Title
Report of the Workshop on an Advanced Soft X-ray and Ultraviolet Synchrotron Source: Applications to Science and Technology

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Report of the Workshop on an Advanced Soft X-Ray and Ultraviolet Synchrotron Source: Applications to Science and Technology

November 13-15, 1985
Berkeley, California

Lawrence Berkeley Laboratory
University of California
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Workshop on an Advanced Soft X-Ray and Ultraviolet
Synchrotron Source:
Applications to Science and Technology

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Contents

Note: The pages are numbered by their chapter numbers.

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ABSTRACT

More than 200 scientists and engineers from universities, national laboratories, and industry met at the Berkeley Conference Center from November 13-15, 1985 to discuss the new research opportunities that would become available with the construction of a synchrotron radiation source optimized for high spectral brightness and high coherent flux at soft x-ray and ultraviolet wavelengths. These investigators found that the generation of such radiation over the proposed spectral range of a few eV to several keV creates entirely new opportunities in biology, chemistry, and atomic and molecular physics, as well as in materials, interface, and surface science and in industrial research and technology. Some of these areas would variously exploit the high intensity available from wigglers or the high brightness and coherence available from undulators, while others would depend on the availability of very short pulses (20-50 picosecond duration) or radiation having adjustable polarization. Workshop leaders representing these diverse interests reached a consensus that the requisite synchrotron radiation facility would have twelve straight sections and would operate at a nominal electron-beam energy of 1.5 GeV. This report presents the findings of nine working groups, six of which focused on the frontiers of their scientific disciplines, and three of which had a technological focus.

Workshop on an Advanced Soft-X-Ray and Ultraviolet Synchrotron Source: Applications to Science and Technology

Berkeley, 13-15 November 1985

Introduction and Summary

Science, containing man's knowledge of the natural world, is based on observation. Even the most elegant of theories derive their substance from experiment. Advances in experimental resources thus provide the foundation for progress in science and its applications in technology, engineering, and medicine.

The earliest observations of natural events were made by eye, with visible light. Galileo's telescope and Huygen's microscope extended the range of human observation to much larger and much smaller objects than could be seen previously; the scope of science was thus greatly enhanced.

Today's observations are usually more indirect than in Galileo's and Huygen's time, and require far more sophisticated means. But light remains an essential probe— albeit extended from the visible to longer wavelengths, as for radiotelescope exploration of the outer reaches of the universe, and to far shorter wavelengths, as for the x-ray spectroscopy of atoms and molecules. It is therefore readily understandable that the advent of a new light source of unprecedented properties should be eagerly anticipated, for it will lead to a rich harvest of previously inaccessible scientific information. A previous example illustrating this point is the development of lasers, which have now become so useful in many areas of science and technology.

At the Workshop held November 13-15, 1985 in the Berkeley Conference Center, more than 200 investigators gathered to discuss the potential uses of a projected synchrotron-radiation source that would produce ultraviolet radiation and soft x rays with properties well beyond anything available in the United States today: very high intensity, extreme brightness, very fast pulses, adjustable polarization, and exceptional coherence. Participants included physicists, chemists, biologists, engineers, and physicians from universities, national laboratories, and industry. Their primary interests were not only in experimental and theoretical basic research but also in applications to new materials, products and devices, and technological topics ranging from diagnostics of heart disease to national defense.

An overwhelming abundance of ideas for investigations with the new source was presented. The enthusiasm of the participants made it clear that many waited with great anticipation for a chance to set up new experiments permitting the measurement of phenomena and effects that are as yet beyond our grasp.

In atomic and molecular physics, the brightness of the new source will permit spectroscopists to measure effects in very dilute gas sources. Relativistic, quantum-electrodynamic, and correlation effects will be readily measurable. Also, the properties of open-shell atoms, atoms in excited states, and highly stripped ions can be studied: These are systems that occur in astrophysical and plasma environments and that may someday serve in x-ray laser schemes. Some of these experiments will involve combinations of the synchrotron source with tunable lasers and with heavy-ion beams, storage rings, or traps. The vibrational structure of molecules will become resolvable, even for core levels. It will become possible to study the dynamics of energetic processes in atomic inner shells, including resonances that occur on a uniquely fast time scale. The high intensity of the light from the new source will allow experimenters to measure spin polarization of photoelectrons— the third crucial quantity in photo-effect (in addition to energy and angle). Thus, the degeneracy in the continuum between the two spin components will be lifted, permitting the complete determination of all transition amplitudes and leading to direct measurements of relativistic interactions in atoms. The brilliance of the source will permit measurements on tiny samples of rare materials, such as the radioactive actinides, whose properties have largely eluded determination in the past because the small available quantities were insufficient for study by traditional means.

In biology and medicine, one of the most attractive potential capabilities of the projected synchrotron radiation source lies in the area of imaging small biological specimens— perhaps even macromolecules. The high brightness and considerable coherence of the radiation from undulators in the new source offer promise for the success of new techniques for imaging of wet, unstained biological samples through x-ray microscopy and holography, contact microscopy, and soft-x-ray diffraction, with sufficiently short exposure times to permit dynamical studies. Utilizing another novel property of the source, biophysicists anticipate switching rapidly between right- and left-circularly polarized light in order to measure, through circular intensity differential scattering, the higher-order structure of polymers in biological systems. Medical researchers look forward to further development of such techniques as noninvasive angiography. Differential coronary angiography with tuned synchrotron radiation is in an exploratory stage. It permits detailed imaging of coronary arteries more rapidly, and with far less risk to the patient than the traditional method involving catheterization.

Interesting applications of the new source are anticipated in the area of chemical dynamics, which encompass all phenomena in which molecules undergo energetic or chemical transformations. As a photolysis source, the synchrotron ring can produce macroscopic yields of vacuum ultraviolet photoproducts. Operated in conjunction with an infrared free-electron laser, the source will be a powerful tool for the study of chemical processes induced by infrared multiphoton absorption. The time structure of the synchrotron light will permit the study of ultrafast processes. For example, the cleavage of the chemical bonds of photoexcited molecules can occur in picoseconds; such processes could be followed through special techniques, utilizing the fast pulses and high repetition rate of the new source. Bond-selective photochemistry will be possible, using a new technique through which specific bonds in large molecules can be cut selectively with tunable ultraviolet radiation, "as with a scalpel." Cluster chemistry is an exciting new field, in which aggregates of atoms or molecules that exhibit the transition between the properties of isolated atoms and those of the solid state are studied.

Here, the new source is ideally suited for measurements of such phenomena as the variation of ionization energies with cluster size, and hence, of the onset of bulk properties as the size of the aggregates increases. Finally, photoionization mass spectroscopy and photoelectron spectroscopy can provide valuable thermochemical data that serve to characterize the structure and energetics of reactive intermediates in chemical reactions. The high ultraviolet output of the new source will make it possible to conduct such studies with unprecedented sensitivity and resolution.

Several of the most exciting applications of the new source lie in the field of materials, interface, and surface science. An outstanding challenge in experimental studies of solid surfaces is the performance of real-time measurements on dynamically changing systems. The high flux and brightness of the radiation from the proposed ring and its sharp time structure will make it possible to study chemical reactions, phase transitions, and the time evolution of excited states, giving new insight into intermediate states and reaction dynamics. For example, time-resolved NEXAFS can be used to observe a phase transition, a chemical reaction of molecules on a surface triggered by the admission of a gas pulse onto it, or a temperature-induced change of an adsorbed species.

Enhanced spatial resolution is another beneficial consequence of the high brightness of the new source; this will make possible a new class of surface analytic measurements, viz., the combination of microscopic imaging and photoelectron spectroscopy. A photoelectron spectromicroscope will provide images in which the contrast is due to differences in molecular species and chemical environment as reflected in the binding-energy spectrum. The range of problems accessible with this approach encompasses virtually all of materials science: analysis of individual grains of polycrystalline samples; correlation of surface chemistry and contrast due to magnetic domains; studies of chemically active small particles on substrates, as in supported metal catalysts; the morphology and surface chemistry of thin-film growth; and finally, studies of the surface chemistry of electronic devices through spatially resolved surface chemisorption, which could be applied to surface modification processes in device fabrication.

Every technical advance in the utilization of synchrotron radiation has given rise to new opportunities in materials and surface science. One dimension that has yet to be exploited in the U.S. is electron-spin resolution. Spin polarization of photoemitted electrons is due to the exchange interaction in magnetic materials, and to the spin-orbit interaction in nonmagnetic materials. For magnetic materials, the opportunities span from very basic questions concerning theories of finite-temperature itinerant magnetism and surface critical phenomena, to applications-oriented areas associated with film growth, and the properties of magnetic memory and recording devices.

The new machine will allow significant advances in core-level spectroscopy, which today represents the mainstream of applied research with synchrotron radiation. Core-level spectroscopy can be applied to understanding many complex materials and interfaces that occur in technological applications. Highlights include the use of core-level shift and intensity measurements in characterizing metal-semiconductor interfaces, and the application of EXAFS and photoelectron diffraction to determine the bonding geometries of a variety of surface and interface systems. A consequence of such studies will be predictive capabilities as to interface formation and materials engineering, both of which are crucial for many areas of high technology, including current development in microelectronics.

The new source furthermore has significant potential for defect spectroscopy of semiconductor interfaces and surfaces, for which no suitable probe now exists. Soft-x-ray photoabsorption studies may be extended to determine the local structure around atoms present in very dilute concentrations in a host system, and this will be an extremely important achievement in surface studies of precursor states, oxidation, poisoning, and chemical reactions on transition-metal catalysts.

Finally, materials science will benefit from the soft x-ray and vacuum ultraviolet scattering capabilities of the new facility. Scattering at these wavelengths is uniquely suited for studying structures which have feature sizes larger than atomic, but this possibility has not yet been exploited. One possible application is scattering from ultra-thin polymer films on solid substrates; these structures are of both scientific and technological interest.

The new source will also offer important opportunities for advanced <u>industrial research and technology</u>. Foremost among these is cutting-edge research in advanced lithography, addressing issues related to 0.25-µm, the lithography for 64-Mbit chips and extending beyond. Central to this aim will be the development of advanced imaging techniques, probably by means of projection optics (rather than proximity printing). Other industrial applications include micromachining, surface scanning, contact transmission microscopy, holography, and polymer characterization and optimization.

Considerable attention was given during the Workshop to <u>new techniques</u> that may become possible with the proposed source, such as laser-synchrotron picosecond-pulse experiments, dynamical diffraction from crystals with glancing-incidence x rays, and the possibility of using the synchrotron-source injector as driver for an infrared free-electron laser. Storage-ring and beamline issues were discussed in some detail.

At the end, working-group leaders met to determine what the optimal parameters for the new facility should be in order to permit the exciting new research and development that had been proposed throughout the Workshop. Consensus was reached on parameters that appear to be thoroughly feasible: Nominally 1.5-GeV electron-beam energy with a current of 400 mA, 12 straight sections in the ring, pulse structure of 20 to 50 psec, with minimum jitter, and a horizontal emittance below 10^{-8} π m-rad. Undulator fundamentals desired from 4 eV to 900 eV, with tuning possible during operation; position and angular stability of the beam should be a small fraction of nominal values of these quantities, beam lifetime should exceed 6 hours, considerable floor space should be made available for experimental apparatus, and the ring design should be flexible so as to permit operation up to 1.9 GeV, and perhaps to as low as 0.75 GeV electron energy. It is expected that machine physicists will be able to complete a conservative final design that meets these requirements, creating one of the potentially most productive and innovative facilities for research and development in the United States.

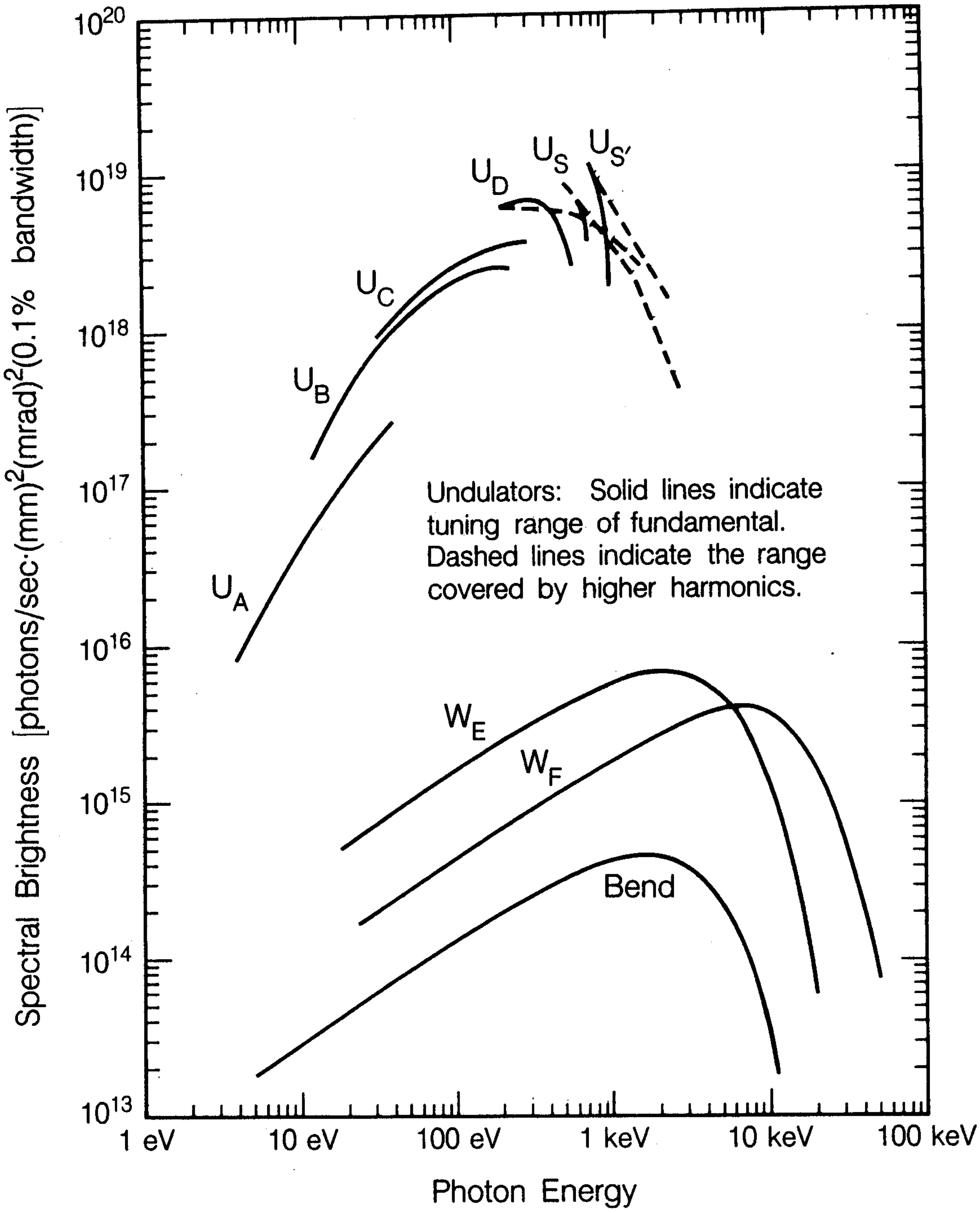
Nominal Storage Ring Parameters

Beam Energy	1.5 GeV
Average Current	400 mA
Horizontal Emittance	$< 10\ \pi$ mm μrad
Straight sections	12
Time structure	20—50 psec
Lifetime	> 6 hours

Other directions for desirable performance:

Flexible lattice design permitting operation to 1.9 GeV, and perhaps as low as 0.75 GeV.
Spectral brightness as high as possible.
Undulator fundamentals extending from as low as 4 eV to as high as 900 eV, with as broad a tuning range as possible.
Bunch lengths as short as possible, with minimal jitter.
Position and angular stability within fraction of nominal widths.
Lifetime as long as possible.
Undulator tuning during operation.
Reasonable horizontal-vertical coupling.
Substantial floor space at and near experimental stations.
Possibility for single-bunch experimentation at some stations.
Future upgrades to include a long UV undulator for FEL research.
Possible use of the injection linac to drive an IR/FEL.

