be a liability to the scientific community and would weaken confidence and support for synchrotron-based techniques. Proper education should be useful in ameliorating these potential problems.

(2) Instrumentation. The development of the following instrumentation and XAFS and other measurement techniques will have immediate and substantial positive impacts on the ability to solve problems in MES:

• *Advanced detector systems.* For certain types of samples, the capabilities of new beamlines exceed those of the detector systems used to obtain the data, so that these capabilities remain under-utilized. The needs are not only for faster, higher count rate detectors, but also for more sophisticated treatment of the data in real time. This last factor is especially important as detectors with very large numbers of elements become available. Such detectors require a computer-controlled set up of the system and the capability of sorting and combining the data streams from all of the channels. Digital signal processing (DSP) is also becoming available for use with these multi-element detector systems, and its use could substantially enhance the ability to extract XAFS data for very dilute elements in highly absorbing matrices.

• *Software for control of beamlines and detectors*. It is necessary to develop software that will provide enhanced and more efficient control of the beamlines and experimental equipment. Without such support, the increased complexity of these new facilities will challenge existing users and possibly preclude new users. This includes software for control of beamline optical components, automated sample controllers, and detectors, including analog electronics and DSP. Such software will also enhance quality assurance for "service" XAFS applications.

• *Radiation safety hardware*. Equipment such as radiation monitoring and survey instrumentation, such as continuous air monitors, is essential for the safe operation of facilities that will accommodate actinides and other radioactive samples, such as SSRL BL-11.

• *User lab facilities.* The science that is being conducted at synchrotron-based XAFS facilities increasingly involves *in-situ* measurements of samples while experiments are being conducted. Such experiments are crucial to the understanding of chemical processes and speciation that occur under environmentally relevant conditions (*i.e.*, in contact with water at ambient temperatures and pressures). Samples for these and other MES experiments often cannot be prepared outside of the synchrotron sources. Thus, there is a pressing need for MES user laboratory space for the preparation and manipulation of samples that are sensitive to transport and aging. These increasingly sophisticated experiments are often accompanied by equipment that is also somewhat sensitive to transport. Since experimental floors at synchrotron facilities are already full with permanently installed instrumentation, there is a need for equipment set-up space and storage lockers.

(3) Methodology. Advances are required in the following XAFS analysis method areas, and will increase the scope of MES problems that can be addressed by XAFS:

• *Advanced analysis and interpretation methods*. The application of software for calculating EXAFS phase and amplitude functions using *ab-initio* multiple-scattering methods has revolutionized XAFS spectroscopy by eliminating the problematic process of acquiring these functions from model or standard compounds as a basis for analyzing XAFS data from an unknown system. The ability to calculate X-ray Absorption Near Edge Structure (XANES) spectra with a high level of accuracy does not currently exist, but it would have a large impact on XAFS-based MES research, since the low analyte concentrations that are characteristic of MES samples often preclude obtaining adequate signal:noise data in the EXAFS region but not in the XANES region. Furthermore, the data acquisition times for XANES spectra are much shorter than for EXAFS spectra, which suggests that XANES techniques will be particularly useful for routine analyses of large numbers of samples and for kinetic studies. The development of spectral libraries, especially for XANES spectra, and a standardized means for evaluating spectra from unknown systems by comparison with the data in the libraries must be developed. Other areas needing attention include the development of robust error analysis algorithms for XAFS results, interpretation of results from systems that contain metal ions in complex mixtures of solid phases or multiple species, which is typical of soil and high-level radioactive waste samples, and more accurate methods for quantifying the coordination numbers of metal ions having anharmonicity and/or asymmetric distributions of atoms in their local coordination environments.

• *Development of structural modeling techniques for solids.* Fissile materials, spent reactor fuel, and waste disposal materials are materials relevant to MES research. XAFS characterization of the short-range structures in these types of materials (as opposed to simple chemical speciation) is highly desirable. Because these solids are typically complex and highly radioactive, characterization of their structures is extremely challenging and may exceed the capabilities of current analysis methods and/or facilities. The development of advanced structural modeling techniques, in which data from diffraction, XAFS, and diffuse scattering are all combined to provide a single, coherent model of the structure, is essential.

(4) Facilities and support for "service needs". Because the analysis and interpretation of XAFS data are more complex than other routine, analytical methods, the successful development of XAFS "service" requires that the method be standardized and partially automated. XAFS methods must be optimized for this type of use, and software should be developed that simplifies data collection, thus increasing efficiency and reproducibility and providing quality assurance.

(5) Research timescales. It is becoming apparent that short timescale engineering approaches are inadequate to address the scale and seriousness of problems associated with remediation of high-level waste and environmental contamination. As previously discussed, solution of such problems requires characterization of the chemical speciation and distribution of contaminants and molecular-level and macroscopic studies of the local environmental factors that affect them. Given the scale and difficulty of such studies, it must be emphasized that research timescales should be 3 - 5 years, rather than the 1 - 2 year time frame that has been more typical in this field. Furthermore, we recommend that there must be flexibility in achieving broad policy and risk

assessment objectives, and given the rapidly evolving and dynamic nature of this field, training of students and associate scientists should be considered to be an essential component of the effort.

2. Assessment of MES-XAFS user time available

The assessment of available user time in 1997 and beyond is difficult because of the assumptions that must be made, including the number of days of operation at each synchrotron light source and the number of experimental stations available for a given technique. It also requires that some assumption be made about the success of general user proposals in the MES area relative to proposals from other disciplines. The estimates presented in Table 6 were generated in consultation with representatives from each of the four laboratories at the Workshop and in discussions following the Workshop. It should be noted that these estimates are for hard x-ray XAFS and micro-XAFS spectroscopy only and do not include time for other types of MES research, including x-ray scattering, x-ray standing wave (XSW) measurements, x-ray imaging, x-ray tomography, and soft x-ray/VUV methods (including XAFS and photoemission spectroscopy, XSW methods, photoeelctron diffraction and spectromicroscopy techniques).

A direct comparison of the number of station days available for MES-XAFS studies shown in Table 6 with those in the Airlie Report (p. 101) is difficult because the latter included all synchrotron radiation methods, both hard x-ray and soft x-ray/VUV, used in MES research. However, because XAFS and micro-XAFS studies currently comprise the bulk of MES synchrotron radiation studies (>80%), a rough comparison can be made. The current estimates of available MES-XAFS station days in 1997 (703 station days) and 1998 (1,108 station days) are well below the estimates in the Airlie Report, which were 1,222 (1997) and 1,427 (1998). The main reason for this difference is the fact that the APS has been slower coming on line than anticipated at the time the Airlie Report was released (January 1996). In addition, even though the number of station days available for MES-XAFS work at SSRL has grown significantly over the past two years, this number is lower than previously anticipated because the proportion of XAFS beamtime currently available to MES vs. other research fields (materials science, biotechnology, chemistry, solid state physics) has reached a steady state. All XAFS beamlines at SSRL and NSLS are oversubscribed by a factor of 1.5 on average, and many well-rated proposals in all fields do not receive beamtime.

Table 6. Estimated Number of Station Days for XAFS and Micro-XAFS Studies at DOE Synchrotron Light Sources*

1996 Use	(number of experimental station days/yr)	Station Days
ALS	(provided beam 186 days x 0.1 experimental stations)	= 19
APS	(provided beam 0 days x 0.0 experimental stations)	= 0
NSLS	(provided beam 220 days x 1.3 experimental stations)	= 286**
SSRL	(provided beam 198 days x 1.8 experimental stations)	= 356
		661
Anticipated Station Days in 1997	(including current + planned stations)	
ALS	(should provide beam 192 days x 0.15 experimental stations)	= 29
APS	(should provide beam 40 days x 1.0 experimental stations)	= 40
NSLS	(should provide beam 220 days x 1.5 experimental stations)	= 330
SSRL	(should provide beam 204 days x 1.7 experimental stations)	= 340
		703
Anticipated Station Days in 1998	(including current + planned stations)	
ALS	(should provide beam 200 days x 0.2 experimental stations)	= 40
APS	(should provide beam 187 days x 1.6 experimental stations)	= 300
NSLS	(should provide beam 220 days x 1.9 experimental stations)	= 418***
SSRL	(should provide beam 204 days x 1.7 experimental stations)	= 350
		1,108
Anticipated Station Days in 1999	(including current + planned stations)	
ALS	(should provide beam 200 days x 0.2 experimental stations)	= 40
APS	(should provide beam 200 days x 3.0 experimental stations)	= 600*
NSLS	(should provide beam 220 days x 2.0 experimental stations)	= 440***
SSRL	(should provide beam 204 days x 2.7 experimental stations)	= 551****
		1,631

** The number of XAFS experimental stations available for MES research includes micro-XAFS stations, but not x-ray scattering, x-ray imaging or soft x-ray/VUV XAFS stations.*
*** The number of XAFS experimental stations for 1998 included 0.3 X11A, 0.25 X19A, 0.25 of X23B, 0.5 X26A*
**** The number of XAFS experimental stations at the NSLS in 1998 and 1999 takes into account the planned upgrade of 0.3-0.5 XAFS beamlines that will be available to MES-XAFS users.*
*****Includes BL-11 which will be available for MES users in early 1999.*

When BL-11 comes on line in early 1999, we anticipate that there should be another 204 station days/year available for MES-XAFS research. Similarly, the upgrading of several XAFS beamlines at the NSLS in early 1998 will provide 0.3 to 0.5 additional station years for MES-XAFS research starting in 1998. In addition, we anticipate that the total number of station days available for XAFS and micro-XAFS research at the APS will approximately double between 1998 and 1999. These changes should result in about 1630 station days available for MES-XAFS research in 1999, which is about the same as the anticipated MES user demand in 1999, based on an extrapolation of the estimates made in the 1995 Airlie Workshop Report. Starting in 1998, MES-XAFS work will be distributed roughly evenly over beamlines at the APS, NSLS, and SSRL.

3. Inventory of hard x-ray XAFS facilities

In the 1.5 years since the Airlie Report was released, there has been no increase in the number of planned XAFS beamlines. Nevertheless, the number of hard x-ray XAFS facilities available for MES research has grown because of a shift in the use of existing synchrotron stations to MES research from other types of work. For example, at SSRL the equivalent of 1.4 experimental stations (out of 7 available) were used for MES-XAFS research in 1995, whereas 1.8 experimental stations were used for MES-XAFS research in 1996, and this number is projected to rise to 2.7 stations in 1999. These observations support the assertion that much MES work, especially of the analytical type, will be performed with existing facilities.

At SSRL, much shared equipment is available for use in MES hard x-ray XAFS experiments. SSRL maintains Stern-Heald-Lytle-type fluorescence detectors, multi-element array detectors and associated electronics, sample cryostats, and a grazing-incidence XAFS apparatus. Two of the 13- element Ge detectors supported by the SSRL Biotechnology Program have been upgraded for higher throughput since the Airlie Report. SSRL has established an actinide handling protocol based on triple containment of samples. Until the containment facilities associated with BL-11 are commissioned, this protocol involves the temporary installation of radiation monitoring and survey instrumentation at the appropriate experimental station for the duration of actinide measurements.

4. Inventory of planned hard x-ray XAFS facilities and new capabilities

a. ALS - There are no current plans for future beamlines optimized for hard x-ray XAFS specroscopy. Soft x-ray/VUV XAFS work will continue on several beamlines, and a number of new soft x-ray/VUV beamlines with XAFS capability are being constructed.

b. APS - An MES actinide experimental support facility is under development at the APS. Facilities currently planned that will be available for users include a variety of detectors, a variety of portable radioactive sample environmental enclosures, a set of available radioactive sample safety protocols, and radiation safety hardware, such as area detectors.

c. NSLS - Currently, the partial or complete refurbishment of three NSLS beamlines is planned, funded by the DOE BES facilities initiative, which may provide up to 0.3–0.5 beamline equivalents for MES. In addition, there are plans to upgrade beamline control software, optics on several beam lines, purchase a 128-element detector system, and increase the XAFS user equipment pool using money from the DOE Scientific Facilities Initiative, NSLS operating funds, and PRT funds.

d. SSRL - The most noteworthy MES facility currently under development at SSRL is the BL-11 wiggler end station, which will be optimized for hard x-ray MES XAFS studies. Funding has been obtained for the purchase of a high speed multi-element detector and signal processing electronics. The experimental hutch includes special sample- and air-handling capabilities that will insure the containment of any spills of toxic or radioactive materials during XAFS studies of such materials. Both the sample containment facility and high speed detectors/hutch electronics suites were funded since the 1995 Airlie Workshop by DOE Scientific Facilities Initiative funding. Inclusion of a microprobe capability to probe approximately 100 $micron^2$ sample features is currently under investigation. The flux density of a microprobe beam would be significantly enhanced should the SPEAR storage ring be upgraded to 17.2 mrad emittance, resulting in a spot size of ≈ 2x3 μm and a flux of ≈ 10^{10} photons/sec. First light from BL-11 is anticipated early in 1999.