Spectral Brightness for an Advanced Soft X-Ray/VUV Synchrotron Radiation Facility Operating at 1.5 GeV



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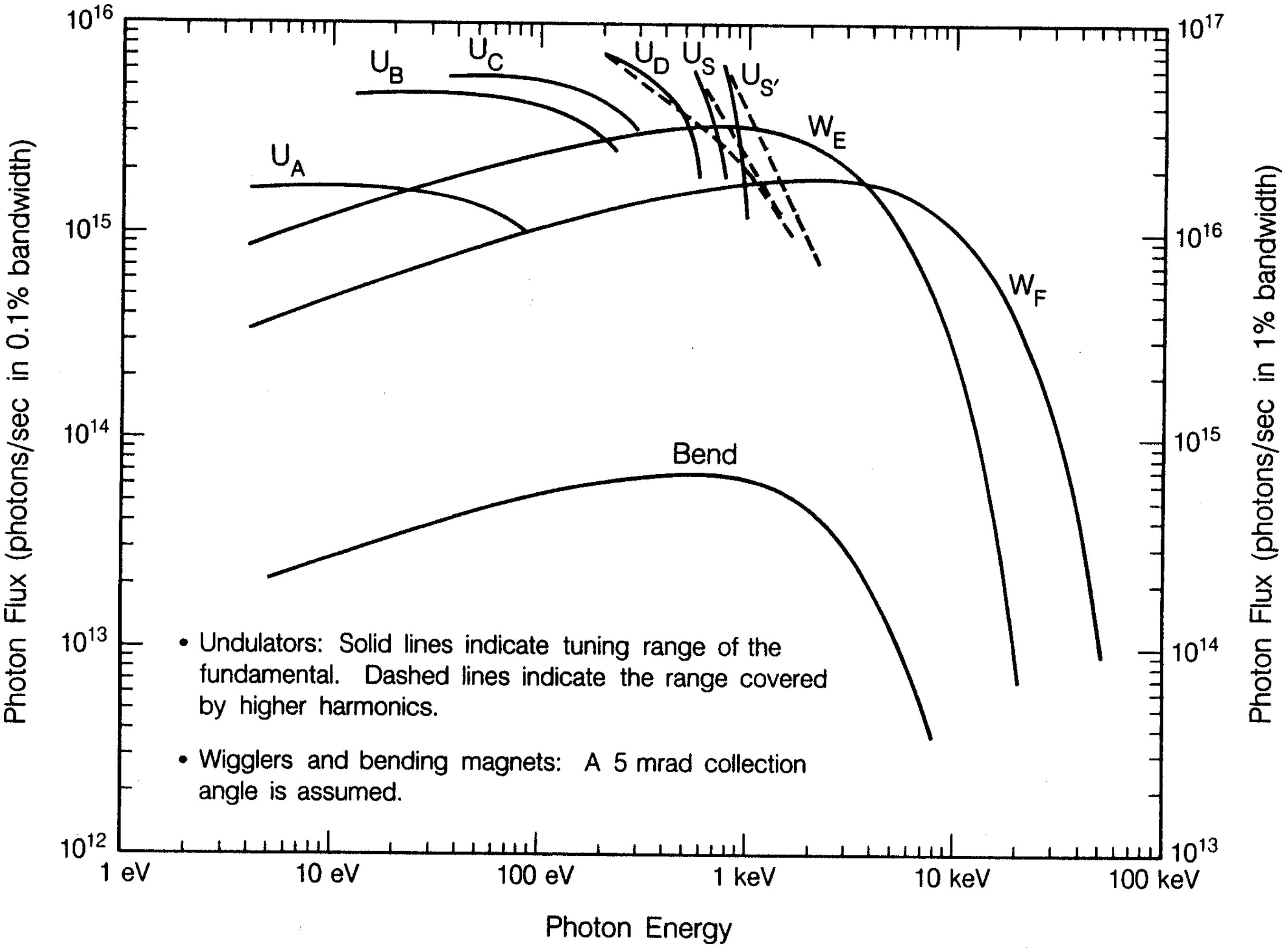
Photon Flux for an Advanced Soft X-Ray/VUV Synchrotron Radiation Facility Operating at 1.5 GeV



- Undulators: Solid lines indicate tuning range of the fundamental. Dashed lines indicate the range covered by higher harmonics.
- Wigglers and bending magnets: A 5 mrad collection angle is assumed.

XBL 8512-12221

PART I. SCIENTIFIC AND TECHNOLOGICAL OPPORTUNITIES

Materials, Interface, and Surface Science

INTRODUCTION

The vacuum-ultraviolet and soft x-ray regime that was opened to experimentation in the last 10-15 years by various synchrotron radiation sources has been a valuable tool in the study of materials, interfaces, and surfaces. The powerful techniques developed and utilized in those years have included surface EXAFS and related techniques, photoemission at an ever-improving level of sophistication and a much expanded range of application, and photodesorption of ions and related techniques. It is furthermore expected that the substantial improvements in the flux and brightness emanating from a 1-2 GeV storage ring based on insertion devices will lead to a considerable expansion and diversification of these existing techniques. Also, experiments that are now wither only barely possible or not at all possible will become feasible. For instance, by trading flux for resolution, ultrahigh resolution photoemission experiments or photoelectron microscopy will be possible. In the valence-band region, a variety of effects in condensed matter physics such as superconductivity, electron-phonon instability, and heavy fermion systems will be probed at their intrinsic energy scale, which has been inaccessible so far. High resolution core-level spectroscopies will allow detailed investigations of crystal and interface growth phenomena. Core levels of important materials such as most common metals and the light elements in organic materials will be probed for the first time with sufficient resolution for chemical analysis of surfaces and interfaces.

The construction of a new ring should be based at least as much on the qualitatively new techniques it will allow as on the expansion of existing capabilities. There will be ample direction for the introduction of new techniques following the commissioning of an insertion-device-based ring. For example, the increased sensitivity inherent in using ~ 10^4 times more light can be applied to study surface and bulk defects and impurities at a physically interesting and technologically relevant level of dilution. Using the currently available sources in this country, this is simply not possible. Another area in which a revolution in anticipated is in the area of magnetic materials. The capability of spin detection in photoemission, combined perhaps with a spatial resolution of less than a magnetic domain size, will lead to a better fundamental understanding of the interplay of geometric, electronic, and magnetic structure, as well as to direct technological applications in magnetic storage. Finally, the new source will enable heretofore impossible studies of dynamical systems via time-dependent studies. These will, for example, probe semiconductor carrier dynamics on a picosecond time scale as well as the sub-millisecond activated processes involved in such diverse phenomena as surface chemical reactions, crystal growth, and nucleation.

Contributors were F.J. Himpsel and S. Kevan (Co-chairmen), W. Eberhardt, N.V. Smith, D.W. Lynch, R.S. Williams, B. Tonner, J.H. Weaver, C.F. Chan, N.J. Dinardo, W. Ellis, N. Edelstein, L. Cox, J. Kortright, C.S. Fadley, J. Bokor, S. Bader, J. Stöhr, and G.J. Lapeyre.

The following pages detail these and other surface- and materials-related experimental capabilities that will be enabled by a 1-2 GeV insertion-device-based storage ring. Table 1-1 summarizes the interconnections between anticipated new capabilities and specific scientific and technological issues to which they can be applied. Each subsection elucidates the immense opportunities that this ring will allow, most of which cannot even be attempted using currently available sources. Each section concludes with details of any special requirements that the proposed science will make on the ring and the facility. The collective needs of the surface and materials science community are summarized in the "User Policy and Facilities" section at the end of this report.

SCIENTIFIC ISSUES

TIME DOMAIN STUDIES

Real-time experiments on dynamically changing systems are certainly one of the outstanding challenges in experimental studies of solids and surfaces. Making use of the increased flux and brightness from such a source, it will be possible to study chemical reactions, phase transitions or the time evolution of excited states in real time. This will give new insight into intermediate states and reaction dynamics. In the following we describe these experiments in the order of increasing time resolution.

Time-Resolved Photoemission and Absorption Fine Structure Studies

One of the exciting new areas of research made possible by such an advanced synchrotron radiation source is in real time photoemission and absorption fine structure (SEXAFS and NEXAFS) studies involving dynamical changes of the sample. The process involved could be a phase transition, a chemical reaction of molecules on a surface triggered by exposure to a gas pulse, or a temperature-induced change of an adsorbed species. Many molecules are known to undergo these chemical transformations with temperature. One example is methanol (CH_3OH) on transition metal surfaces. At very low temperatures, the molecule adsorbs intact and forms methanol ice. Upon a slight annealing, a methoxy species forming a bond between the oxygen and the surface is known to be the predominant state adsorbed. Further heating removes the hydrogen atoms of the CH_3 group. Finally a CO species is left on the surface that is eventually desorbed or dissociated. This is only one example, but it illustrates nicely the multitude of possibilities for real time studies. In real-time spectroscopy, we would be able to detect reaction intermediates and also determine activation barriers and rate constants.

Under present conditions it is possible to measure a photoelectron spectrum within 0.1 or 0.01 sec using a parallel detection scheme. Making use of the increased intensity and smaller spot size of an undulator beamline it would be possible to reach a time resolution several orders of magnitude better. NEXAFS and SEXAFS spectra are presently recorded by stepwise scanning the photon energy. In the future a monochromator/sample arrangement could be designed where the x-ray beam

Table 1-1.

New Capabilities

1. Time domain	2. Spatial resolution	3. Spin-polarization	4. Ultrahigh energy and momentum resolution	5. Advanced core level spectroscopy	6. Dilute systems, defects	7. Soft x-ray scattering	Issues
X			X	X	X		1. Electronic structure: • Bonding at surfaces/interfaces • Fermi level pinning in semiconductors (ohmic contacts, indirect doping, traps) • Energy bands
	X	X	X	X			2. Magnetism and superconductivity: • Magnetic materials (information storage, permanent magnets) • Heavy Fermions
X	X			X		X	3. Surface chemistry: • Heterogeneous catalysis • Processing of microstructures (etching, growth)
			X	X	X	X	4. Materials Engineering: • Polymers, organic materials • Composite materials (grain boundries, alloys) • Epitaxial layers (superlattices, strained layers)

is dispersed across the sample such that different points (lines) on the sample correspond to different photon energies. For example, a 1-cm-long area on the sample could correspond to a 300 eV photon energy range. By suitably imaging the electrons originating from the 1-cm-long area onto an area-sensitive detector (e.g., via a magnetic field), an entire absorption spectrum could be recorded at one shot. It appears that with the intensities of the new source NEXAFS/SEXAFS spectra could be recorded in a 1-10 msec period. This would allow one to study not only the above mentioned cases where the rate of temperature rise must be adjusted to the time resolution, but also events that follow a sharp stimulus, such as the admission of a small quantity of a second species in a well defined gas pulse or the application of a laser beam on the surface.

Time-Resolved Studies of Excited States

On a faster time scale, the time-structure of synchrotron radiation is unique for the study of dynamical phenomena directly in the time-domain. The realization of bunch lengths as short as 5 psec would allow the direct study of processes on this time scale. Tunable laser sources which produce intense visible, near-infrared and near-ultraviolet pulses of similar duration may be used to prepare excited material which would then be probed by synchronized vacuum-ultraviolet or soft x-ray radiation from the synchrotron. Several diagnostic techniques would be appropriate for such studies. These include angle-resolved UV photoemission spectroscopy (ARUPS), x-ray photoelectron spectroscopy (XPS), EXAFS, and x-ray scattering. Figure 1-1 illustrates preliminary UPS results in which laser-excited states in InP are observed in photoelectron spectra and their time-dependent decay studied. There is a wealth of phenomena that could be studied with such techniques. Some guidance may be obtained by examining what has already been done by purely optical techniques in the field of picosecond laser physics. However, the use of synchrotron radiation techniques offers the possibility of the measurement of physical phenomena that can be obtained in no other way. For example, time-resolved ARUPS would be capable of measuring both the energy and momentum of non-equilibrium carrier distributions in highly-excited semiconductors. Another example is time-resolved x-ray scattering, in which strain fields and heat flow in laser-heated crystals could be directly determined as a function of time.

It is important, however, to recognize the special experimental requirements which must be addressed in actually realizing the potential of time-resolved laser-synchrotron experiments. The laser source must be temporarily and spatially synchronized with the synchrotron. In addition, to obtain an adequate signal in any measurement of a laser-excited process will require sufficient laser flux per shot to produce a substantial level of excitation. Present limits in laser technology will typically dictate a maximum laser repetition rate of 1-10 kHz. With typical synchrotron radiation bunch repetition rates of ~ 10^3 to 10^5 kHz, this means that the effective synchrotron flux usable for such measurements is reduced by 2-4 orders of magnitude. This constraint immediately points to the need for high flux. A second consideration is that of brilliance. The spot on a sample which is probed by synchrotron radiation must obviously be smaller than the laser-excited spot. This

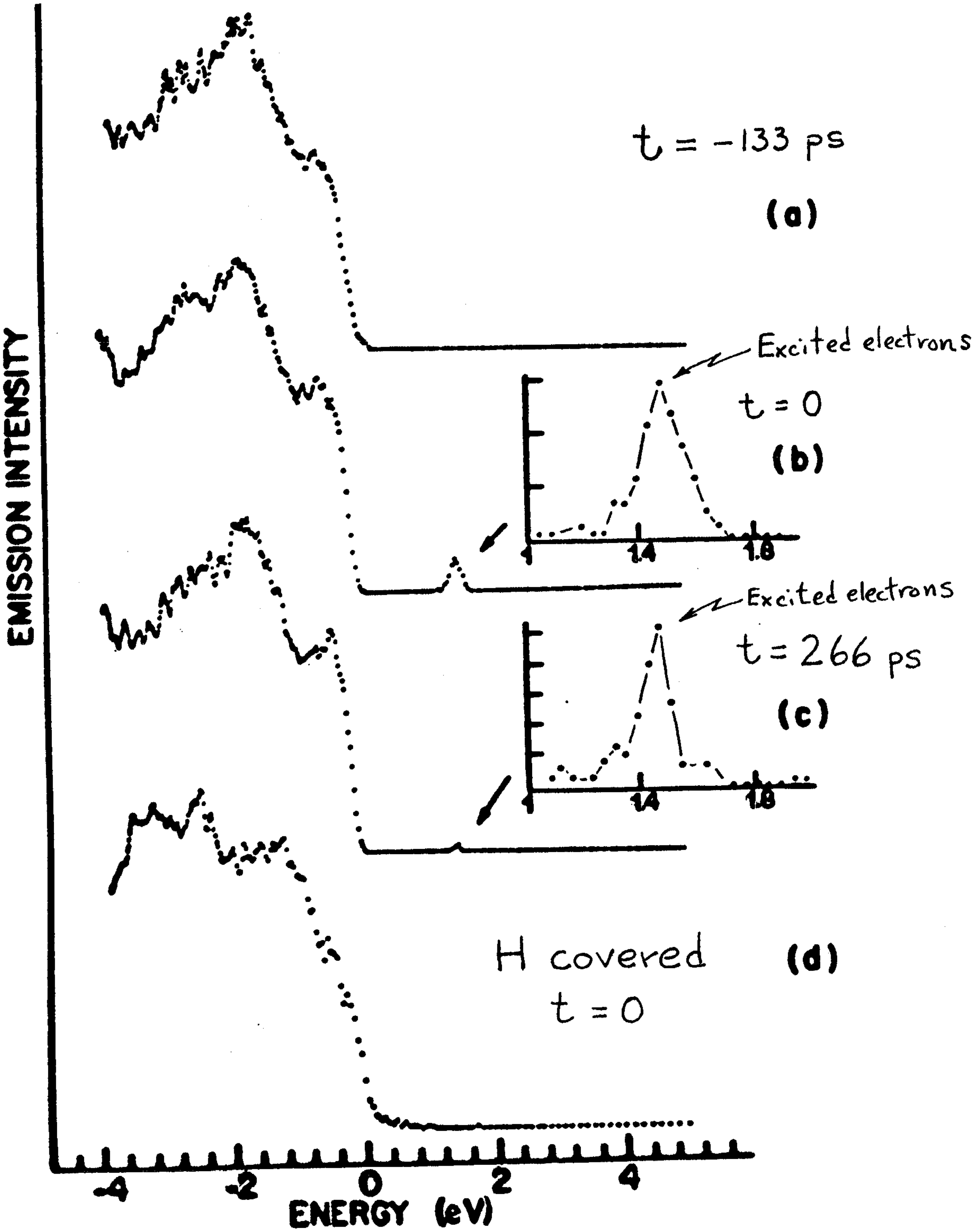


Figure 1-1. Time-resolved photoemission spectra for InP(110) (532 nm pump fluence: 0.5 mJ/cm^2)

then requires a spot size at the sample of the order of 50 μm or better to make efficient use of the available laser flux. Finally, the period between the synchrotron beam pulses must be regulated with a precision within one part in 10^7 in order for such laser-synchrotron experiments to be feasible.