5. Recommendations for new hard x-ray XAFS facilities

Short term facilities needs (1-3 years). In the 1.5 year period since the Airlie Report was released, no new major hard x-ray XAFS beamlines, other than those under construction or planned, will be required to meet anticipated user demand. However, as noted above, many of these facilities will require enhancements in user support and instrumentation available for MES work in order for users to effectively utilize beamlines. As a guide to funding requirements, this working group recommends the following schedule for purchase or upgrade of equipment. The justification for this equipment was discussed in section V.A.1.

- Purchase/upgrade of high throughput/high energy resolution detector systems at the rate of 1 per year per facility.
- Purchase/upgrade of specialized sample handling and containment equipment, and improved beamline optics at the rate of 1 beamline per year per facility.
- Development of a major new capability on existing beamlines (*e.g.*, time-resolved XAFS, high-resolution powder diffraction, grazing-incidence XAFS, x-ray scattering facilities) at the rate of 1 per year per facility.

The needs listed above could be met by providing on the order of $1M in capital equipment funding per year per synchrotron source for support of MES work. This support could also be leveraged with support for other kinds of research, *i.e.*, structural biology or materials science.

Long term facilities needs (3–5 years). If the new research areas and the service component grow as we anticipate, it is likely that 3–5 new XAFS facilities will be needed over the next five years, half of which will be equivalent to BL-11 at SSRL or the APS ID stations. An annual review of this need should be performed so that the long lead times required for construction of these beam lines are planned to coincide with increasing user demand.

6. Assessment of operations/user support needs for XAFS beamlines

a. ALS - More general user support is needed for researchers who wish to make XAFS measurements or use beamlines in general. Specialized experimental equipment and facilities for MES research are needed. The need for MES user support on spectromicroscopy beamlines at the ALS is especially critical because the UHV techniques are often new to new synchrotron radiation users and they are much more complicated than spectroscopy and microspectroscopy techniques at ambient conditions. Thus several new staff members at the ALS will be needed to handle the increased demand for beamtime by MES users.

b. APS - An MES actinide experiment support facility is currently under development at the APS. No details were available at the time this report was submitted to the DOE.

c. NSLS - The NSLS is currently in the process of refurbishing the equivalent of 0.3 - 0.5 beamlines for MES use. This will require operations support similar to the SSRL model proposed below.

d. SSRL - The XAFS spectroscopy working group has developed a model for the SSRL MES program staff and operations requirements. This model includes operations support of SSRL BL 11, which is dedicated to MES research, and support for MES users on other SSRL beamlines (including BL's 2-3, 4-1, 4-2, 4-3, and 6-2) as described above in section IV.A.1. The requirements in the model are projected from comparison to the SSRL biotechnology program and programs at other synchrotron facilities.

<u>SSRL MES staff model</u> (“fte” is defined as full-time equivalent)

1 fte staff scientist
1 fte beamline engineer
1 fte beamline electrical/mechanical technician
1 fte SSRL radiation/laboratory technician
1/2 fte SLAC radiation technician (provided from existing SLAC staff)
1/2 fte computer programmer/systems manager

<u>SSRL MES operations equipment requirements</u>

Radiation safety hardware: continuous air monitors, other survey and monitoring equipment

EM&S: maintenance and expendable supplies (*e.g.*, office supplies)

B. HARD X-RAY MICROPROBE ANALYSIS, MICROSPECTROSCOPY, AND IMAGING WORKING GROUP

Summary of Findings

1. Activity level of the science

It is now widely accepted that specific information on chemical speciation and transformations is prerequisite to the development of a comprehensive understanding of toxic element behavior in soils. This information is required to properly predict contaminant fate in the environment, to develop effective and rational remediation strategies, and to provide realistic and accurate risk assessments. Unfortunately, our understanding of the importance of chemical speciation has advanced more rapidly than the analytical capabilities to determine it, particularly in complex systems such as soils, sediments, and waste-forms. The limits of existing techniques to address specific problems related to chemical speciation of toxic elements in such complex samples have been exceeded for well over a decade. Conventional methods of investigating chemical speciation lack the sensitivity required and usually prohibit investigation under environmentally relevant conditions, for example, on moist samples using minimal or no chemical pretreatment. In contrast, synchrotron-based microanalytical techniques provide the potential for determining the chemical speciation of a wide variety of toxic elements in moist soil samples, waste-forms, and biological specimens with little or no chemical pretreatment at detection limits that, on the average, exceed those of conventional methods by several orders-of-magnitude. Further development and deployment of synchrotron-based microanalytical techniques will allow environmental scientists working on a range of problems at DOE sites to provide the fundamental information required to address critical issues relating to waste site and waste-form characterization, waste disposal methods and management, and questions arising from newly emerging technologies related to treatment and remediation of contaminated sites.

In recent years it has been demonstrated that synchrotron-based microanalytical and micro-XAFS spectroscopy can provide chemical speciation at spatial resolutions $\leq$ 10 µm. Research efforts in this area have utilized these techniques to determine spatial distribution maps of contaminants and their specific chemical bonding environments. Studies have included the determination of U speciation in contaminated and chemically remediated sediments from the Portsmouth, Oak Ridge, Fernald, and Savannah River (SRS) Sites, the determination of Cr oxidation states in cementitious waste-forms generated at the SRS, the determination of contaminant metals associated with groundwater colloids from the F-Area at the SRS, tree ring analysis of specimens from a wetland on the SRS impacted by the F-Area and H-Area contaminant plumes, the location and chemical forms of Ni, Se, and As incorporated in turtle shells and hyperaccumulating plants collected from a variety of contaminated environs at the SRS, and the mechanisms of tetraphenylboron degradation on soil mineral phases relevant to the Defense Waste

Processing Facility (DWPF) at the SRS. These studies have demonstrated that unprecedented insights can be gained from these techniques that can be directly applied to problems associated with biomonitoring, waste management, and with remediation activities at former DOE weapons production and research sites.

There is an increasing interest in the environmental, earth, biological, and material sciences in the ability to conduct spatially resolved XAFS spectroscopy for chemical speciation of heterogeneous natural and synthesized samples. The small x-ray beam size of X-26A at NSLS, affords the potential to probe heterogeneous samples at a scale more likely to reflect homogeneous domains within the complex mosaic compared to conventional beam lines where the beam size is typically in the tens to hundreds of mm or cm size range. Many environmental applications of x-ray fluorescence and x-ray absorption near edge structure (XANES) spectroscopy have already been successfully conducted at X-26A at the NSLS, and the interest in this capability is expanding rapidly, especially among scientists working in the molecular environmental science area, on problems related waste management within the DOE complex (Airlie Workshop Report, 1995). Extension of this micro-scale capability to extended x-ray absorption fine structure (EXAFS) spectroscopy is required to provide more specific and detailed chemical speciation information on these complex samples. Interest in this capability among researchers in the environmental, earth, biological, and material sciences is significant. Although this capability is planned for the GeoSoilEnviro-CARS beamline currently under development at the Advanced Photon Source (APS), we believe that there is an immediate need to address complex problems associated with environmental management and restoration activities at DOE sites using this advanced technology. Furthermore, there are many applications for which the existing X-26A beamline at the NSLS, or the plannned micro-XAFS facility on BL-11 at SSRL is most appropriate. The demand for synchrotron-based microanalytical techniques will ultimately be much greater than the beam time available at the APS for support of environmental management and restoration activities, particularly as the application of these techniques becomes more ‘routine’ (DOE Workshop Report, 1995). Additionally, there are a number of technical obstacles in implementing spatially resolved EXAFS spectroscopy that need to be addressed currently at beamline X-26A at NSLS. Thus there is a growing need for additional micro-XAFS facilities at U.S. synchrotron sources.