The combination of these requirements with the desire to achieve a short bunch length of the order of the 5-20 psec that is the time scale of interest clearly point to the need for a new, high-brilliance storage ring source which can be operated in a highly stable mode with this bunch length. No presently running storage ring has this combination of characteristics.

SPATIAL RESOLUTION

The high brightness of such a source will make possible a new class of surface analytic tool: combined microscopic imaging and photoelectron spectroscopy. In brief review of prior work of this type, the imaging of surfaces using photoelectrons has a history extending to the very beginnings of electron microscopy. Additional developments in electron optics during the 1960's resulted in routine resolutions of a few hundred angstroms. Advances in recent years have added to this imaging capability the ability to simultaneously record photoelectron energy distributions from microscopic regions of a sample. Although important improvements have been achieved in the form of UHV technology and modern electron energy analysis, a critical need exists for high flux densities of photons at the sample to fully realize the combined potential of photoelectron spectro-microscopy (PESM).

The photoelectron spectro-microscope provides images whose contrast is due to differences in molecular species and chemical environment, as reflected in the binding energy spectrum. This is an important adjunct to SEM experiments, which detect atomic species, but are not sensitive to chemical environment. The PESM technique also subjects the sample to relatively low exposure of charged particles (only photoelectrons and lower-energy secondaries), which avoids the local heating effects, surface diffusion, and decomposition that can accompany microprobes making use of electron bombardment.

There are several approaches to photoelectron microscopy under development. As in electron microscopy, there are two general classifications of the technique: scanning microprobes and imaging microscopes. The scanning instruments use a focused beam of UV/soft x-ray light to provide the spatial resolution. The resolution limit will thus be set by the focusing optics, typically a zone-plate. The electron detection is done straightforwardly with conventional energy analyzers. The drawback to a scanning device is that is it difficult to change magnification, and real-time imaging is not possible. Imaging instruments use the emitted photoelectrons themselves to provide the magnification and resolution. Two imaging techniques have proven successful: magnetic projection and focused electrostatic lenses. Both techniques permit energy-resolving the magnified image. Topographical contrast mechanisms of the two microscopes are complementary: local magnetic or electrostatic fields.

The range of problems that could be studied with this technique is as broad as materials science itself. We consider a few:

Polycrystalline Samples. Many phases of alloys are difficult to isolate as single crystals for study with conventional surface probes. The PESM would enable analysis of individual grains in a polycrystalline sample.

Magnetic Materials. Contrast due to magnetic domains could be correlated to surface chemistry within a given sample and in a single experiment.

Small Particles. Chemically active small particles on substrates could be isolated, and their chemical/electronic properties studied. This will be useful in studies of supported metal catalysts.

Thin-Film Growth. The morphology and surface chemistry of thin-film growth is an extremely active area in surface science. The PESM would enable one to identify growth mechanisms with simultaneous lateral and depth resolution, while monitoring chemical effects due to interface compound formation or inter-diffusion.

Surface Chemistry of Electronic Devices. Spatially resolved surface chemisorption studies should have a major impact in research on chemical sensors. They should also be applied to the study of surface modification processes in device fabrication.

The PESM is a device that clearly benefits tremendously from tunable, high-brightness photon sources. A realistic initial goal for combined imaging and energy-resolving capability would result in a 1 µm spatial resolution with 1.0 eV energy resolution. Simple conservative extrapolation of current yields on synchrotron sources sets a requirement of 10^{14} photons/sec/$(mm)^2$ of monochromatic photons at the sample. Photon energies should cover 50-1000 eV. Assuming a 1% monochromator efficiency, proposed undulator fluxes exceed this flux by an order of magnitude. This conservative estimate neglects inherent gains from the use of multidetection energy analyzers. These factors should ultimately reduce the resolvable features to 0.1 µm with the flux available from this new ring.

SPIN-POLARIZED PHOTOEMISSION

Although every technical advance in the utilization of the characteristics of SR has given rise to new opportunities in materials and surface science, one dimension that has yet to be exploited in the U.S. is electron-spin resolution. The spin polarization of photoemitted electrons is due to either the exchange interaction in magnetic materials, or to the spin-orbit interaction in non-magnetic materials. In the latter case circularly-polarized radiation is generally needed, and even atomic resonance phenomena can be explored. For magnetic materials, the opportunities span a range from very basic questions concerning theories of finite-temperature itinerant magnetism and surface critical phenomena, to very applications-oriented areas associated with film growth and the anisotropy of magnetic memory and recording devices. Indeed, a committee of the National Academy of Sciences-National Research Council recently strongly endorsed the need to foster basic research in magnetism in order to strengthen the declining U.S. role in magnetic technology [R.M. White, Science 229, 11 (1985)].

Virtually all conventional photoemission techniques have spin-polarized analogues. Spin-polarized angle-resolved photoemission can be used to map majority and minority energy bands of single-crystal ferromagnets, while angle-integrated studies can be directed toward the valence bands of amorphous and polycrystalline materials. Figure 1-2 shows results from a recent spin-polarized angle-resolved photoemission study of the ferromagnet iron. Core-level spectroscopy also can serve to differentiate species-dependent and surface-vs-bulk dependent magnetic properties. The secondary electron polarization provides additional complementary information on the average magnetization of multicomponent materials.

A few examples of the exciting research possibilities in spin-polarized studies will give a sense of the rich rewards that could be expected. Many of the actinide elements have magnetic properties that arise from partially filled 5f shells, but the details of their properties have not been explored. The magnetic properties at the surface of a semi-infinite solid can be totally different than that for the bulk. Non-magnetic materials can have magnetic surfaces; magnetic materials can have enhanced magnetic moments at the surface, or have magnetically "dead" surfaces, or have a different type of surface magnetic order compared to the bulk. The surface can have a higher ordering temperature than the bulk, giving rise to true two-dimensional magnetic monolayers. Magnetic monolayers, bilayers, trilayers, etc. can also be produced artificially via epitaxy. In this manner also natural lattice constants can be altered, almost at will, and new or otherwise unstable phases can be synthesized. The advent of supercomputers permits theoretical predictions to be made, based on local-density theory and total-energy calculations, that serve as a challenge and stimulus for experimental studies.

A 1-2 GeV synchrotron based on insertion devices is necessary for such studies in order to properly exploit the rich opportunities presented by such low-dimensional magnetic phenomena, and epitaxial "atomic engineering" capabilities. The reason for this is that the optimal efficiency of spin detectors is only ~10^{-4}, despite dramatic recent advances in spin-detector technologies. This means that to perform spin-polarization analysis with the same ease that conventional photoemission is presently performed, an increase of 10^{4} in photon intensity is needed. In order to utilize spin detection coupled to the next generation of high-energy and momentum resolution experiments, or to utilize high brilliance to focus the radiation within a single magnetic domain, even the extraordinary capabilities of advanced light sources will be heavily taxed.

Spin detection can be accomplished utilizing the left-right scattering asymmetry due to the spin-orbit interaction, when a spin up (down) electron back scatters off of a high-Z target. In conventional "Mott scattering," the energy-analyzed photoemitted electron is accelerated to ~120 keV and its orbital motion experiences a rapidly-varying electric field due to the Coulomb field of the nucleus of a gold target. Alternatively, in low-energy electron scattering (~120 eV) the field inhomogeneity is due to the electron cloud of the gold target. At

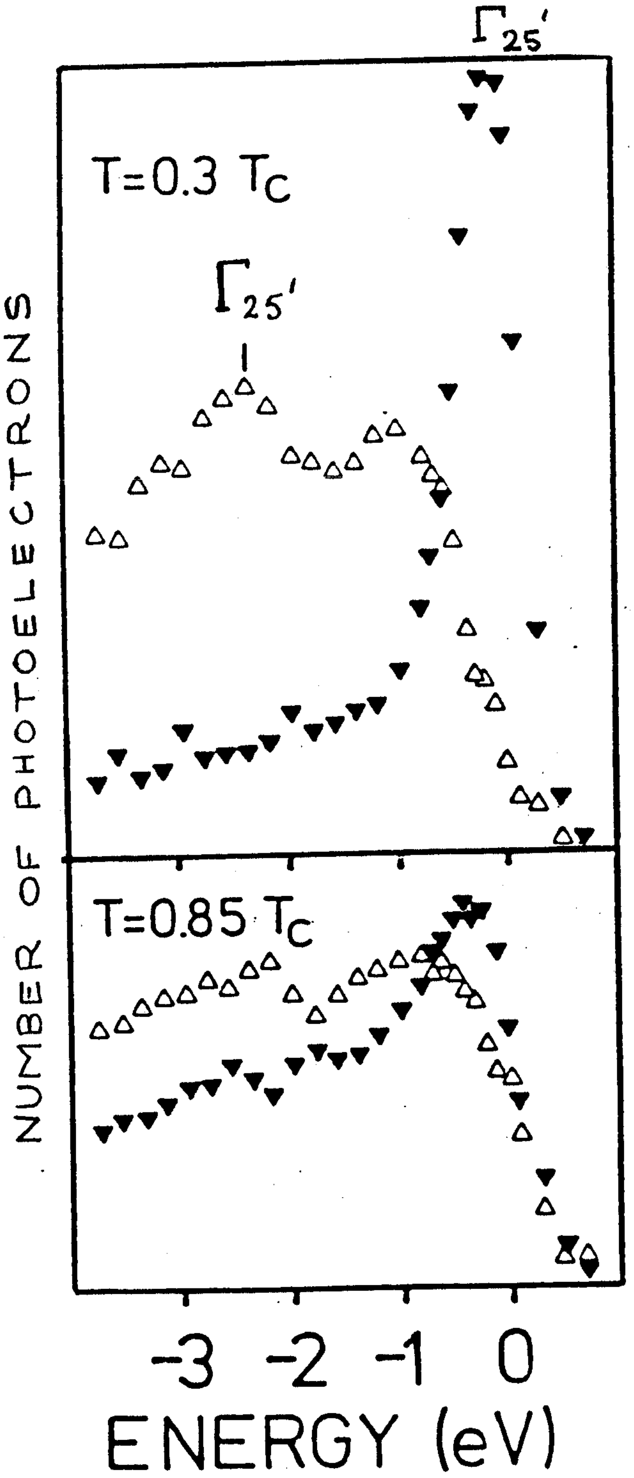


Figure 1-2. Spin-resolved band in iron.

Rice University, very compact Mott detectors have recently been made, making them relatively easy to interface to a fixed-position electron spectrometer. New ultra-compact low-energy spin detectors of an NBS design should even be readily attachable to movable angle-resolved spectrometers.

The insertion device needed for such experiments is a weak field undulator, for which the first harmonic can be adjusted between ~10-100 eV. This can be achieved via a tunable gap and utilizing a movable pin-hole pre-monochromator. The undulator is a hybrid rare-earth-cobalt magnet with 100 poles and a 5-cm period. The exciting properties are its outstanding brightness, and, as shown in the figure, the ability to utilize significant π-polarized as well as σ-polarized light, by going off axis (that is, perpendicular to the plane of the storage ring). Significant circular polarization should be present as well. The monochromator can be based on toroidal or plane grating principles. The need exists to combine simulations of the SR characteristics with ray-tracing codes conventionally used to optimize monochromators, in order to obtain an optimally matched undulator-monochromator beamline.

An additional type of experiment capable of providing unique information on magnetic materials is core-level photoelectron diffraction from multiplet-split core levels. Such core levels exhibit peaks that can in many cases be associated uniquely with photoelectrons of definite spin orientation, thus providing an <u>internal</u> source of polarized electrons so that no external spin detector is required. The different way in which spin-up and spin-down photoelectrons scatter and diffract from the overall ionic or atomic spins in a magnetically-ordered material can then be used to detect the type of short-range order present, and to study its dependence on temperature. This technique should be applicable to both antiferromagnetic and ferromagnetic systems. The overall question of when short-range magnetic order disappears is one of long-standing controversy, and a better understanding of it will assist in the development of higher-density magnetic storage materials. These experiments will require tunable, polarized radiation from ~200-1300 eV and very high fluxes to permit adequately resolving such core peaks against high backgrounds in an angle-resolved experiment.

ULTRAHIGH ENERGY AND MOMENTUM RESOLUTION

Higher resolution has always led to new physical insights, and valence-band photoelectron spectroscopy with synchrotron radiation has been no exception. Recent work on heavy fermion systems demonstrates this. These systems have very large T-linear specific heat coefficients, implying very large effective masses, and display a complex interplay between tendencies toward superconductivity, magnetic ordering and the Kondo effect. The present picture of these systems as based on many-body theory is far from being in final, or even satisfactory, form. Current models suggest a ground state and low-lying excited states composed of highly correlated 4f or 5f electrons, resulting in a very narrow (1-10 meV) many-body resonance in the f spectral weight at the Fermi energy. A U5f peak has indeed been found at the Fermi level in UBe_{13} from recent photoemission data obtained at a temperature of 20 K and with a reasonably low 0.13 eV energy resolution. To make direct contact with many-body theory, similar measurements must be made at lower temperatures and with an energy resolution almost certainly better than 10 meV. Such measurements could be made on a variety of heavy fermion systems. For single crystals, angle-resolved photoemission could be used to reduce the contributions from the non-f electrons and to search for dispersion in the f-derived Fermi-level resonance. Spin polarized measurements are also desirable in those systems exhibiting magnetic behavior at low temperature. All of these measurements that are so important for the validation of the theory of interacting electrons in solids require both very high resolution and high photon flux in the 20-150 eV region. Utilizing the 3d → 4f or 4d → 5f resonances in the f-photoemission cross sections also demands a high performance beamline in the 800-1500 eV photon energy range.

Other areas where very high energy resolution of ~ 1-10 meV complemented by very high momentum resolution are important are in accurate studies of Fermi surface effects in various systems. These include phase transitions and reconstruction driven by electron-phonon coupling (superconductivity, charge density waves, etc.), many-body effects in the photohole state, and subtle momentum broadening effects due to trace impurities and defects. The energy scale on which one expects changes in these experiments is that typical of phonons. Extending momentum resolved photoemission into this regime will further integrate the technique into a wide variety of condensed matter physics fields.

The ultrahigh energy- and angular-resolutions required by these studies can be best achieved by reducing the source diameter without loss of photon flux, i.e., by using a higher-brilliance source of synchrotron radiation such as an undulator on a new 1-2 GeV storage ring. Such studies will require a very high-performance soft x-ray monochromator in order to satisfy the stringent resolving power ($\Delta E/E \sim 10^{-4}$) requirements in the soft x-ray regime. By reviewing existing soft x-ray monochromators, it is found that the major limitation on the resolving power is due to the figure error of optical elements instead of the overall aberration of the monochromators. Although by applying spherical optical elements one can substantially solve this problem (a sphere is the most accurate element that can be manufactured), the achievement of resolving powers as high as 5000 is still a very difficult task. A new 1-2 GeV high-brilliance source with small σ and σ' definitely will increase the chance of achieving this goal, simply because the effective diffracting area is much reduced and there is thus a high probability of finding a spot with high figure accuracy locally on the grating surface.

ADVANCED CORE LEVEL SPECTROSCOPY

Core level spectroscopies of various types represent the main stream of applied research at today's UV/soft x-ray synchrotron radiation sources. In comparison to valence spectra, it is often easier to interpret core-level spectra, and thus to determine various bonding parameters (e.g., charge transfer, oxidation state, coordination, bond lengths, and bond angles). Such infromation can lead to a better understanding of many complex materials and interfaces that occur in technological applications. With current synchrotron radiation sources, only about half of the elements of the periodic system can be accessed via suitably sharp (~ 0.1 eV intrinsic width) core levels, since at photon energies above about 250 eV the achievable monochromatic photon flux is too low by about two orders of magnitude. With photon energies up to a minimum of ~1000 eV, the sharpest core level of every element can be measured, including the presently unaccessible 3d and 4d metals (e.g., titanium, iron, nickel, copper, silver) and the light elements so important in organic- and bio-chemistry (carbon, nitrogen, oxygen, fluorine). As highlights, we mention the use of core-level shifts and intensity measurements in characterizing metal-semiconductor interfaces, and the application of photoelectron diffraction and EXAFS to determining the bonding geometries of a variety of surface and interface systems.

To characterize a reaction interface fully, it is necessary to follow the changing environments of the constituent atoms as a function of the chemical and physical properties of the overlayer/substrate with ultrahigh resolution core-level photoemission. Coverage-dependent and temperature-dependent studies will show the onset of reaction, the development of reacted species, the interaction among them, the role of defects, grain boundaries, kinetics and thermodynamics of systems which can be both laterally and vertically heterogeneous. Access to a high flux, stable, small-spot source in the photon energy range 100-1000 eV with instrumental resolution better than the natural linewidth is necessary. A consequence of such studies will be predictive capabilities as to interface formation and materials engineering, both of which are crucial for various high technology applications, including developments in microelectronics and the fabrication of stable ohmic and rectifying metal/semiconductor contacts.

An additional dimension of advanced core-level spectroscopy that will be capable of considerable new development and a wide variety of applications is core-level photoelectron diffraction. In this experiment, photoelectrons are emitted from the core levels of different atoms in an ordered specimen (e.g., atoms in the crystal, at a shallow-interface, or on the surface), and the directional- or energy-dependence of the photoelectron intensity is measured. A very closely related type of measurement discussed in more detail in a later section is EXAFS or surface EXAFS, in which the core-level excitation probability is monitored as a function of energy. Prior studies have demonstrated the capability of both photoelectron diffraction and surface EXAFS for determining the atomic positions and molecular orientations at surfaces and during interface formation. For example, adsorbed atoms/molecules, stepped surfaces with catalytic activity, and epitaxial overlayers such as metal-on-metal, metal-on-semiconductor, and semiconductor-on-semiconductor systems have been studied. The photon energies required are in the range from 200 eV to 3000 eV to enable the study of a range of core levels, and current synchrotron radiation sources do not yield sufficient flux to do such experiments at both high energy and high angular resolutions. Improvements in energy resolution will permit resolving chemically-shifted core levels (e.g., metal in silicide and metal in an overlying metallic cluster) and thus studying the diffraction or EXAFS from each type of species separately. Higher angular resolutions of ~±1° will also yield finer features in photoelectron diffraction patterns, and thus much greater sensitivity to atomic structure.

DILUTE SYSTEMS/DEFECTS

Defect Spectroscopy of Semiconductor Interfaces and Surfaces

The physical behavior of semiconductors and the limit in the electrical performance of devices is strongly dependent on defects. Defects are as important at interfaces as in the bulk. They determine such phenomena as trapping of charge carriers, electrical barriers due to Fermi-level pinning, band offsets, etc. Yet there is no spectroscopic probe to clearly identify defect states. Suitable experimental methods could be developed with very high flux sources, for example, photoemission spectroscopy (PES) in which fluxes many orders of magnitude greater than those presently available may be needed. Several factors indicate the need for these greater fluxes: the low concentrations of defects, with at least three orders of magnitude necessary to compensate; and a resolution requirement of less than 50 meV, which implies an order of magnitude or more to be feasible. Since the defect signals are small with respect to the dominant "bulk" emission, the typical background signals arising from scattered higher-energy electrons also need to be much reduced. Control of the background may necessitate double-dispersion instrumentation for both the photon and electron optics, which further increases the flux requirement. The basic spectroscopic approach could be either to look for structure above the valence-band maximum or at core thresholds. The core-to-threshold transition, involving in this case a defect state at the conduction band minimum, is detected through the decay of the resulting core hole. The states involved in the decay process can be probed with several types of measurements. These mechanisms have been studied for intrinsic semiconductor states and more recently for gas-phase samples, where the method has been called deexcitation electron spectroscopy. In the case of solids, the defect-derived signal would ride on top of the substrate signals, which means very high counting rates would be needed to obtain good signal-to-noise ratios. Some modulation or difference technique may be also required to aid in picking out such small defect signals. The fluxes produced by such a next-generation source should make it possible to develop spectroscopies for studying such defect states.

Soft X-Ray Photoabsorption Studies

The determination of the local structure around atoms present in very diluted concentrations is an important problem in surface science as well as materials science. In particular we focus on the first and second row elements (C,N,O,...,Al, Si,P,S). The capability of being able to describe the local environment around these atoms is a fundamental issue in many areas of research. These include chemisorption properties of organic molecules on catalytic transition metal surfaces and semiconductor physics problems such as lattice relaxation, precipitation, clustering, and the metal-to-insulator transition of impurity atoms in a semiconductor crystal host. A unique way to obtain this type of structural information is by K-edge extended x-ray absorption fine-structure (EXAFS). The potential of this technique for these problems has been recognized for some time and a large amount of work on the C, O, and S K-edges of atoms or molecules chemisorbed on surfaces has been performed with existing soft x-ray (300-3500 eV) sources. These studies are typically carried out by monitoring the elastic or inelastic Auger electron yield produced by the non-radiative recombination of the excited core hole. The detection limit of these techniques is a surface atomic concentration of about 5 × 10^{14} at/cm^2, which corresponds to ~ 1/4 of a monolayer.

This detection limit is determined by the signal to background ratio (STB) which can be conveniently defined as the K edge-jump to background ratio at the absorption edge and which is for ~ 1/4 of a monolayer approximately 10%. This means that the EXAFS amplitude, which is typically <10% of the edge-jump is then less than 1% of the total collected signal. The general procedure for increasing the STB ratio and thereby the detection limit is to somehow decrease the background, which, for the case of Auger electron detection, is due to unavoidable elastic and inelastic electrons produced by substrate excitations. One way to reduce drastically the background is to monitor the fluorescence yield (FY) of the radiative recombination channel of the excited core hole as a function of photon energy. Unfortunately, for the K and L shells accessible with soft x rays, the fluorescence yield is only a few percent or less of the Auger yield, and therefore experiments on low-Z atoms have not been attempted until very recently. At the S K-edges the STB ratio obtained with FY detection was found to increase by a factor of 10 and at the C K-edges by a factor of 20 over the Auger yield detection. This means that by FY detection the detection limit can be improved to a 1/100 of a monolayer or ~2 × 10^{13} at/cm^2! The remaining problem in using FY detection at this point is the signal to noise ratio (S/N). For example, using a gas flow proportional counter the S K-edge FY SEXAFS spectrum of c(2×2)S on Ni(100) was measured using the JUMBO monochromator at SSRL with a monochromatic photon flux of 2 × 10^{10} photons/sec. Figure 1-3 summarizes these results. Collecting 0.1 Sr of solid angle, the count rate to the S K edge jump was 3000 counts/sec at the absorption edge. The c(2×2) S overlayer on Ni(100) corresponds to 1 × 10^{15} at/cm^2. Although the detection system is able to measure 2 × 10^{13} at/cm^2 with sufficient STB, the experiment cannot be done because the count rate will be only 60 counts/sec. Limitations in photon flux are even more severe for the C K edge. Experiments at the BESSY storage ring in Berlin using the SX-700 monochromator with about 5 × 10^{11} photons/sec yielded only 100 counts/sec edge jump for about two monolayers of ethylene on Cu[100]. The FY detection mode presents other advantages with respect to Auger yield. In particular, by using an energy dispersive detector, there are no interference problems, such as those due to substrate core-level photoelectrons, that can make Auger yield EXAFS experiments impossible for many interesting systems.

Another unique characteristic of soft x-ray FY EXAFS is its "bulk" sensitivity. Photons in the 300-3000 eV energy region penetrate 1,000-20,000 Å in medium atomic-number materials. Therefore we can perform EXAFS studies of dilute impurities in host materials. Assuming an absorption length λ_o = 1 μm and the surface detection limit σ_o = 2 × 10^{13} at/cm^2, the minimum concentration that can be measured is

$$\rho_o = \sigma_o/\lambda_o = \frac{2\times10^{13}}{10^{-4}}\ \text{at/cm}^3 = 2\times10^{17}\ \text{at/cm}^3$$

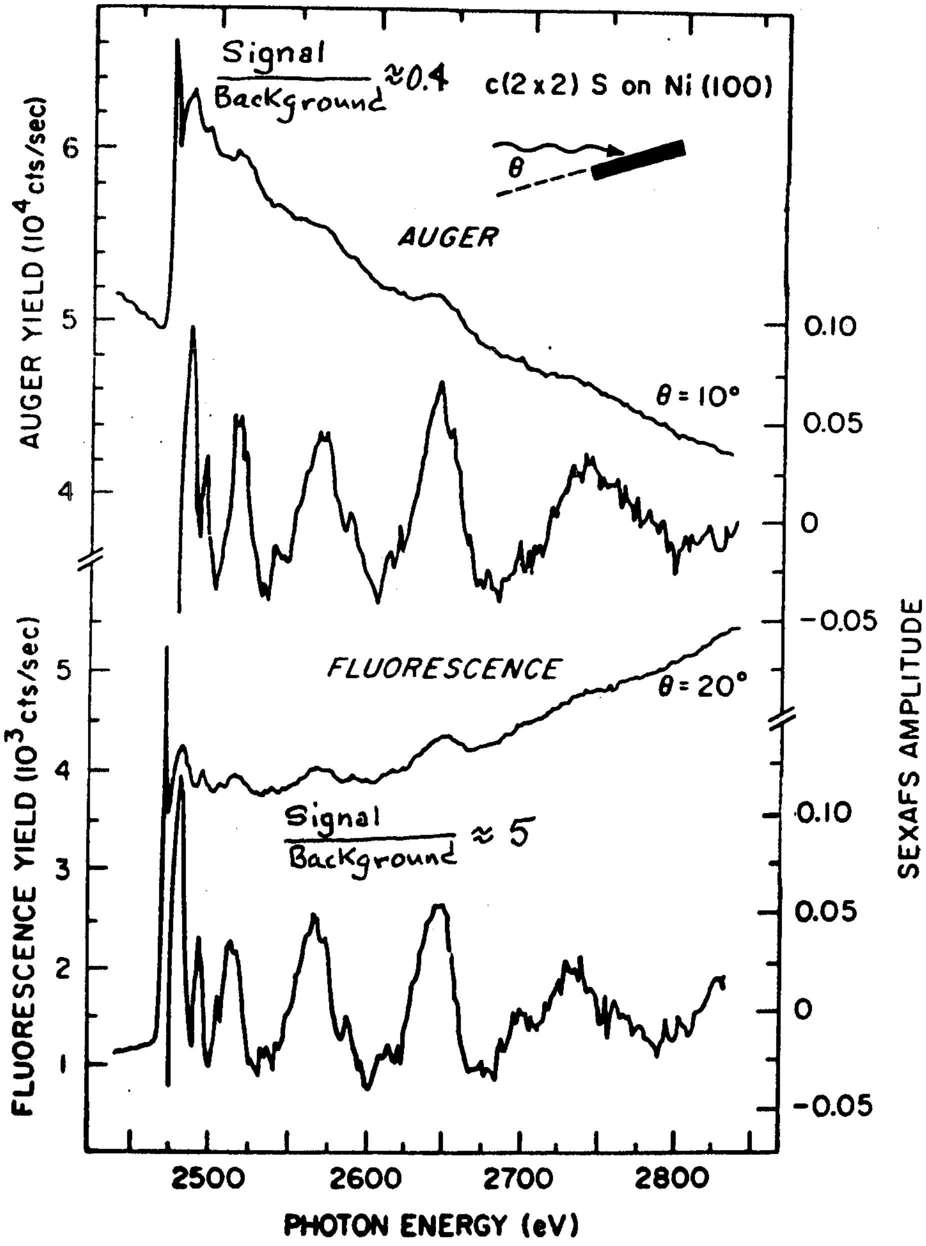


Figure 1-3. Comparison between Auger and fluorescence detection of SEXAFS.

It thus appears immediately that FY is capable of measuring the structure around important impurity atoms like Al, Si, P, S in semiconductors. In fact, the EXAFS signal of S impurities in GaAs crystals doped by S ion implantation has been measured down to concentrations of ~ 1 × 10^{19} at/cm^3, at which point this study started to be limited by poor S/N ratios.

In conclusion, by soft x-ray FY detection we have today the experimental capability to measure diluted species on surfaces down to 2 × 10^{13} at/cm^2 and in the bulk down to 2 × 10^{17} at/cm^3. This has an enormously important potential in surface studies of phenomena such as precursor states, oxidation, poisoning, and chemical reactions on transition metal catalysts. Referring to the research on impurity atoms, it also should be noted that there is no other current technique except EXAFS that is able to provide a detailed and complete description of the local structure up to at least the second atomic shell around an impurity atom. These studies can address fundamental and technological problems like precipitation, lattice relaxation and diffusion. To perform these experiments in the mentioned concentration ranges a monochromatic photon intensity greater than 10^{13} photons/sec/eV over the 300-3000 eV range is needed. Other very important issues are a beam lifetime above 6 hours and high spatial stability of the electron beam. Also, if we could obtain another two orders of magnitude in photon flux, it would become reasonable to put a monochromator between the sample and the detector in order to overcome the detector saturation problems occurring when substrate fluorescence lines are present (an example is P impurities in silicon).

SOFT X-RAY AND VUV SCATTERING

X-ray scattering probes electron density fluctuations, and has traditionally used wavelengths of the order of 1 Å to probe the atomic structure of matter at large scattering angles (wide-angle scattering) and to probe larger-scale structure such as phase separation at extremely small angles (small-angle scattering). Soft x-ray and VUV wavelengths are uniquely suited to study structures having feature sizes larger than atomic by scattering and have yet to be exploited for these experiments. One reason for this is that high absorption at these wavelengths limits the effective sample size and hence the scattered intensity. With the high fluxes available from a new source sufficient scattered intensities will be obtained, and the limited sample size can be used to advantage to study thin films or intrinsically small samples. Other advantages of scattering with soft x-ray or VUV photons are 1) the ability to choose the wavelength appropriate for a given size structure, 2) a lower available K-range, 3) the ease of performing scattering experiments at higher angles, and 4) the possibility of anomalous scattering from important low-Z elements.

An exciting class of experiments that will be made possible with very high fluxes of soft x-rays is scattering from thin surface layers. Similar experiments will be performed for ultra-thin polymer films on solid substrates. These structures are of both scientific and technological interest. Soft x-rays could be used to study inter-chain correlations as well as the scattering resulting from phase-separated mixtures of polymers. High fluxes are necessary for these samples because they are very small (perhaps limited by absorption) and because their electron density is relatively low. Dynamic studies of structural changes on heating are extremely important and require even higher fluxes, as do differential anomalous scattering studies to obtain chemical information. Electron density differences in phase separated samples are small--an additional need for high fluxes.

Many other examples of soft x-ray or VUV scattering experiments that can be realized with high fluxes of these photons can be given. Scattering from biological cellular units or cells themselves could be a much easier technique than microscopy or holography. Because these structures are amorphous, these experiments will require extremely high fluxes. Another class of experiments to exploit soft x-ray or VUV scattering is the study of surfaces and structures on surfaces. Analogous to grazing incidence diffraction (GID) at hard x-ray wavelengths, soft x-ray GID experiments could probe lateral and/or vertical correlations of roughness on surfaces, large molecules on surfaces, clusters or islands on surfaces, and the like. Like thin polymer layers on surfaces, structures larger than atomic-scale in dimension in thin insulating, semiconducting, or metallic films could be studied with scattering techniques. Clearly, such soft x-ray and VUV scattering techniques are ripe for exploitation that would benefit greatly from a new low-energy synchrotron source.

See "User Policy and Facilities" section for a discussion of the user policy concerns of this working group.

Chemical Dynamics

SELECTED RESEARCH OPPORTUNITIES

In a broad sense, the subject of chemical dynamics encompasses all phenomena in which molecular species undergo energetic or chemical transformations. These phenomena range from the bimolecular reactions of ions with small molecules in the interstellar medium to the complex and cooperative phenomena that occur in enzyme catalysis. While the methods used to study such processes are very different, the objectives are usually remarkably similar. These include identifying the reactants, reaction intermediate(s) or transition state(s), and products; characterizing the important features of the potential-energy surface that influence the reaction dynamics; and examining the utilization and disposal of energy during the course of the reaction. Even the most complex of chemical systems can usually be broken down into elementary steps involving localized reaction sites or specific reactive intermediates that can be described in exquisite detail.