C. SOFT X-RAY/IR MICROSCOPY-SPECTROSCOPY WORKING GROUP

a. Soft X-ray Microscopy/Spectroscopy - Summary of Findings

There is an on-going expansion of soft x-ray microscopy/spectroscopy beamline facilities nationwide. However, the over-demand for beamtime by programmatic efforts and the specialization of the facilities will continue to significantly limit MES researcher access in the foreseeable future. There is large potential for the application of soft x-ray microscopy/ spectroscopy techniques to important scientific problems in MES, and initial MES activities are already well-underway at several SR facilities. Some of these microscopy/spectroscopy efforts include the speciation of Mn in aqueous cell environments, the investigation of surface chemistry of minerals, and the micro-characterization of actinide materials. Although soft x-ray SR science is an unfamiliar field to most environmental scientists, it is an emerging area of MES research that has several unique capabilities for addressing environmental problems. For example, soft x-ray/VUV techniques are traditionally applied to surfaces (now including "wet" surfaces), bulk systems, and hazardous materials, and they are the exclusive direct probes of the light elements C, N, and O.

The entire MES community needs to be made aware of the scientific opportunities and capabilities in the soft x-ray/VUV region. This could be achieved by holding a workshop focusing on MES issues and problems that can be addressed by soft x-ray/VUV SR techniques. Such a workshop was held in late March at the ALS. One important result of this workshop was the recommendation to the construct two dedicated microscopy/spectroscopy MES beamline facilities at the ALS.

1a. Activity level of the science

There is intense activity in the soft x-ray microscopy/spectroscopy field within the general user community at all facilities (ALS/NSLS/SSRL). The scientific activity level is clearly limited by access to beamline facilities and funding for operational personnel at the beamlines. More beamline facilities with existing technologies are needed. Continued technical development of microscope technologies is needed for improved spatial resolution on future beamline facilities. There is also the need to secure funding for the construction of microscopy beamline facilities that will enhance all scientific programs and will be especially beneficial to MES research. Funding support for microscopy/spectroscopy efforts are largely from the Materials Science Division of DOE and internal funding from SR light sources.

2a. Assessment of user base

There is large MES participation on BL X1 at the NSLS and BL 3-3 at SSRL. In addition, smaller, initial MES activities are beginning at the ALS. There are so few beamtime opportunities available to MES users that the MES user base is difficult to accurately define at this point.

However, the potential MES user base is inferred as large based on the scientific utility of soft x-ray/VUV techniques and applications in the thrust areas of MES-related research.

3a. Inventory of existing soft x-ray microscopy/spectroscopy facilities

Each of the currently existing facilities is extremely useful and each has demonstrated scientific utility for MES related research in the soft x-ray energy region. About 0.5 of a BL year is used at NSLS X1A-B for on-going MES work. Similarly, about 0.4 of BL 3-3 at SSRL is used each year for MES research. At the ALS, distributed over several microscopy/spectroscopy beamlines, it is currently estimated that MES in this topical area utilizes about 0.2 BL year.

Technical progress in this area is being fairly aggressively translated into beamline endstations or into new beamline sources that may provide increased opportunities for MES via the general user programs. However, none of the new soft x-ray/VUV beamline facilities are focused on the specific needs for MES research and mainline programmatic investigations other than MES will utilize most of the newly available beamtime. Technical improvements of the microscopes in spatial and corresponding spectroscopic capabilities are viewed as essential to the MES research community.

The current inventory of soft x-ray/VUV beamlines and beamtime is insufficient for users from all disciplines (NSLS is overbooked by ≈2X, SSRL is at the fully subscribed level on BL 3-3 and BL 8-1 and is ≈2X oversubscribed on BL 10-1, the soft x-ray/VUV beamlines at the ALS are oversubscribed by ≈2X, and ALS BL 6.0.1 is fully subscribed). This situation is particularly acute for emerging MES researchers who must compete for this limited beamtime resource. There is little doubt that full MES participation will be limited in the forseeable due to inaccessibility of beamtime and lack of experience in the soft x-ray/VUV energy regime by MES users. There are significantly more microscopy/spectroscopy endstations than there are of beamline sources capable of providing full, independent operation of these endstations.

Table 7. Existing Soft X-ray/VUV Beamlines, Major Uses, and User Demand

ALS	1.0	BL 6.0.1 (CXRO microscope)	[fully subscribed]
	1.0	BL 7.0.1 (STXM, Fluorescence, general use, XAFS, μESCA	[over-subscribed by ≈3X]
	1.0	BL 9.3.1 (XSW, XAFS, no spatial resolution, 2.5% MES usage)	[fully subscribed]
NSLS	3.0	BL X1A, BL X1B, X-24A (STXM, SPEEM, XSW, XAFS)	[over-subscribed by ≈ 2X]
SSRL	1.0	BL 3-3 (XAFS, XSW, PES, no spatial resolution, 40% MES usage)	[fully subscribed]
	1.0	BL 8-1 (PES, 5% MES usage)	[near fully subscribed]
	1.0	BL 10-1 (PES, 1% MES usage)	[over-subscribed by ≈ 2X]

Total existing soft x-ray/VUV beamlines used or potentially useful for MES research: **9.0 BL**

4a. Inventory of planned soft x-ray/VUV beamlines and new capabilities

6.5 new soft x-ray/VUV beamline sources and microscopy/spectroscopy endstations are currently being built. Although these capabilities will be added to the beamline inventory in FY'97, the overdemand will still exist. MES researchers will continue to have limited access to these facilities, as will general users. The new facilities will provide improved microscopic/ spectroscopic capabilities in specific areas, but will not meet the demand of general users. None of the new facilities has been constructed with MES considered as a primary scientific program.

Table 8. New Soft X-ray/VUV Beamlines and Major Uses

ALS:	1.0	BL 4.0.1/2	PEEM (magnetic microscopy)
	1.0	BL 4.0.3/4	Magnetic spectroscopy
	1.0	BL 6.3.1	Reflectometry (Intel Corp.)
	1.0	BL 7.3.1.1	Microdiffraction/spectroscopy (internal)
	0.5	BL 11.3	SPEEM (polymer STXM, not useful for MES research)
NSLS:	1.0	BL X13	Novel soft x-ray magnetic microscope that will double as a conventional microscope (FY'97 operation)
SSRL	1.0	BL 5-2 VUV studies in the 10-40 eV region	
Total new soft x-ray/VUV beamlines (Completed in FY'97 or FY'98):			**6.5 BL**

5a. Recommendations for new soft x-ray/VUV spectroscopy/microscopy facilities

Because of the heterogeneous nature of many environmental samples, including both natural and synthetic samples, microscopy and micro-spectroscopy are becoming essential methods of MES research at synchrotron radiation facilities. Information on the spatial distribution of chemical species and the need to study samples of limited size or on selected sample locations is very important. In many respects, the high spatial resolution capability of microscopy is much further developed in the soft x-ray/VUV region in comparison to the hard x-ray region. The core levels of the low-Z environmentally important elements (C,N,O) are directly accessible in this region. Furthermore, nearly every element has an electron energy level within this ≈50-1500 eV range, suitable for investigation by photoemission and or absorption spectroscopy. Environmentally relevant processes often occur at interfaces and the soft x-ray regime has traditionally been the realm of surface science. Many important environmental surface interactions take place at aqueous interfaces, and soft x-ray microscopy/spectroscopy techniques are making great progress working with “wet” systems, as demonstrated recently at the ALS.

The 6.5 soft x-ray/VUV microscopy/spectroscopy beamlines that will come on line shortly, even when combined with the 9.0 existing soft x-ray/VUV beamlines, will not satisfy the demand for beamtime by soft x-ray/VUV users from all disciplines, based on current oversubscription rates of the existing beamlines. This statement is especially true for MES researchers who are just beginning to understand the potential of synchrotron radiation in the soft x-ray/VUV energy region for certain classes of MES research. Additional soft x-ray/VUV beamline facilities must be built to accommodate general user demand as well as the growing demand by MES users. Existing and new soft x-ray/VUV facilities have not been tailored to MES research, nor is it likely they will be given the severe over-demand for these facilities. Thus we strongly recommend the construction of two new soft x-ray spectroscopy/microscopy beamlines at the the ALS for MES research that would take advantage of this source's very high brightness. One would be optimized for simultaneous spectromicroscopy (using a zone plate) and x-ray emission spectroscopy (using a high-resolution grating) on environmental samples. The other would be optimized for soft x-ray spectroscopy in the 1-3 keV energy range. These proposed beamlines are described in detail in the white paper in Appendix E.

6a. Assessment of operations and user support needs

There is a critical need to maintain and provide a high level of user support at all microscopy/spectroscopy beamline facilities for the most efficient use of these scarce resources. Not only are these types of beamlines technologically complex, the MES scientific issues are diverse and complicated, and the shortage of these beamline facilities necessitates the most efficient operation possible. Furthermore, most new MES users will initially require assistance and training for a period of time. Excellent user support will make good scientific use of allocated beamtime and will help ensure that data are properly analyzed in a timely fashion.

The staffing model for such a beamline facility centers on a dedicated beamline scientist and a technical support associate. A postdoctoral fellow is also needed to provide enough scientific effort to run the beamline facility around the clock. The beamline facility should have a laboratory staging area for equipment and a basic preparation laboratory to support general MES user needs. In view of the fact that many MES experiments may involve hazardous materials, at least a 0.2 FTE should be included in the operational scheme to provide direct safety support.

b. Infrared Spectroscopy - Summary of Findings

The field of infrared synchrotron radiation (IRSR) science is rapidly expanding, with several new spectrometers and microscope endstations being fabricated. Microspectroscopy techniques will likely have the most impact in MES because of the ability to probe heterogeneous media. The method is non-destructive, allowing for the study of living cells. New beamline facilities at the ALS (1) and NSLS (4) will complement the two existing operational beamlines on the VUV ring at the NSLS. One of the beneficial aspects of the IRSR efforts is that they are compatible with most soft x-ray SR light sources (assuming adequate beam stability) and are regionally available. The availability of beamtime for general users (including MES users) is anticipated to be about two beamline-years at the NSLS and 0.5 beamline-years at the ALS. Best estimates of programmatic MES users at the two existing NSLS beamlines is between 5 and 10%. There appears to be sufficient beamtime for the next few years for MES expansion into this field. Workshops to demonstrate the utility of IR and microscopic techniques to the MES community are needed to develop a long term customer base for this type of spectroscopy.

1b. Activity level of the science and level of research funding

The first MES users have emerged in the last year at NSLS and constitute about 10% of the activity of a single beamline. The program to investigate fluid and gas inclusions in mineral specimens is one example. There are additional MES programs focused on environmental aspects of mineralogy and polymer science. IRSR beamline facilities for MES research are perceived to be under-utilized. Outside of the MES field, there has been an influx of research support through two funded DOE Scientific Facilities Initiative programs. Furthermore, a MSD-DOE 2% Initiative for infrared studies of complex metals will staff and maintain a programmatically focused beamline facility for the next several years, as well as a CRADA. The funding of non-MES programs in IRSR will provide sufficient opportunities for the envisioned beamtime needs of MES users in the next two to three years. Operational support for the beamlines after the SFI and 2% funding expires will need to be secured. Therefore, in approximately 2-3 years' time, MES operations on IRSR beamlines will require support.

2b. Assessment of user base

The present active MES user base at NSLS constitutes ≈10% of the operation of a single IR beamline. There has been a large over-subscription of the existing IRSR beamlines at the NSLS and potential MES users would have difficulty receiving beamtime as a result. The potential user base is not known, but is probably substantial. Therefore, with expanded availability, the number of MES researchers will increase as scientific opportunities in this area become known. A carefully planned workshop on IRSR science at the ALS or NSLS would help in assessing the current MES user base and in attracting new MES users.

3b. Inventory of existing IRSR facilities

There is currently 1.0 operating IRSR beamline at the NSLS (U4IR). New and existing IR beamline facilities will meet the perceived MES needs for the next 2-3 years. As the participation in the IR field increases by both general and MES users, a shortage of MES beamtime opportunities could occur in 2-3 years.