There is an enormous number of applications of synchrotron radiation in studying the rates, mechanisms, and energetics of chemical reactions and characterizing the structure and energetics of reactive intermediates. Only a few of these can be highlighted in this report as examples that represent specific interests of the workshop participants. The recently issued National Academy of Sciences report, "Opportunities in Chemistry,"* provides broader perspectives of current activity in the field of chemical dynamics.

<u>Bond Selective Photochemistry</u>. The idea of using photochemical techniques to selectively excite and effect reactions of specific bonds in molecules is usually frustrated by energy transfer processes that redistribute energy before reaction can occur. Recent studies have shown that excitation of electrons to antibonding orbitals of specific chemical bonds from nearby atoms with nonbonding orbitals can result in selective bond cleavage, making it possible to observe processes that would never be achieved using thermal activation. These excitations, to repulsive states, occur in the vacuum ultraviolet between 4-10 eV. The intense output of an advanced synchrotron source in this energy region will facilitate the detailed study of bond-selective photochemistry of isolated molecules using molecular beam techniques. With fluxes in excess of 10^{15} photons/sec it will be possible to explore the generality of this phenomenon on a preparative level, on surfaces, and in condensed phases. Another promising and general approach to achieving bond selective chemistry involves the combined use of single infrared photon excitation followed by vacuum ultraviolet photodissociation. An infrared

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Contributors were J. Beauchamp (Chairman), Yuan Lee, T. Baer, M. Bowers, D. Trevor, C.B. Moore, M. Berry, A. Bradshaw, Chen C. Hsu, R. Sander, M. Cornacchia, and H. Lancaster.

*"Opportunities in Chemistry," Committee to Survey the Chemical Sciences, G.C. Pimentel, Chairman, National Academy Press, Washington, D.C., 1985.

FEL in conjunction with VUV output of the source will provide exciting opportunities for such studies.

Cluster Chemistry. The use of pulsed supersonic beams in conjunction with laser evaporation techniques has made it possible to generate and study clusters of virtually any chemical composition and size. Studies of the structural, electronic, and magnetic properties and the chemical reactivity of these species as a function of cluster size is currently an area of intense activity in many laboratories. Of fundamental interest is the variation in ionization potential with cluster size and the observation of the onset of bulk properties. An advanced synchrotron source, with enchanced output in the 4-10 eV region, is ideally suited for the accurate determination of these parameters. Results obtained to date suggest that small clusters have highly specific reactivity that can be correlated with their ionization energetics. The possible applications of these results in the design of novel catalysts and new materials with unusual magnetic and electronic properties are a source of enormous excitement in the chemical and materials science community.

Structure and Energetics of Reactive Intermediates. Photoionization mass spectrometry and photoelectron spectroscopy are capable of providing valuable thermochemical data useful in characterizing the structure and energetics of reactive intermediates. The high output of a new source in the 4-30 eV region will make it possible to conduct such studies with unprecedented sensitivity and resolution. For example, the heat of formation of the radical SiH_2, an important intermediate in the chemical vapor deposition of silane, has an uncertainty of nearly 20 kcal/mole. Photoionization measurements can provide the heat of formation of this species to better than 0.5 kcal/mole. The field of organometallic chemistry has grown enormously in the past decade. The selective activation of carbon-hydrogen bonds by coordinately unsaturated transition metal complexes offers exciting new possibilities for the development of new catalysts for preparing derivatives of hydrocarbons under mild conditions. The description of these processes requires a knowledge of the strengths of metal-carbon bonds, which cannot be determined using conventional approaches. Newer techniques involving photoionization mass spectrometry and photoelectron spectroscopy are able to provide this badly needed data base. The intense output of an advanced synchrotron radiation source along with the temporal characteristics of the radiation will make it possible to determine ionization energetics of reactive intermediates with a resolution of 1 meV!

Studies of Ultrafast Chemical Phenomena. It is well recognized that energy transfer processes and chemical reactions can occur on a subpicosecond timescale. New techniques that improve the time resolution available for the study of ultrafast phenomena open new vistas in studying the rates and mechanisms of chemical reactions. The combined use of picosecond laser techniques with the short light pulse available from a new source will make it possible to use pump-probe techniques to conduct wide ranging studies of the dynamics of energy transfer processes and chemical reactions in the gas phase, on surfaces, and in condensed phases.

SOURCE CHARACTERSITICS

There is not presently a substantial community of chemical physicists in the area of chemical dynamics that is participating in the use of synchrotron light sources. For many applications, existing synchrotron sources offer little advantage in comparison to other sources of vacuum ultraviolet radiation that can be dedicated to specific applications in individual laboratories. These include high intensity atomic and molecular line sources, rare-gas continua, and an increasing number of tunable and fixed frequency laser sources of vacuum ultraviolet radiation. In additon, laser multiphoton ionization techniques can selectively access specific states of atomic and molecular ions. While these sources offer solutions to specific problems, they are not suitable for use over a wide spectral range and have temporal characteristics that prevent many applications.

A synchrotron radiation facility designed for optimum photon performance in the vacuum ultraviolet spectral region can significantly modify this situation and result in an enormous increase in user interest and participation in the area of chemical dynamics. The desirable and in several cases unique characteristics of an advanced soft x-ray and ultraviolet synchrotron source are discused below.

High Intensity. The source will provide photon fluxes that are more intense (for a given resolution) than conventional laboratory sources by three to four orders of magnitude. This will make it possible to conduct routine measurements of photoionization efficiency curves and photoelectron spectra with unprecedented sensitivity. Photon fluxes in excess of 10^{15} photons/sec are sufficient to interact efficiently with low density targets such as ion beams and can serve as macroscopic yields of vacuum ultraviolet photoproducts. It is highly desirable to have an undulator optimized for narrow bandwidth and low harmonic content at long wavelengths. This will facilitate wavelength-selective preparative photolysis and materials processing without a monochromator.

Excellent Performance at Long Wavelengths. Synchrotron sources are noted for their ability to provide tunable vacuum ultraviolet and x-ray radiation over a wide range of wavelengths. The photon energy range 4-30 eV is of primary interest for studies in chemical dynamics. Operation at 1.3 GeV and the use of an appropriate undulator provides enchanced photon output in this region. In addition to the high intensity, it is the superior performance at long wavelengths that makes the new source a unique and attractive facility for studies in chemical dynamics.

Compatibility with Free Electron Lasers. The use of a linear accelerator to fill the booster ring permits use of this device, once the synchrotron is loaded, as an injector for an infrared free-electron laser. The final design of an advanced light source should incorporate a by-pass arm with an ultraviolet free electron laser optimized for long wavelength operation. The IR and UV FEL's will greatly facilitate pump-probe experiments when used in conjunction with the output of the synchrotron light source. An IR FEL operating with high peak power in the 2-10 micron region would be a powerful tool for the study of chemical processes induced by infrared multiphoton absorption, used either alone or in conjunction with the synchrotron source.

Temporal Characteristics of Radiation. A synchrotron source is optimized for a short electron bunch length will give light pulses which are approximately 25 pioseconds long. Achievement of the shortest possible pulse is essential in the design of the experiments to study ultrafast processes. For example, the cleavage of the chemical bonds of photoexcited molecules can occur on a picosecond time scale. These processes can be followed by splitting the beam and passing a portion of the radiation through an optical delay line before it is allowed to interact with the molecular system. The design of novel pulse compression and expansion devices that can be inserted before and after an undulator would provide even shorter pulse lengths and further improvements in time resolution. For many applications involving time dependent studies, the high repetition rate of the fully loaded synchrotron causes difficulty. It is essential to provide capabilities for selectively shunting a single bunch of electrons through an undulator to provide a single pulse of vacuum ultraviolet radiation. To take advantage of the short pulse length for the study of ultrafast phenomena using a picosecond probe laser, it is necessary to synchronize the output of the probe laser with the output of the synchrotron source. The stability of the rf drive facilitates the accomplishment of this objective. The short output pulse of the machine also enhances the detection of zero energy electrons formed in photoionization processes. This makes it possible to record threshold photoelectron spectra of specific molecular species in mixtures with unprecedented resolution (1 meV!). Finally, it is noted that an increasing number of experiments in chemical dynamics are being performed with pulsed rather than cw molecular beams. This reduces the gas load on the experimental apparatus and makes it possible to carry out unique time-resolved experiments that are well-suited to make unique use of pulsed-light sources.

Polarization of Radiation. The polarized output of the synchrotron facilitates studies of phenomena such as molecular photodissociation processes, where observation of product angular distributions can provide information relating to the symmetry of the excited state.

Atomic and Molecular Science

In this field of fundamental importance, photoionization studies must be carried out on inherently dilute targets that consist of free atoms and molecules. This aspect alone requires a high-intensity, very bright photon source. Further, the need to examine detailed features of the atomic and molecular structure, such as multiplet and vibrational levels, requires a photon source capable of providing high resolution over a wide energy range. A storage ring that is optimized for the operation of insertion devices can provide much higher intensities, brightness and resolution than is presently available, potentially leading to major advances in atomic and molecular science. Not only will the scope and the reliability of present studies be expanded, but entirely new classes of experiments will become feasible.

The photoelectric effect provides a versatile and sensitive probe of the electronic structure and dynamics of atoms and molecules. This probe would be vastly enhanced by the capabilities of the proposed new source, allowing us to probe the basic interactions between photons and quantum states and delineate the details of the electronic, vibrational, and rotational structure. Photoabsorption, photoelectron, Auger-electron, fluorescence, and ion studies during the last decade have given us new insights, but a thorough understanding and widely applicable theoretical models are still lacking. Experiments with a new photon source that can provide orders-of-magnitude greater brightness and resolution than is now available will open up new opportunities and help to attack many unsolved problems. These include *inter alia* electron interactions in open-shell atoms, vibrational and rotational interactions in molecules, fragmentation pathways of excited molecules, autoionization processes, two-electron excitation processes, spin polarization in both atoms and molecules, dynamics of excited states, resonance states near absorption thresholds, studies of extremely small quantities, and the electronic structure of clusters and ions. The feasibility of investigating clusters and ions represents truly a quantum leap, allowing us to study, respectively, the transition from the isolated atom to coordinated aggregates and the dynamic behavior of any charge state and any element via its isoelectronic equivalent.

Results from these advanced experiments are of paramount importance to establish systematics and to improve the theoretical models that include relativistic effects and many-body interactions. But the results will also provide basic information in other fields as, for example, material and surface science, catalysis, chemical reactivity, aeronomy, astrophysics, and plasma physics.

Some of the scientific opportunities presented and discussed by the working group are described below in greater detail.

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ATOMIC STRUCTURE AND DYNAMICS

Photon interactions offer unique advantages over other collision processes for studying atoms, molecules, and ions. Because photons are absorbed, the focus of study is the target. Energy resolution is good. Because of electric-dipole selection rules, only a small number of final states are allowed. Synchrotron radiation permits measurements over a large energy range, which is essential for comparison with theory. Photoionization results are also useful in interpreting results of other collision processes. Finally, photons are easily polarized. The processes discussed below require higher photon fluxes than are currently available to permit experimental results that are precise enough to distinguish among alternative theoretical approaches. Experimentally, a high photon flux is imperative because of the low number densities of the targets, and a high brilliance is needed because the target volume examined by various dispersive apparatus is very small. Only a high resolution comparable to the natural widths of the atomic levels can provide results with the highest degree of distinction. In numbers, 10^{12} to 10^{13} photons per s mm^2 mr^2 within a bandwidth of 0.01 Å are required at the sample for most of the frontier experiments in atomic physics.

Some of the most important topics lie in the area of photon interactions with open-shell atoms, ions, and excited neutrals. The measured quantities are (a)the total photoabsorption cross section, (b) the partial cross section for producing specific ionic states using the techniques of photoelectron and fluorescence spectroscopy, (c) the probability for producing doubly and multiply charged ions, (d) angular distribution of photoelectrons from single and double ionization events (no measurements have ever been made on the latter), and (e) spin polarization of the photoelectrons.

Novel Targets. Combining *laser-excited atoms* with synchrotron radiation, one can study photoionization of excited states. These have large size and hence large cross sections, but the target is usually very thin. Experimental results would test theoretical predictions of (1) multiple Cooper minima in excited-state photoionization cross sections as well as (2) unusual variations in the angular distribution parameters and the relative strength of the ℓ_o+1 and ℓ_o-1 channels.

Open-shell atoms are a new area for theoretical and experimental study. As was the case for closed-shell atoms, a combined theoretical and experimental attack will be crucial for rapid progress. Theories of open-shell atom cross section, branching ratios, and angular distribution asymmetry parameters differ significantly from one another, particularly near ionic thresholds. Experimental results will help theorists sort out the correct approaches.

The study of photoionization of *high-Z elements* will test theoretical approaches to relativistic interactions with greatest possible sensitivity. Given the high brilliance expected from the new source, even the *actinide elements* which, due to their radioactivity and limited availability, must be studied in extremely small quantities (10 mg or less) can be investigated over a wide energy range. Such work will also allow the delineation of the electronic properties of the chemically significant 5f, 6d and 7s electrons.

The study of *ions* isoelectronic to open-shell atoms may be one of the easier ways to understand open-shell atom photoionization. More generally, the study of ions isoelectronic to neutral atoms permits one to deduce the importance of electron correlation relative to the nuclear central potential, thereby allowing one to identify better those features that are caused by electron correlation.

Many-Body Interactions. *Double photoionization* measurements are very significant tests of theory. Most useful would be measurements with smaller experimental uncertainties and high energy resolution of the two electrons in order to determine the subshells from which the two electrons are ejected. For photon energies just at and above the double ionization threshold of H^- or He, experimental measurements of the angular distribution would test recent theoretical predictions. Specifically, theory predicts for finite energies above the threshold a Gaussian distribution of the two-electron probability distribution about the most probably relative angle, $\theta_{12} = \pi$. It also predicts different angular distributions for singlet and triplet L = 0 initial states.

Experimental measurements of *photoionization plus excitation* would aid theory in predicting excitation probabilities. Current results for production of He^+ (n = 2) show qualitative agreement between theory and experiment. However, there remain significant quantitative discrepancies between alternative theoretical predictions as well as large uncertainties in the experimental data. This is particularly pronounced for the 2p/2s branching ratio. Alignment measurements of excited ionic states would provide additional sensitive tests of alternative theories.

Experimental study of features is a severe test of autoionization features is a severe test of theoretical understanding. In some cases, such as the 3p → 3d resonance in the 3d spectra of the transition metals, autoionization simply dominates the spectrum. In other cases, the description of narrow autoionization resonances requires the inclusion of interactions not usually considered in describing the broad absorption spectrum. Experimental parameterization of partial cross sections, branching ratios, β parameters, and spin polarization parameters within autoionization resonances permits so-called "complete experiments" within a narrow energy range, which give detailed information on the nature of the resonances.

Experimental study of *inner-shell ionization* near threshold permits detailed information on many-particle interactions and the limits of the two-step model that separates excitation from deexcitation. For example, the *resonant Raman effect* epitomizes this breakdown: here, a photon of exactly the right energy (within the lifetime width) promotes an atomic electron to an excited state, which decays through an x-ray or Auger transition; all of this occurs in a single step. The emission line exhibits linear dispersion and sub-natural linewidth at resonance.

When an atom is ionized by a photon that exceeds the threshold energy, *post-collision interaction* provides a mechanism that bridges excitation and deexcitation by feeding energy from one to the other, smoothly linking resonant Raman scattering at threshold with the two-step mechanism at high energies. Post-collision interaction arises when the slowly receding photoelectron is still within, or near, the residual singly charged ion as Auger decay occurs.

Clearly, the fundamental understanding of atomic transitions will be advanced by a description that unifies the formation and decay of autoionizing and inner-shell vacancy states. The initial theoretical efforts are still at a conceptual stage where quantitative predictions are not easily extracted, and where the guidance of experimental data is of the essence for further elaboration.

Experimental study of weak subshell cross sections provides information on interchannel interactions. Interchannel interactions are usually weak on an absolute source. However, when a high-intensity channel interacts with a low-intensity channel, the low-intensity channel is often driven by the high-intensity channel. Besides highlighting inter-channel effects, measurements of weak subshell cross sections also permit the uncovering of the important spin-orbit and other relativistic interactions and even dipole-forbidden transitions.

Measurement of photoelectron spin polarization is of increasing importance to theory. Firstly, it provides direct measurement of relativistic interactions in atoms. Secondly, when combined with partial cross section and photoelectron angular-distribution measurements, it permits the complete determination of all transition amplitudes, both magnitudes and relative phases. Such measurements, which can be undertaken only at a very intense photon source, are the most stringent tests of theoretical models.

MOLECULAR STRUCTURE AND DYNAMICS

Molecular science has benefited significantly over the past decade from refined photoionization studies. Fundamental understanding of molecular physics as well as chemically significant insights have been stimulated by innovative experiments. For example, the concepts of channel interactions and the development of multi-channel quantum defect theory (MQDT) were motivated largely by photoionization measurements. Also, ubiquitous effects due to potential barriers, e.g., dramatic oscillator-strength redistributions and Franck-Condon breakdown, have had great impact in other areas such as physical chemistry. However, present instrumental capabilities restrict the growth of these fundamental molecular studies, and an improved excitation source is essential for (a) the sustained growth of these important studies, (b) the experimental base on which theoretical advances critically depend, and (c) the initiation of entirely new experiments.

Many of the experimental approaches and requirements parallel those applied to the studies of atoms. However, the presence of vibrational and rotational structure as well as the possible fragmentation of the excited molecule place a premium on high resolution and the measuring devices and methods used for the analysis of the various ionization products. The study of weaker processes that are so important for highlighting interchannel effects will require a high photon flux. The availability of a wide energy range, spanning 10 eV to several keV, is not only important for similar reasons as discussed for atoms but is crucial for uncovering phenomena that are intrinsic to molecules. For example, the nature of the molecular bond is best studied at the lower energies, say up to 100 eV, but phenomena that are localized to an atomic site of the molecule must be studied at higher energies by way of the ionization of core electrons. In another example, the effect of shape resonances on the various possible partial continuum channels should be explored by photoionization of the valence electrons at low energy and the different core electrons (s,p,d) at high energy.

Angle-Resolved Photoelectron Spectroscopy. The measurement of the electron abundance with respect to the photon polarization allows deduction of the partial cross section for the process and of the photoelectron angular distribution parameter. The experimental data are directly related to theoretically significant quantities which in comparison give stringent tests of the theoretical model used. As a consequence these measurements give dynamical information about the motion of the electrons in the molecule and the correlation of their motion in the molecular potential. These experimental data are indispensable to test theoretical formulations of initial and final wavefunctions and the pertinent correlations. This interplay between experiment and theory is the only way to improve our understanding as well as the theoretical models, which up to now have remained at the relatively simple single-channel level due to the great complexity of the molecular systems.

The new source, with its high intensity and resolution, will allow for the first time fundamental measurements in molecular systems to test the predictive ability of multi-channel quantum defect theory in systems such as H_2 and N_2. The theory accounts for the channel interactions that lead to autoionization, predicts the branching ratios and asymmetry parameters across autoionizing resonances, and clarifies competition between dissociation and autoionization. To make definitive tests of the theory, measurements with better than 0.01 Å resolution will be required and, due to the low cross section, fluxes on the order of 10^{12} photon/sec must be provided at the target. These measurements form a prototype basis for many molecular systems and are the type of experiment necessitated by expectations of advances in the field. Another area that depends critically on high resolution is the observation of ligand field splitting on core levels of main-group and transition-metal compounds. These ligand field splittings provide a new method for obtaining bonding information in organometallic compounds.

It is most desirable to study oriented molecules as a function of angle between the molecular axes and the polarization vector. Such experiments can be devised in the future with suitably prepared beams. The results would enormously increase our understanding of the molecular structure and would translate angular studies into a whole new domain of information.

Photoelectron measurements will serve as a basis for the various efforts by theoretical groups in calculation of cross sections for complicated molecular systems. High resolution and brightness are essential to be able to measure photoionization cross sections for a wide range of molecular systems over an extended energy range. These measurements are important also for their practical consequences in other areas such as radiation damage assessment and atmospheric physics.

Coincidence Measurements. To completely characterize photoeffect in molecules, both the excitation and deexcitation processes must be delineated and the interconnecting pathways must be established. An important avenue is given by placing photoelectrons or Auger electrons in coincidence with the fragment ions. Although high photon intensities are not necessarily beneficial for this type of experiment, high resolution undoubtedly is. These data will provide information on neutral and cationic potential surfaces and the associated vibrational dynamics. Theoretical treatment of this refined information on dissociative photoionization is still in its infancy, but tremendous advances in this area can be expected from these new studies.

Spin Polarization of Photoelectrons. The measurement of the spin orientation of a photon-emitted electron results in a complete determination of all scattering parameters for a dipole-allowed transition. As a result, precise tests of calculations are possible with all experimentally determinable quantities as constraints for comparison. Additionally, the details of spin effects in molecular dynamics can be elucidated for a complete understanding of the processes and potentials involved in photoionization. At the present there are no experiments of this type being performed in the United States and the unique capabilities of new source will make attractive possibilities in this area.

Fluorescence is a valuable probe of molecular photoionization for two reasons: First, it serves as the most general probe of the ionic alignment, which reveals both spectroscopic and dynamical properties from the body-frame polarization cross sections. Second, it is an extremely sensitive measure of the energy deposition in the ion when the fluorescence is energy-resolved. In fact, fluorescence polarization has been used already to study intra- and interchannel coupling in N_2 photoionization, while dispersed fluorescence has revealed rotational distributions in recent studies. These measurements demonstrate the utility, desirability, and feasibility of refined fluorescence studies, and serve as the springboard for the next generation of experiments.

Dilute Systems. Molecular photoionization studies have been tremendously useful for elucidating the electronic and geometrical structure of common molecules and atoms. However, the extension of these methods to the study of many chemically and physically important species has been blocked due to the lack of a sufficiently bright excitation source. The problem is that many such systems, e.g., open-shell atoms, molecular radicals, negative ions, atomic ions, and atomic clusters, cannot be created with the high sample densities mandated by currently available excitation sources or by internal constraints such as thermal decomposition of molecules at elevated volatization temperatures. The motivations for such work comes from many different scientific and technological disciplines. For example, chemistry and astrophysics rely strongly on a detailed understanding of highly reactive molecular radicals, and technological interest in atomic clusters is intense.

HIGH-RESOLUTION X-RAY SPECTROSCOPY

The high brilliance of the new source will expedite high-resolution studies of atomic systems in the 500-5000 eV range and beyond. To increase the resolution and in part compensate for lifetime broadening, doublely differential spectroscopies can be developed where monochromatic x rays are used to excite a system with the resulting emission studied through a dispersive device. An undulator with a tunable magnetic field would be an excellent source for these studies and along with appropriate crystal monochromatization, energy resolution of or the order of 0.1 eV could be obtained in the suggested excitation range. This technique represents a decisive advance in resolution in x-ray spectroscopy and can be applied to a wide range of physical and chemical problems.

ATOMIC PHYSICS WITH STATIONARY IONS AND ION BEAMS

Using a high-brilliance photon source, ions can be studied in extremely small quantities within an ion trap or as slow ion beams. Some of the ramifications of such studies have already been pointed out in the context of atomic dynamics. Spectroscopic information on multiply charged ions is also highly important for the interpretation of effects in plasmas which are produced in diverse ways in the solar environment, Tokomaks and laser-induced bursts. In a unique application of intense synchrotron radiation, ions can be produced inside ion traps in high charge states and, most significantly, with kinetic energies much lower than obtainable by other methods. These ions can then be used in situ or extracted as a beam to serve for precision ultra-low-energy collision experiments. An entirely novel way for studying multiply charged ions with photons, or electrons, would be offered by the combination of such a new source and a separate heavy-ion storage ring.

EXPERIMENTAL REQUIREMENTS

Most of the envisioned experiments require a flux of 10^{12} to 10^{13} photons per second incident on the sample which has a cross section of typically 0.1 × 0.5 mm. This photon beam should have a bandwidth of 0.01 Å over most of the photon energy range which spans 10 eV to approximately 10 keV. Provisions for scanning the photon energy should be made. For the benefit of coincidence measurements, a multi-bunch mode of operation is indicated. The wide range of energies should be covered under optimum conditions which implies access to different beamlines and a facile switchover of the setup. Many of the new experiments will cross laser or ion beams with the photon beam. The additional apparatus will require ample space at the end of the beamlines.

Biology and Medicine

INTRODUCTION

A low energy (1.3 to 1.5 GeV) ring that maximizes vacuum uv and soft x-ray radiation while minimizing power loading at higher energies is just what the biologists are looking for. Most transitions of bonding electrons occur in the vacuum ultraviolet (VUV); the large intensities from a high-brightness synchrotron source are important for circular dichroism, linear dichroism, and fluorescence measurements. Imaging of many types would use x-ray radiation in the water window. Differential scattering of circularly polarized light (CIDS) pinpoints the parameters for the chiral structures found in cells, while differential absorption of circularly or linearly polarized light enhances the sensitivity and contrast in microscopy. High brightness for soft x rays would allow imaging of biologically significant samples that may be unstained and "wet" by a variety of techniques. X-ray holography might produce three-dimensional images of organelles. Soft x-ray diffraction could produce patterns for single specimens. Stereo images of cells might be obtained in several ways. In the medical field, a 1.5 GeV source in conjunction with a 5-tesla wiggler would produce sufficient quantities of radiation at 33 keV for noninvasive coronary angiography at a competitive cost to techniques requiring a dangerous operation.

VACUUM UV RADIATION

At present there are no conventional VUV sources that are broadly tunable with a flux in excess of about 10^9 photons/sec. Biologists are interested in the chemical properties of molecules as observed in the excitations of valence shell electrons. Thus they need VUV radiation in the 2000 to 1000 Å range and would favor a 1.3 to 1.5 GeV ring. High spectral resolution is not always required, so that bandwidths of 0.5% are often adequate for "monochromatic" light. Within reason, the aperture size is also not important. However, high fluxes of at least 10^{14} photons sec^{-1} are important for differential techniques such as circular dichroism and linear dichroism. Rings with more than 1.5 GeV would create large amounts of power that might preclude their use with biological samples. Furthermore, it is necessary to scan the spectrum and scanning the entire range from 3000 to 1000 Å is desirable for biological molecules. In order to avoid the problems inherent in eliminating higher energies, the best solution would seem to be a U_A undulator provided that the user controls the gap with a stepping motor for scanning purposes, and rapid scanning over most of the range is available.

CIRCULARLY POLARIZED LIGHT AT THE WATER WINDOW

Both differential scattering and differential imaging of circularly polarized light from 280 to 530 eV will yield important information about biological materials. Both techniques require a beam line with crossed undulators (K-J Kim's device) for making circularly polarized

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Contributors were W.C. Johnson (Chairman), J. Kirz, and A. Thompson.

light. The device must chop between right and left polarizations at some reasonable frequency and must be tunable for this energy region.

Circular Intensity Differential Scattering (CIDS) gives the chiral parameters for the secondary and higher order structures found for polymers in biological systems. Differential absorption of circularly or linearly polarized light enhances the sensitivity of imaging by doubling the information content and increasing contrast.

ELEMENTAL MAPPING BY ABSORPTION MICROANALYSIS

Absorption edges in the soft x-ray range can be used to map the distribution of various elements in a specimen. Two images are formed, one on either side of an absorption edge. The quantitative elemental map is made by analyzing the differences between the two images. The method has been used so far only to map major constituents, such as calcium in bone. Both scanning microscopy and contact microscopy have been used, and resolution better than 0.25 μm has been demonstrated.

With a high brightness source and a high resolution monochromator elemental mapping can be expanded in directions of considerable biological interest:

a) With high statistics digital images, attainable by scanning microscopy, one should be able to map elemental constituents of physiological interest (e.g., calcium and potassium in muscle).

b) With any of the imaging methods it should be possible to exploit the small chemical shifts in the absorption edges, to map the location of certain elements in a given chemical state, and to create separate maps for them.

c) It should be possible to improve the resolution in the elemental maps to order 100 Å.

SOFT X-RAY IMAGING

A high brightness 1-2 GeV source will open up new possibilities in soft x-ray imaging. Many imaging techniques require coherent illumination, while others need high intensity.

There is particularly great interest in the possibilities for imaging wet biological specimens with resolution in the 100-500 Å range, possibly extended to three dimensions. The wavelength range 23 to 43 Å (often called the water window) is ideally suited for that purpose, since water is relatively transparent here. Undulators with periods around 3 cm on a 1.3-1.5 GeV ring would provide an ideal source for such investigations. The output from such undulators contains very high coherent flux, with wavelengths tunable over the region of interest, without excessive radiated power. The importance of minimizing total power is closely connected with the need for high resolution monochromators, which are sensitive to thermal distortion. The most promising approaches to three-dimensional imaging of wet biological specimens are discussed below.

X-Ray Holography. The first attempts at developing this technique (primarily in Japan) were limited by the lack of coherent flux. More recent work, especially by Howells et al. using the U15 beamline at Brookhaven's NSLS, have yielded promising results on simple systems, but are still limited by available coherent flux. For work of relevance to biology, this limitation must be removed. The proposed source, with a short period undulator and a high resolution monochromator provides exactly what is required. In usable, coherent power, the source is superior to the U15 beamline by about 5 orders of magnitude! The transverse resolution of the reconstructed hologram should eventually achieve values in the 200 to 400 Å range.

Soft X-Ray Diffraction. It was pointed out by Sayre that the structure of any specimen should be reconstructable from its diffraction pattern by the methods of x-ray crystallography, provided the diffraction pattern can be recorded. For a non-crystalline specimen the pattern is weak, especially at large angles, and, since the illumination must be coherent, the method demands very high coherent flux. Initial tests indicate that diffraction patterns from small biological specimens can indeed be observed. The ultimate resolution of this approach is half the wavelength of the incident radiation, or about 15 Å. The coherent power from a short period undulator is necessary to develop this method. In view of the substantial exposure involved, the method will require specimens that are not easily damaged by radiation.

Contact Microscopy. High resolution contact microscopy, developed by Feder et al., has already succeeded in providing stereo images. This technique needs more flux to allow "flash" imaging of live (and motile) specimens. A wide beam (~ 5 cm) is desirable to accommodate large specimens.

MINIMALLY INVASIVE CORONARY ANGIOGRAPHY

Transvenous coronary angiography using synchrotron radiation is being developed by a group from Stanford, SSRL, and LBL as a possible technique for imaging coronary arteries with much less risk than current methods.

Currently a very dangerous procedure utilizing an arterial catheter is used to deliver contrast agent to the coronary arteries. Using synchrotron radiation it may be possible to introduce the iodinated contrast agent by an injection in a peripheral vein. Greatly enhanced sensitivity is achieved by acquiring digital images above and below the iodine K edge (33 keV) and then logarithmically subtracting those images. Initial images have been taken at SSRL of the coronary arteries of an anesthetized dog. Next year it is planned to study human subjects with this system.

Even though this experiment uses 33-keV x rays, this important medical problem can be studied at this facility using a superconducting wiggler. Assuming that a (7.5 mrad) beam (15 cm wide at 20 m) was available from this insertion device, the flux available at 1.9 GeV, 400 mA, 5 tesla is a factor of more than 200 greater than is estimated to be required for angiography. It appears to be possible to operate successfully at 1.5 GeV. Results from patient studies next year should be able to accurately estimate the acceptable limits of machine operation.

CONCLUSIONS

1. A 1.5 GeV ring appears to be a good compromise which gives a reasonable flux in the vacuum uv and soft x ray region without undue power loading from higher energies.
2. Beamlines should be made available to the biological community for vacuum uv spectroscopy and soft x-ray work in the water window.
3. For much of the imaging program short period undulators (such as D or S) would be best.
4. Vacuum uv spectroscopy requires high flux and rapid wavelength scanning with a modest (< 0.5%) bandwidth.
5. Users will need control over the gaps on the undulators used on their beamlines.
6. One or more beamlines should have a device for chopping between right and left circularly polarized light.
7. Components (such as monochromators, detectors, windows) should be available for one-of-a-kind experiments by users. Sophisticated apparatus should be available for data collection and analysis.
8. Provision should be made for blocks of time on call for biologists who have successfully prepared rare and fragile samples.