Existing IRSR beamlines: NSLS - 1.0 beamline; ALS - 0.0 beamlines

4b. Inventory of planned IRSR facilities and funding sources

Four new IRSR beamlines at the NSLS should be completed by the end of FY'97, bringing the total there to six fully dedicated IRSR beamlines, two with an end station and a side station. Thus a total of 6.0 IRSR beam stations at the NSLS will soon be available. The ALS will have a single IRSR beamline operational by the end of FY'97. These facilities have an appropriate blend of IR microscopy (≈ 50%) and the more conventional IR spectroscopy (≈ 50%) endstations, each with particular strengths. However, there is specialized equipment development needed for anticipated MES experiments, such as attenuated total reflectance cells. Regional needs will likely drive the development of additional IRSR beamlines or specialized facilities to satisfy these needs.

Table 9. Existing and New Infrared Synchrotron Radiation Beamlines

NSLS:	6.0 beam stations (BL's U4IR, U2A, U2B, U10B, U10A, U12IR)* Funded by SFI, MSD-DOE 2% initiative, CRADA, and NSLS internal support.
ALS:	1.0 beam stations (BL 1.4) Funded by ALS internal support
Total IRSR beam stations by the end of FY'97:	**6.0 at NSLS, 1.0 at ALS**

* Five new IR beamlines are expected to be on-line by the end of FY'97.

5b. Recommendations for new IRSR facilities

There is no immediate need for new IR facilities at the NSLS or ALS to support MES research. However, MES usage of IR facilities at the NSLS should be monitored to substantiate need for operational funding in the near future.

6b. Assessment of operations and user support needs

There is the distinct possibility that with the growth in MES usage and the distinct likelihood of the termination of beamline support from other sources, that funding will be needed to preserve MES activities in the IRSR area. Funding would be required in beamline operations support and for beamline scientists or technicians. Funding for MES-specific instrumentation should be included as part of this support.

D. SURFACE-SENSITIVE METHODS WORKING GROUP

Summary of Findings

- There has been an approximate doubling of MES research on soft x-ray/VUV beamlines at the NSLS and SSRL during the past two years, and an aproximate tripling of MES research on soft x-ray/VUV beam lines at the ALS.
- The number of beam stations used over the past year for soft x-ray/VUV research MES research is currently about 0.3 at the ALS, 0.25 (exclusive of x-ray/IR imaging) at the NSLS, and about 0.4 at SSRL. Another 0.5 beam stations at the NSLS are currently being used for MES research.
- The most significant growth areas for MES soft x-ray/VUV research are
    - Scanning transmission x-ray microscopy (STXM) of biological samples
    - L-edge spectroscopy for speciation determination
    - Photoemission/photoelectron diffraction studies of oxide and sulfide surfaces
    - X-ray standing wave studies of oxide and sulfide surfaces
- There is a significant growth potential in the following areas:
    - X-ray emission spectroscopy
    - Development of differentially pumped experimental chambers so that wet samples can be studied using soft x-ray wavelengths more routinely.

1. Activity level of the science

During the past two years, there has been a significant increase in the use of soft x-ray/VUV methods for MES research. The data in Table 10 document the usage of soft x-ray/VUV facilities at the ALS, SSRL, and NSLS for the past year.

2. Assessment of user base

This is the first detailed investigation of this growing field that had just begun to emerge at the time of the Airlie Report. It's too early to assess the user base.

3. Inventory of existing surface sensitive SR facilities

See section 1 above

4. Inventory of planned surface sensitive SR facilities and funding sources

See section 1 above

5. Recommendations for new surface-sensitive SR facilities

Based on the current user interest level in and availability of soft x-ray/VUV facilities available for MES research, we recommend that one new beamline at the ALS be constructed in the 50-1500 eV energy range that is optimized for surface-sensitive x-ray emission spectroscopy and spectromicroscopy. This recommendation is developed in more detail in the white paper in Appendix E.

6. Recommendations for user support for soft x-ray/VUV facilities

Because of the complicated nature of most soft x-ray/VUV experiments, these facilities require more user support than most other types of experimental facilities for MES research by the general user community. As recommended in section C.6.a, several staff scientists will be required to provide the heavy level of support required for general users, including those from the MES community, of these facilities.

Table 10. Usage Level of Soft X-ray/VUV Beamlines for MES Research*

Source	Beam Line	Main Usage	% Time for MES Research
ALS	4.0.1/2	under construction	0%
	4.0.3/4	under construction	0%
	6.1.2	Biomicroscopy	10%
	6.3.2	Soft XAFS, XPS	5%
	7.0.1/2	STXM/PED	10%
	8.0	PRT -Emission Spec	0%
	9.0	Gas phase studies	0%
	9.3.1	SEXAF, XSW	0%
	9.3.2	PED, XPS	5%
	10.3.1	X-ray microprobe	10%
		Total	**40% of a BL**
NSLS	X1A	STXM, SPEEM	25%
	X1B	STXM, SPEEM	25%
		Total	**50% of a BL**
SSRL	1-1	PES	0%
	1-2	PES	0%
	3-3	SEXAFS, XSW	40%
	5	PES	0%
	8-1	PES	2%
	8-2	PES	2%
	10-1	PES	1%
		Total	**45% of a BL**

* A total of 1.35 soft x-ray/VUV beamlines is currently available for MES research.

E. ES&H/OPERATIONS WORKING GROUP

Summary of Findings

A relatively large scientific community is currently involved in basic and applied science centered on actinide-containing materials. For historical reasons, many of these researchers are conservative in their experimental approach, and hence slow to realize the enormous potential of synchrotron-based techniques in their research. For example, the widely tunable, high energy photons available from modern synchrotron sources provide the capability for a variety of non-destructive experiments on impure, non-crystalline, and very small samples. These are exactly the types of samples that the actinide researcher must manipulate. The impact of synchrotron-based experiments is just now beginning to be realized within the actinide community, and we anticipate a growing interest in synchrotron-based studies of actinide materials, which is expected to increase significantly over the next several years. Synchrotron-based research is expected to have an important impact in areas such as decontamination/decommissioning, health/ecology/risk, waste forms, fissile materials and storage, spent nuclear fuel, subsurface characterization, waste characterization, waste treatment and destruction, plutonium stabilization, and cleanup. With these changes in mind, there will be an increasing need for access to expertise, infrastructure, and safety protocols for working with actinide elements at synchrotron facilities.

The relatively high energy photons (>5 keV) used for most experiments on actinide-containing samples permit rigorous sample encapsulation. Therefore, the radioactive material can be encapsulated at the home institution and transported to the light source, the experiments performed, and the samples transported back to the home institution. All of this is currently done without the need for open-sample procedures and for protocols to be in place at the synchrotron laboratory. However, adherence to these sample-management procedures does not obviate the necessity for strict safety protocols at the beamline where radioactive samples are being run. There remains the need for radiological monitoring, emergency procedures, and special sample transport and handling protocols. For example, actinide work at SSRL employs an air exhaust system that has continuous air monitors (CAMS) which can be accessed remotely at any time. The set-up, calibration, and maintenance of these monitors must be carried out by appropriately trained personnel. The protocols for performing experiments require intensive participation from radiological personnel. In addition, the transport of samples to and from the synchrotron site requires Special Materials personnel to assure quantity limits are not exceeded at the facility, and that all samples are shipped according to the strict requirements set forth by DOE and the DOT. Overall, these procedures add to the staff burden for performing synchrotron-based experiments.