Note: See "User Policy and Facility Parameters" section for a fuller discussion of conclusions 7 and 8.

Industrial Research and Technology

X-RAY LITHOGRAPHY

It is anticipated that by the time new soft x-ray synchrotron source will go on line (5 years from now), it will be the synchrotron facility required for cutting-edge research in advanced lithography. The primary issue anticipated for the new facility will be advanced imaging techniques (e.g., by means of projection optics) rather than proximity printing. Specifically, the high-current, high-brightness source, tunable in the 250 eV to 1500 eV spectral range, will be utilized to address issues relating to 0.25-µm lithography for 256-Mbit chips extending down to 0.17-µm lithography likely to be required for 1-Bbit chips. It is expected in the interim that present lithography research systems will be developed into pilot systems and then into volume production systems around 0.5 µm using compact synchrotron and plasma sources. These appear to be adequate for 64 Mbit, and the transition from optical to x-ray lithography is likely to occur at this level. Other issues include advancement of the application of insertion devices necessary to maintain production-scale throughput at decreasing feature sizes, electron beam wobbling for exposure field enlargement, and improvement of the mechanical stability of step-and-repeat stages for next-generation exposure systems. The new source will provide the necessary training environment in these areas of research and development, thus satisfying what is anticipated to be a critical national need if this country is to remain competitive technologically. For the same reason, the U.S. industry is encouraged to form a consortium to address these issues in a cooperative fashion as is done in Europe and Japan.

In the following discussion, the requirements on electron storage ring and photon beamline design are presented. In order to provide the spectral flexibility necessary for advanced lithography research in the areas of mask and resist, the 8 to 15 Å wavelength range is recommended. Normal-incidence projection optics will need wavelengths above 30 Å due to the loss mechanisms in the optical elements. A tunable undulator (configuration D at 1.9 GeV beam energy appears to be the appropriate choice) should be able to cover this spectral range with sufficient intensity. A grazing-incidence mirror should be implemented to provide the option of high-energy cut-off as needed. In addition, a separate bending magnet beamline might be required to satisfy the anticipated high beam-time demand by users wishing to fabricate test circuits. The exposure field needs to be about 5 × 5 cm^2 to be relevant for application purposes. This should be achieved by means of electron-orbit modifications (e.g., beam wobbling). An alternative solution could be a two-dimensional scanning mirror arrangement, which, however, may introduce intensity losses and degradation problems and is therefore less attractive. In order to minimize the area of the exit window, a

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Contributors were R. Jaeger (Chairman), S. Laderman, P. Pianetta, M. Sogard, and G. Williams. Discussions were held with F. Cerrina, A. Neureuther, D. Rose, W. Turnbull, and J. Warlaumont. Critical comments by T. Barbee were greatly appreciated.

mechanism needs to be implemented in the beamline design that provides a synchronous motion of exit window and beam (at the lithography facility of BESSY [Berlin], the whole beamline is moved at present). The beamline design has to provide efficient He pumping to allow for the use of He as mask-cooling and/or beam-transport gas. An all-vacuum section will be required for the development of projection optics. It is anticipated that the users will provide their own exposure stations. A minimum-configuration station including an aligner (without stepping capability) appears to be appropriate for staff training and unequipped first-time trial users.

APPLIED MATERIALS CHARACTERIZATION

The new VUV and soft x-ray synchrotron radiation source would significantly contribute in two key areas of materials characterization in support of advanced industrial materials development. First, it would provide an exciting opportunity to promote a major advance in the application of white-light x-ray topography to studies of bulk structural defects and thin-film stresses. A wiggler would supply a bright beam in the range of 7.5 to 12.5 keV without introducing strong harmonics. The intensity should be more than enough to overcome the critical barriers presently existing for real-time white-light topography of semiconductor materials with high spatial and temporal resolution. Second, as surface, near-surface and thin-film material requirements for semiconductor technologies become more stringent, the use of advanced chemical analysis techniques such as those discussed in the surface science and materials science groups of this workshop will likely gain importance. By advancing such techniques, training material scientists, and increasing the opportunity to perform experiments in these areas, the advanced facility would significantly contribute to critically important technologies such as surface and thin-film preparation.

OTHER APPLICATIONS

Besides the important industrial applications presented in the preceeding sections and discussed in detail by the working group, other opportunities of industrial interest present themselves. Major topics are micromachining, surface scanning, contact transmission, microscopy, holography, polymer characterization, and optimization. Micromachining utilizes lithography to fabricate microscopic physical structures primarily out of silicon. New types of mechanical transducers as well as chemical-specific transducers are possible. Arrays of microscopic channels etched into silicon provide the means for gas flow centrifugation (e.g., for isotope separation). Some of these structures require extremely high aspect ratios in the resist that can only be achieved with x-rays harder than those used for the replication of electronic device structures. Microscopy in conjunction with element selectivity ("microprobe") is extremely important for the characterization of technologically important materials structures. All x-ray imaging techniques should benefit from a better understanding of the polymers used as image medium. An increased polymer research in the soft x-ray regime is therefore encouraged.

A synchrotron facility for industrial research needs to satisfy several organizational and technical requirements, as set forth in the "User Policy and Facility Parameters" section.

New Techniques and Opportunities

This group consisted of two subgroups, one on novel experiments and new techniques and the other on the possibilities for incorporating a free electron laser (FEL) into the new synchrotron radiation facility. The goal of the novel experiments and new techniques subgroup was to identify source characteristics that were important for a widely varied group of forward looking experiments and to discuss new approaches to problems such as magnets, undulators, optics, and short synchrotron radiation pulse production. The FEL group considered possible facility variations or future upgrades that provide radiation of greater coherence. The following topics were discussed.

Laser-Synchrotron Picosecond Pulse Experiments. Present laser technology in the pulse width range accessible using a new synchrotron radiation source (8 ps to 90 ps proposed bunch lengths for different options) provides 5-ps pulses at approximately 1000 Hz repetition rate, with 10-20 microjoules per pulse, for a peak power of 2-4 MW covering the spectrum from the near IR to the near UV. For laser-SR pulse experiments such as angle resolved photoemission the SR source should have the shortest possible pulse width (certainly less than 20 ps). The radiation pulses must be phase stable to allow stable coincidence timing. The SR source must have high brightness to allow a 50 micron or smaller spot size at the sample, and must have a short and long term pointing stability of better than 50 microns at the sample to ensure overlap with the focussed laser beam, which can be a diffraction limited spot. This also demands some kind of precision beam alignment system, since overlapping small beams of invisible radiation is non-trivial. In addition, a beam knock out system to switch on and off the SR beam would be highly desirable, and is absolutely necessary for some experiments.

Excited-State Spectroscopy. Advances in high-resolution spectroscopy of atoms and molecules, as well as spectroscopy of excited states, is at present limited by source brightness and spectrometer resolution. The range of photon energies of interest is approximately from 5 eV to 200 eV. The areas identified as important are:

1) Autoionizing resonances
    a) Flux required: 10^{14} photons/sec in 0.01 eV bandwidth.

2) Selective excitation
    a) Flux required: 10^{15} photons/sec in 0.01 eV bandwidth.
    b) Selectable circular polarization.
    c) low sample atomic density of $<5 \times 10^{10}$ atoms/cc.

The circular polarization requirement could be met using K-J. Kim's proposed crossed polarized undulator system.

High Pressure X-Ray Diffraction at 20 keV. This work requires high photon energy to penetrate the diamond anvils used in high-pressure cells.

Contributors were B.M. Kincaid (Chairman), R. Laderman, P. Pianetta, M. Sogard, G. Williams, T. Barbee, K. Halbach, J. Bokor, D. Ederer, M. Howells, M. Nichol, T. Jach, D. Rose, W. Colson, D. Deacon, K-J. Kim, J. Murphy, and H. Wiedemann.

In addition, very small x-ray beam size is necessary (<0.1 mm) along with small divergence for precision crystalline x-ray diffraction work. The lifetime of the high-pressure samples is often limited, thus requiring large fluxes to take diffraction data rapidly. This adds up to a requirement for a high brightness source of short wavelength x rays. This could be met by wigglers with 1.9-GeV operation.

Dynamical Diffraction from Crystals with Glancing Incidence X-Rays. These experiments represent the prototype of a new generation of diffraction measurement likely to become common at synchrotron light sources in the future. They offer the following advantages: 1) direct visualization of the dispersion surfaces determined by dynamical diffraction in the crystal; 2) surface diffraction channeled along only the surface region of the crystal; and 3) x-ray standing waves which permit the determination of adsorbate position parallel to the crystal surface. It is the ability to control both the incident angle of the x rays on the crystal and the diffraction angle which makes these extra features possible.

The method and theory has been conclusively proved in recent experiments at HASYLAB (by S. Brennan, P. Cowan, T. Jach, M. Bedzyk, and G. Materlik). However, strict requirements for small beam divergence (5 μ rad vertical, <60 μrad horizontal) have severely limited the photon flux on the surface of the crystal. The methods used to produce x-ray beams with small divergence require a synchrotron light source with low emittance and high brightness. There is a need for a source at least 100 times brighter than the one used for the experiments (DORIS, Hamburg) and in fact 10 times brighter than the present available source (NSLS, Brookhaven). The new source would appear to fit these needs if equipped with wigglers and undulators that would extend the radiation into the 5-10 keV energy region.

Magnet Technology. K. Halbach presented a summary of recent work on permanent magnet systems, including a discussion of the basic performance numbers for hybrid undulators, and new methods for achieving higher fields, controlling saturation in the steel, and controlling undulator field error tolerances.

Undulator Tolerances. B. Kincaid discussed his recent work on the effects of undulator errors on the radiation spectrum. There was an extended group discussion of various methods of timing or tuning very long undulators using the output radiation. The main message of Halbach and Kincaid was that undulator design must include careful control and understanding of tolerances, and that long undulators will require special design techniques, including segmentation, multiple trims, and use of the spectrum for tuning the undulator.

Multilayer Optics. The optics necessary for multipass operation of FELs or manipulation of insertion device generated light must withstand demanding operational conditions. Any such optical system must have high strength, thermodynamic stability, low thermal expansion, high radiation damage resistance, and yield high throughput and resolution performance.

Recently, multilayer optics of high enough quality to be used as elements in synchrotron applications have been demonstrated. These new structures have the capability to be engineered and formed onto curved surfaces and can be used as transmission optics as well as in reflection.

Radiation resistance and thermal stability can be achieved by using materials such as a silicon carbide as substrates. This material has good polishability and is now available in large shapes.

Multilayer structures will operate at wavelengths of approximately 30 Å to 800 Å at normal incidence. Presently observed reflectivities in the range of 20% to 50% in the VUV and XUV region are expected to improve so that better than 50% reflectivity will be achieved over the 30 Å to 800 Å range.

These will generally be broad band pass optics with resolution of from 1:10 to 1:100. Recent work on multilayer gratings shows great promise for increasing this resolution to 1:1000 or better. Work is in progress on Mössbauer nuclear scattering x-ray optics that could lead to extremely high spectral resolution $(1:10^8)$. This high resolution requires an undulator source in order to get useful output flux.

Multifacet Metal Mirrors. A multifacet metal mirror concept for an XUV FEL resonator has been proposed by Newman at Los Alamos. The basis is quasi total *external* reflection of s-polarized beam at angles larger that the critical angle $(\theta < 60^\circ)$. Metals are spectral regions where the optical constants n and k are sufficiently less than unity are candidates. Metals such as Al $(\lambda \geq 35$ nm), Si $(\lambda > 35$ nm), and Rl $(\lambda =$ 10-14 nm) provide over 50% retroflectance for configurations of 6 to 9 mirror facets. Potential hazards include oxidation and carbon film growth as well as substrate roughness. The effects of these will be examined in the coming year at Los Alamos.

Use of New Source Injector Linac for Slow Positron Beam Source. The new source injector linac could be used to provide a user facility for slow positron beam research during the long idle times between fills of the storage ring. The linac beam produces fast positrons by pair production in a target, which then thermalize in a moderator. Thermal positrons then diffuse to the surface of the moderator and escape. Some positrons form positronium at the surface. The study of low energy positron physics has grown rapidly in recent years, with several groups around the world mounting serious research efforts. There is sufficient demand at the present time to justify a user facility slow-positron beam.

The optimum use of the injector for positron beam work would require the following operating parameters:

1) high energy $\geq$ 100 MeV)
2) high peak beam power $\geq$ 10 kW)
3) high rep rate (approx 1000 Hz)
4) a short pulse structure to minimize heat loading.

In addition, a user facility slow-positron beam needs lab space, shielding from primary radiation and available when facility is running, and a multi-port slow positron beam transport system accommodating user experiments. These requirements may require some kind of collaborative effort on the linac over the above the new facility requirements.

Soft X-Ray Lithography--The Future. If all technical problems involving masks, resists, substrates, etc. are ignored, even though they are "semi-insurmountable problems" at present, the physics of the x-ray lithography exposure process sets certain limits on the wavelengths to be used. For optimum resolution a narrow range near 1 keV is the only choice. The MCFS (minimum controllable feature size) then turns out to be from 0.5 micron to 0.25 micron, assuming a reasonable tolerance budget in a real industrial lithography application. This resolution demands major advances in 1 keV optical elements. Even if high brightness sources were available tomorrow, the optics would still be the problem.

RF Buncher-Debuncher System for Bunch Compression. A system for compressing the electron bunch in time before an insertion device and then expanding it again after the insertion device should be investigated as a way to make very short light pulses.

Method of Chopping the X-Ray Beam on a Picosecond Time Scale. Use one undulator and a sub-millimeter wavelength RF or laser source to bunch the electron beam on a short distance scale within the main bunch. Then use this bunched beam in a second downstream undulator to produce chopped or modulated undulator light.

FREE ELECTRON LASER (FEL) SUBGROUP SUMMARY

The FEL subgroup explored options for a FEL-based VUV and XUV facility as a part of the new source. The basic assumptions of the group was that FEL experiments now underway (i.e., Stanford, Los Alamos) will lead to a usable VUV (1000 Å to 500 Å and higher harmonics) laser. If the new machine were designed to incorporate such a device as an upgrade option, a unique and valuable source of tunable coherent light could be provided for the scientific community.

The FEL requires somewhat different operating parameters for the storage ring, including operating at 1 GeV and 0.75 GeV with a single high current electron bunch. In addition, a longer straight section (~20 meters) is required.

The bypass scheme proposed in LBL white paper LBL-18945 (K-J. Kim, ed.) can provide this long straight section. This scheme also allows single pass short wavelength FEL operation, possibly to ~100 Å wavelength, as described in the LBL report. The same straight section could also be used for light source undulators, time sharing the electron beam with the normal bend magnet sources and straight section insertion devices. Some of the ideas proposed for the long bypass straight section were:

1) A single long undulator (~1000 periods). This assumes that the problem of tolerances discussed by Kincaid and Halbach can be dealt with.

2) Several shorter undulators in a dog-leg arrangement serving multiple beam lines.

3) Co-linear undulators for multiple wavelength operations.

The FEL group also considered use of the injector as a driver for an infrared (IR) FEL.

The injector could be used to drive a 1 to 10 micron range FEL similar to the one recently developed by Madey's group at Stanford. Providing space for this would cost very little, and the FEL radiation produced could be provided to users. There was a strong support for this idea.

The subgroup's recommendations are that a staged approach to the FEL facility be adopted, so as to minimize disruption of the normal scientific user program.

1) First, the bypass design and machine operating conditions should be established.
2) Machine components common to both the bypass straight section and the standard ring design should be installed when the ring is built.
3) Complete the installation of the bypass system and the light source insertion devices in the bypass.
4) After FEL technology has been proven useful in the VUV and XUV ranges, and consistent with user demand, install the FEL system.

This staged approach should provide maximum scientific benefit with minimum interference with the main goals of the new facility.

PART II. TECHNICAL DESIGN CONSIDERATIONS

Storage Ring Issues

INTRODUCTION

The task of the Supporting Group on Storage Ring Issues was to interact with the user community, translate their requirements into machine parameters, and identify the important machine-related R&D issues raised by these requirements. No effort has been made by the group to select or prioritize among potentially conflicting requirements.