The existing and newly-funded facilities that will come on-line in the near future (SSRL: BL11; APS: PNC-CAT, GSECARS-CAT, BESSRC-CAT, and MR-CAT; ALS) are expected to provide adequate beamtime for XAFS work over the short term (< 5 yrs). We envision a growing demand on beamlines devoted to microprobe, infrared, x-ray standing wave, scattering, and diffraction experiments. In contrast to the situation regarding hardware, the operations support for the existing beamlines is currently inadequate, and is expected to become critical as the user base continues to grow. In addition to the standard beamline staffing requirements, there is a need for safety protocols and health physics technicians trained in monitoring alpha-active materials, nuclear and hazardous materials storage requirements, and nuclear material tracking, and quality assurance. Whereas these requirements will demand increased personnel, the extent of the burden, both to the facility staff and to the users, can be minimized if there is cooperation among the light sources. We recommend that a modicum of standard operating protocols be developed and employed by all the labs for experiments involving radioactive samples. We envision that a set of baseline protocols could readily be tailored by individual researchers to benefit from an optimized work-load. To develop these protocols, we recommend that scientific and ES&H personnel from all US-based synchrotron sources meet to discuss and devise a baseline set of routine controls and procedures for handling radioactive materials. The requirements and procedures particular to each synchrotron, for example the Actinide Facility at the APS or BL 11 at SSRL, could then be expanded from this standard set of protocols.

Appendix A. Invitation Letter to SSRL Workshop Participants

Dr. Paul Bertsch
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P.O. Drawer E, Bldg. 737A
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Dear Paul:

I recently spoke with you by telephone about the workshop you have been invited to attend on Molecular Environmental Science & Synchrotron Radiation Facilities. It will be held at SSRL on Friday (Jan. 17) and Saturday (Jan. 18). As I indicated in our conversation, the workshop was requested by Dr. Robert Marianelli of DOE-BES-Chemical Sciences and Dr. Roland Hirsch of DOE-BES-OHER, and its main purpose is to bring the 1995 Airlie Report on synchrotron facilities for molecular environmental science (MES) research up to date. To remind you what we concluded at the Airlie Workshop, I have enclosed Chapter 7 from the Workshop Report. This updating should include a revised assessment of the synchrotron radiation facilities at DOE-supported labs available for MES research, including those that have been planned or proposed since the Airlie Workshop and those that have received funding from the DOE Facilities Initiative and/or the recent Environmental Management Science Program. We have also been asked by Bob and Roland to provide revised estimates of the MES user bases at each of the laboratories and the types of users (i.e., large groups with significant funding, small groups with less funding, and/or individual users with even less funding, and the levels of experience of different groups). The purpose of these revised estimates of the MES user base is to provide DOE with a sense of what levels of operations support might be needed over the next five years at the various synchrotron radiation facilities devoted in whole or in part to MES research. One specific topic that we have been asked to assess is the need for MES-synchrotron radiation facilities in the soft x-ray and VUV areas. A list of the invited workshop participants is enclosed.

With these objectives in mind, I would like you to come to the workshop with as much relevant background material as possible, including information on the status of the facility you represent in the MES area, any plans for expansion of or changes in the facility that will affect MES research, detailed information about the MES user base at your facility, and any ideas you might have about the need for new MES-synchrotron facilities. A list of MES users and the titles of their projects over the past five years at your facility would be an excellent starting point for assessing the user base. Compiling a list of this type from each of the labs would also help us in determining the relative popularity of the different synchrotron methods in MES research and the types of problems different groups are working on. Thus, I urge you to try to collect as much of this type of material as you can in the short time before the workshop. Because of the relatively short duration of the workshop (1.5 days), having this background material available at the beginning of the workshop is essential. My hope is that we will generate a short report at the workshop that provides DOE with the requested information. We will have both Macintosh computers and PC's with Microsoft Word 5.1 for word processing, so you should bring material on disk in Microsoft Word format if possible.

The workshop will begin on Friday morning (Jan. 17) at 8:15 in the SSRL-LOS Building main conference room (Third Floor) with a continental breakfast. We will begin discussions at about 8:45 and will continue through a working lunch. You should be prepared to make a brief presentation about your facility and research area, what's being planned, information on the MES user base at your facility, and thoughts on what new MES-synchrotron radiation facilities are needed over the next five years and the exciting science that will justify these new facilities. Following lunch, we will break up into smaller working groups to begin preparing sections of the workshop report. We will have dinner at 6:30 pm at the Stanford Faculty Club, and after that you can retire to your motel. The enclosed list of accommodations should give you some choices of motels. I urge you to make reservations as soon as possible. We will begin work again on Saturday morning at 8:15 am with a continental breakfast and additional presentations on some of the conclusions we have reached at that point. Lunch will be provided on Saturday about noon, and the workshop will break up shortly after lunch with a final summary presentation. For those of you who wish to depart for home on Saturday, Jan. 18, we should be done by about 1:30 pm.

Bob Marianelli has agreed to pay the travel (economy) and per diem expenses for university types, but he expects workshop participants from the DOE labs to pay their own travel/per diem expenses out of existing budgets. SSRL, through DOE-BES funding, will provide meals during the workshop. University types should submit their expense reports to SSRL for reimbursement duriing the workshop.

I look forward to seeing you on Friday morning, January 17, and to a productive day and a half. The results of this workshop will almost certainly become an important part of the the soon-to-be-held BESAC review of synchrotron radiation facilities in the U.S., so it is important that we provide DOE with the most objective survey of existing MES synchrotron facilities, needed facilities, estimates of funding needed to operate these user facilities, and MES user bases that we can.

Thanks for agreeing to participate in this important review.

Best regards,

Gordon E. Brown, Jr., Chair
SSRL Workshop on Molecular Environmental Science and
Synchrotron Radiation Facilities

Main Findings of 1995 DOE-MES-Airlie, VA Workshop

• X-ray absorption fine structure (XAFS) spectroscopy and micro-XAFS are currently the most useful synchrotron-based methods for defining metal contaminant speciation and spatial distribution in complex environmental matrices.

• Soft-x-ray and infra-red spectromicroscopies are potentially very useful for studying the speciation and distribution of organic contaminants in soils.

• A survey of MES users shows that the number of available synchrotron beamlines for MES research (the equivalent of 3.6 full-time experimental stations, nationally) is currently saturated by this group.

• This survey also indicates that future demands for beam time in this research area will double in the next three years.

• Completion of the equivalent of 3.25 planned MES beamline stations at SSRL and APS over the next three years will not likely meet this increased demand after 1998 because of anticipated needs for service work on environmental samples and new research directions.

• Controlled clean labs built around or adjacent to environmental science experimental stations at synchrotron sources are required to permit safe sample handling, minimal sample preparation, and safe experimental studies on highly toxic and radioactive samples. Funding for these labs is a high priority.

• Funding for personnel at planned environmental science beamlines is needed to provide user support and training, technical development, equipment supervision and maintenance, and environmental safety and health needs.

Conclusions from 1995 MES User Survey and 1995 Workshop Estimates of MES Beam Time Availability

- **The estimate of 1996 usage in station days/year for MES research matches the current requirement, based on the MES user survey.**

- **The beam stations currently available for MES research (none of which are fully dedicated to this research area) are fully subscribed. MES beam time demand is being satisfied at the expense of other types of research.**

- **The MES user survey suggests a demand doubling timescale of 3 years for existing research areas. This will lead to a near-term shortfall of station days for MES research.**

- **Planned beam stations to be devoted in whole or in part to MES research will double the supply of beam time in about 1998. This is about the same time that the demand for MES beam time will double.**

- **This conservative estimate suggests the need to consider soon an increase in the number of beam lines devoted to MES research and/or increased efficiency in the use of existing beam lines.**

- **New research directions (e.g., soft x-ray and IR microscopy of organic and biological samples) and potential demand for service operations may produce a severe beam time supply shortfall.**

Supply of and Demand for Beam Time for Environmental Research
(from 1995 Airlie Workshop Report)

Synchrotron Facility	Technique or Group	Stations (current)	Stations (under construction or planned)
NSLS	XAFS (conventional)	1.0	
	XAFS (spatially resolved)	0.5	
	Scattering	0.1	
	Microprobe and tomography	0.5	
SSRL	XAFS (conventional)	1.0	
	Environmental Research (B11)		1.0
CHESS	XAFS (conventional)	0.3	
ALS		0.2	
APS	CARS		0.75
	PNC		0.5
	BES		1.0
Total Stations		3.6	3.25
Number of Station Days Available		~660 days/yr ('94) ~704 days/yr ('96) ~728 days/yr ('97) ~728 days/yr ('98)	~520 days/yr ('96) ~700 days/yr ('97) ~880 days/yr ('98)
Number of Station Days Required (Survey Results)		~720 days/yr ('94)	Anticipated to increase to ~1450 days/yr by 1998

Appendix C. SSRL Workshop Agenda

Agenda for the
Molecular Environmental Science & Synchrotron Radiation Facilities Workshop

Stanford Synchrotron Radiation Laboratory
Stanford, CA
January 17-18, 1997

Friday, January 17

8:00-8:30	Continental Breakfast at SSRL
8:30-8:50	Introductory Remarks and Organization of the Workshop (Gordon Brown, Stanford University and SSRL)

MES Facilities/Research Reports

8:50-9:10	Overview of the Advanced Light Source (Neville Smith, ALS)
9:10-9:25	Examples of MES Research at the ALS (David Shuh, LBNL)
9:25-9:45	Overview of the Advanced Photon Source and GSECARS-CAT (Mark Rivers, CARS)
9:45-10:00	PNC-CAT at the APS and MES Research at PNNL (Ray Stults, PNNL)
10:00-10:15	Plans for MES Research at the APS and ANL (Lynda Soderholm, ANL)
10:15-10:30	Overview of NSLS and MES Research at the NSLS (Eric Johnson, NSLS)
10:30-10:45	IR Microscopy Facility at the NSLS (Larry Carr, NSLS)
10:45-11:00	Coffee Break
11:00-11:15	Hard X-ray MES Studies at the NSLS (Paul Bertsch, SREL)
11:15-11:30	X11-A PRT at the NSLS (Dale Sayers, NCSU)
11:30-11:45	MES Facilities at SSRL (Tom Rabedeau, SSRL)
11:45-12:00	Examples of MES Research at SSRL (Gordon Brown, SSRL)
12:00-12:15	MES Actinide Research at SSRL (Steve Conradson, LANL)
12:15-12:30	Discussion
12:30-1:15	Working Lunch

ES&H/Operations Issues

1:15-1:30	Safety Issues in Actinide Research (David Clark, LANL)
1:30-1:45	ES&H Considerations in MES Research at SSRL (Ian Evans, SSRL)
1:45-2:00	The Biotech Model for User Support at SSRL (Britt Hedman, SSRL)

2:00-5:30 **Working Group Meetings**

Objectives: To evaluate existing or planned facilities in the following areas, to review MES user bases at US-DOE synchrotron radiation facilities, and to recommend needed facilities and operations/user support.

A. XAFS Spectroscopy Working Group (Bargar, Conradson, Hedman, Sayers)
B. X-ray Imaging Working Group (Bertsch, Rivers)
C. Soft X-ray/IR Microscopy-Spectroscopy Working Group (Carr, Johnson, Myneni, Shuh)
E. X-ray Standing Wave/Surface Scattering/Photoelectron Diffraction/ Photoemission Spectroscopy Working Group (Brown, Rabedeau, Smith)
F. ES&H/Operations Working Group (Clark, Evans, Soderholm)

6:30-8:30 Dinner, Stanford Faculty Club

Agenda for the
Molecular Environmental Science & Synchrotron Radiation Facilities Workshop

Saturday, January 18

8:00-8:30	Continental Breakfast at SSRL
8:30-8:45	Report from the X-ray Spectroscopy Working Group
8:45-9:00	Report from the X-ray Imaging Working Group
9:00-9:15	Report from the Soft X-ray/IR Microscopy-Spectroscopy Working Group
9:15-9:30	Report from the X-ray Standing Wave/Surface Scattering/Photoelectron Diffraction//Photoemission Spectroscopy Working Group
9:30-9:45	Report from the ES&H/Operations Working Group
10:00-11:00	Discussion of Findings and Recommendations from the Working Groups
11:00-12:30	Completion of Working Group Reports
12:30-1:30	Working Lunch
1:30-2:00	Concluding Remarks

Appendix D. Names and Addresses of SSRL Workshop Participants

LIST OF PARTICIPANTS
DOE MOLECULAR ENVIRONMENTAL SCIENCE & SYNCHROTRON RADIATION FACILITIES WORKSHOP

JANUARY 17-18, 1997
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