BASIC MACHINE DESIGN AND PERFORMANCE GOALS

The basic machine is a periodic lattice comprising a number of straight sections which accommodate insertion devices. Proposed numbers are 12 straight sections each 6 m long and a beam energy in the range of 1-2 GeV. A high brightness is generally needed and a high photon flux is a basic requirement. The incorporation of the above design features involves the following studies:

- lattice for optimum brightness and minimum error sensitivity
- beam dynamics and lifetime
- beam position stability and control
- injection efficiency
- RF design
- vacuum considerations
- component optimization

Suggested studies concern the trade-offs between beam energy, performance (for instance, brightness and lifetime) and insertion devices.

OBJECTIVES AND ENHANCEMENTS

Wishes have been expressed by various working groups to enhance the basic design for special purposes.

Bypass. The addition of a bypass to accommodate either a long undulator for single pass FEL operation or a conventional undulator to minimize line width. On a pulsed basis, this could also be used for time-of-flight experiments, where long and variable time intervals between pulses are required. The main R&D issue here concerns the reproducibility and stability of the orbit on a pulse to pulse basis for the experiment in question and specifically for the other users. This mode of operation is incompatible for simultaneous multibunch conventional operation.

Contributors were M. Cornacchia (Chairman), L.N. Blumberg, E. Gianfelice, K. Halbach, A. Hofmann, A. Jackson, K-J. Kim, P. Morton, H. Lancaster, L. Palumbo, H. Wiedemann, and M. Zisman.

Improved FEL Capability. The utilization of the first 50 MeV of an injection linac would allow the generation of infrared FEL radiation. This seems to be an issue requiring application of conventional technology and should therefore be straightforward.

SPECIFIC R&D ISSUES

Overall Detailed Performance Evaluation. Although the fundamental feasibility has been established, additional effort is required to optimize the overall performance of the facility and its components. No fundamental problems are anticipated, but preconstruction R&D is required for detailed design of some components.

Beam Position Stability and Reproducibility. A general requirement is the tight stability of the beam position and angle (of the order of the beam size and divergence). Some R&D effort is necessary in order to develop and optimize feedback systems, as well as beam diagnostics.

RF System. A useful field of research concerns the optimized shape of the RF cavities to minimize high order mode losses.

Vacuum System. Improved understanding of the gas desorption and beam cleaning processes will help the optimization of the system.

Impedance Studies. A program of impedance evaluation and measurements is necessary. Low impedance and stable longitudinal motion are demanded by the users' requirements of short bunch length with minimal jitter. An improved understanding of the beam-environment interaction will provide the necessary input for the design of instability correcting systems.

Heat Load and Stress Analysis. Such analysis of vacuum chamber components must be done in order to insure the safe operation of the facility.

Experiments in Existing Facilities. Experiments on existing storage rings are highly desirable to verify the design codes used for new facilities. Specifically, continuing studies of

- dynamic aperture
- impedance
- injection efficiency
- beam characteristics

will strengthen the data base for the machine design.

Effect on Beam Parameters of Insertion Devices. The impact of wigglers and undulators on the emittance, lifetime, and energy spread should be studied and limitations established.

Beamlines

INTRODUCTION

A key element in the successful exploitation of the new storage ring photon source is the availability of beamlines, which can deliver monochromatic light to an experiment without degrading the beam quality. Fortunately, we are in a position to address this challenge with a certain amount of hindsight. The first generation of beamlines that were built for high brightness dedicated sources (NSLS, BESSIE, etc.) have now been operating for some time and we are in a position to see where the limitations to their performance come from. In virtually all cases the limitation comes from the quality of the figure and finish of aspheric (cylindrical, toroidal, paraboloidal or ellipsoidal) optical surfaces. The surface imperfections have arisen largely from optical fabrication tolerances, but the role of distortions due to photon beam thermal loading is becoming more important. Now that we understand the overriding priority that must be given to these issues there are a number of relatively straightforward strategies that we can use to ensure that the next generation of beamlines are free of limitations due to optical surface quality. The simplest one is to avoid the use of aspheric surfaces altogether and build beamlines using only flat and spherical surfaces. These can easily be fabricated with tolerances considerably better than needed and this provides one solution to the fabrication problem. Other approaches require improvements in methods of fabrication and the related technology of surface metrology. The thermal problem can be solved by applying active cooling to the optical substrates.

The consequence of these evolutions in design will be that, compared to present beamlines, the next generation will have different layout, more horizontal deflections, more cooling, more use of the Rowland Circle, but, most important, less technological uncertainty.

The beamlines working group has studied the various areas where improved technical capability is desirable and apart from the optical surface question discussed above we have identified two other general areas of high importance: 1) the beamline/storage-ring/insertion device interface and 2) the fabrication of dispersive elements, gratings, multilayers, zone plates, etc. In the sections that follow we elaborate on these issues and make specific recommendations for the assignment of R and D resources. We also initiate an information gathering exercise on the optical surface question that will lead to reports and analyses of the present status of this technology at a special workshop on the subject at Brookhaven in May 1986. Finally we report some discussions and recommendations on the organization of users into effective units for beamline developments.

Contributors were M. Howells (Chairman), R. Ryan, A. MacDowell, S. Hulbert, G.K. Tirsell, A. Thompson, F. Cerrina, J. Cerino, S.T. Kulkarni, E. Hoyer, P.Z. Takacs, P. Cowan, M. Hettrick, and W. Warburton.

RESEARCH AND DEVELOPMENT PROGRAM

We propose the following 10 items in Table 8-1 below for immediate initiatives or on-going R and D programs. They are listed in our priority order and are discussed at greater length in the sections that follow.

Although progress on these items will be highly beneficial to the light source program they should not be construed as potential obstacles to progress. On the contrary we believe that there are no "show stopping" problems facing us at present.

Table 8-1. R and D Program Summary.

	Item	Target Institution
1.	Design, construction and operation of real heat resistant mirrors, gratings and crystals.	Collaboration with scientifically motivated projects.
2.	Finite element modeling of thermally loaded optical surfaces, etc. Refinement of technique, experimental verification, networking to a wider community.	BNL and/or LBL
3.	Beam/Beamline/insertion device alignment, feedback systems and their signal measuring devices, gap scanning, suppression of effects on e^- beam.	Host institution of the accelerator
4.	Application of novel materials and techniques to synchrotron radiation optical components.	Small business/national lab*
5.	Computer modeling by optical ray tracing, refinement of technique, networking to a wider community.	F. Cerrina, University of Wisconsin
6.	Instrumentation for figure measurement of grazing incidence optics.	Small business/national lab*
7.	Develop a U.S. source of ion etched diffraction gratings for synchrotron radiation.	Small business*
8.	Develop a U.S. source for high resolution diffractive optics, especially zone plates.	Business/national lab*
9.	Detectors	Detector group at host institution
10.	Special beamline for optical component testing.	Ideally one at each facility but most cost-effective open port is Wisconsin.

*Small business/national laboratory joint ventures are especially to be encourages in these areas.

1. Design and Construction of Heat Resistant Beamlines

The proposed light-source facility will include undulators of very high brightness and wigglers of moderately high power output. The primary issue of beamline design is to hold the required tolerances in the presence of this power loading on optical elements--mirrors, gratings, crystals, and multilayers. Secondary issues arise because of the need for cooling these elements in a UHV environment whilst carrying out arc-second angular tuning.

A great deal of progress has been made in solving these generic problems in the present generation of beamlines and further advances are being made in theoretical studies of design approaches for even more challenging situations. However, this work will always be incomplete until the designs have been demonstrated in a serious operational environment. Therefore our first priority is that we must do more than studies. We must build real heat-resistant beamlines and components and utilize present radiation sources to prove the technology that we plan to use for the next generation of synchrotron radiation facilities.

2. Thermal Loading of Optical Components

X-ray optical elements on beamlines of a 1-2 GeV synchrotron will be subjected to significant power densities and power density gradients and we need to improve our skills in dealing with these problems. The major issues that need to be addressed are thermal stability of materials, new materials research, computer simulation, and cooling methods.

Thermal Stability. The thermal stability of focusing elements is particularly important because they must maintain arc-second accuracy over the area that the beam strikes under the varying heat loading conditions of a typical fill cycle. If these components are thermally distorted it will lead to an apparent loss of source brightness. The thermal stability of monochromator elements is particularly important since the wave length calibration and spectral response can be affected.

Both laboratory and synchrotron research facilities need to be developed to measure thermal distortion under conditions that simulate the heat load from planned beamlines. Instrumentation such as an infrared camera and an optical interferometer will be required to measure temperature and surface profiles of components. A laboratory facility using either an electron or ion beam source could study the following:

a) VUV mirrors and gratings under realistic power levels.
b) New materials with better thermal properties.
c) Properties of new monochromator elements like synthetic multilayers for long term stability under varying power levels.
d) Different cooling geometries.
e) Validation of computer modeling of optical elements.

On a synchrotron beamline a facility should be provided for viewing mirrors and monochromator elements with an infrared camera as they are illuminated by the synchrotron radiation beam. This facility would provide a way to test and validate the calculated thermal and x-ray performance of optical elements.

New Materials Research. The physical properties of materials used for optical elements often determines their thermal performance. New materials need to be evaluated for use as optical elements. Some of the properties that must be considered are the following:

a) Thermal conductivity
b) Coefficient of thermal expansion
c) Ultrahigh vacuum compatibility
d) Machinability, capability for brazing, welding, etc.
e) Tolerance to thermal cycling
f) Stability under radiation loads
g) Grain growth of polycrystalline materials
h) Stability and cleanability of optical surfaces

Computer Simulation. As well as experimental measurements an effort to refine and extend our present computer simulation capability is required. Improved capabilities are are needed in the following areas:

a) Calculations of the incident power spectrum and how it is absorbed in the optical element.
b) Performance of finite element analysis of various cooling geometries to trace the heat and stress profiles through the volume of the optics.
c) Prediction of the loss in output performance due to thermally induced effects.
d) Arrangements to enable the modeling capability that is presently available at LBL and BNL to become more widely accessible to the community through the support of suitable liaison personnel and networking capability.

Cooling. A variety of different cooling methods are potentially useful for these optical elements. Some of these are:

a) Turbulent water cooling
b) Heat pipes
c) Liquid-metal coolants
d) Cryogenic cooling schemes

These are essentially engineering issues and should be addressed in the context of a concrete design problem.

3. Stability and Alignment of Beamlines and Insertion Devices

We cannot overemphasize the importance of beam stability. We suggest that the beam position needs to be stable at the level of ± 1/4 σ at the entrance slit of the monochromator and at the source. This stability is needed in both horizontal and vertical planes for low K insertion devices. In order to attain the necessary stability the beamlines must be instrumented with monitors of very high positional resolution, and high gain-bandwidth feedback. Such monitors would need to be superior to those presently used and some development work should be initiated in this area.

Due to the peaked nature of undulator spectra, it will probably be necessary to vary the insertion device gap as the monochromator is scanned, both under user control. This continuously changing field must be so well compensated that it has no detectable effect upon electron beam size or position or upon other photon beamlines. Hence we strongly recommend that electron beam/insertion device interaction dynamics be given a high priority as a storage ring design issue and be addressed early in the overall program.

4. R&D Effort in Novel Materials Techniques and for Optical Components

We recommend an R and D effort to develop new materials and fabrication techniques that will alleviate the surface roughness and thermal distortion problems. In particular there is a need to assess the suitability of new and improved materials for optical component fabrication, e.g., ceramics (SiC), metals, special surface treatments (CVD coatings, sol gel application, lower surface treatment), multilayer coatings. In addition, there is a need to develop improved polishing methods based on recently developed techniques for measuring surface roughness, and to develop methods of in-situ cleaning of optical surfaces. Most suppliers of optical components do not have the resources to support a materials development effort. A cooperative arrangement between the national laboratories and optics suppliers would be the most efficient way to develop new techniques and transfer them to the manufacturing community.

5. Ray Trace Analysis

A crucial part of the development of advanced optics for the new high brightness sources will be prediction of the optical system performances. This must be achieved by means of an accurate and reliable computer simulation of the optical system, including an accurate modeling of real sources (bending magnets, wigglers, undulators). The code must be capable of predicting the effects on the system performances of non-ideality factors; this is particularly crucial for the case of high resolution monochromators and spectrometers.* The important problem of power distribution on the optical surfaces must also be addressed in an improved way, particularly for wigglers. The program must be able to generate an output that can be used in a finite element analysis code in order to calculate the surface distortion; this can then be fed back in order to calculate the effect on the system performances.

The new codes will be based on SHADOW, developed at the University of Wisconsin by F. Cerrina.† User-friendliness will be further improved by extending the use of graphics and menu-oriented input. Essential to an efficient use is the timely distribution of new features and improvements to users of the program, as well as the availability of good documentation. This will be achieved by a) preparing a user's manual, b)

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*The advent of diffraction limited optics will require the inclusion of physical optics, i.e., the Fresnel image formation.

†SHADOW already includes some of these features but must be further extended and improved in order to satisfy all the requirements.

distributing a newsletter by mail and c) through the use of computer networks.

6. Instrumentation for Figure Measurement of Grazing-Incidence Optics

The unconventional optics (aspheric, grazing incidence, etc.) that are normally used in soft x-ray beamlines require nonstandard measurement techniques and most optical fabricators cannot afford to develop the needed instrumentation. This is the basic reason why these items have sometimes been unsatisfactory in the past. We recommend an R&D effort (1) to develop a low-cost commercially available instrument for optical-figure measurement and (2) to apply this instrumentation to mirror fabrication. Until arc-second surface tolerances have been achieved and verified with reliable instrumentation this type of surface should not be used on a high brightness storage ring such as the new facility.

7. Develop a U.S. Source of Ion-Etched Diffraction Gratings for Synchrotron Radiation

Diffraction gratings that satisfy the optical and materials specifications required by VUV and soft x-ray beamlines are not currently available at reasonable prices and delivery times and not available in the U.S. at all. We recommend R&D support to develop local (U.S.-based) sources of ion-etched diffraction gratings that meet these requirements. The availability of such support would encourage companies to develop advanced methods of producing gratings on both conventional and novel substrates.

8. Diffractive Optics

An increasing number of experiments have a requirement for soft x-ray lenses (zone plates) and transmission diffraction gratings. It is expected that his number will increase in the future provided a reliable supply of these items can be established. At present the best U.S. diffractive optics are made by electron beam writing but although a very high level of expertise has been established the zone plates and gratings that are produced are available on a scientific collaboration basis only. We recommend that the zone plate availability problem be studied and R and D support given so as to sustain the present expertise and promote wider availability of zone plates and gratings in the future.

9. Detectors

The increase in source brightness provided by an advanced new machine will permit experiments with higher spatial, time and/or energy resolution. Full utilization of this new capability, however, will require improvements in detectors to match the performance of the source-plus-beamline. Obviously, experimentalists associated with specific experiments need to be deeply involved with setting the goals for this development but the host facility should also coordinate and participate in R and D aimed at producing the required devices. This should be a natural outgrowth of high energy physics detector programs and needs to be supported sufficiently early in order to bear fruit in time for the turn-on of the new machine.

10. Test Beamline

In view of the importance of verified high performance for the next generation of beamlines, we recommend that an optical component testing facility be estabilished on one of the operating storage rings and be available to the community nationally. Such a facility should have sufficient infrastructure in place that rapid turn around of test optics could be achieved.

COMPUTERS, SOFTWARE, AND BEAMLINE ORGANIZATION

The group's comments on general purpose computers and appropriate beamline organizational units are included in the "User Policy and Facility Parameters" section.

User Policy and Facility Parameters

A facility optimized for high spectral brightness insertion-device-based beamlines differs from present bend-magnet-based synchrotron radiation facilities in that there are a limited number of insertion devices, and the beamlines to handle the high photon fluxes tend to be more expensive. For example, with 12 straight sections for insertion devices and 2-3 high performance beamlines per insertion device, some 30 such beamlines could be developed. Some users believe that the individual institution participating research team (PRT) concept, in which research groups get a long term commitment for a significant portion of dedicated beamline use in exchange for providing the funds for the beamline, would be inappropriate for such beamlines. Basic research by small groups would suffer if only "wealthy" consortia could afford PRT beamlines. A more appropriate model for high-performance beamline allocation might be that used by NSLS for the insertion-device beamlines whereby multi-institutional affinity groups could build the beamline and work stations, and in return would receive some predetermined fraction of available beam time. It was agreed that a policy on beamline assignment would have to be carefully thought out for a new facility, and that a workshop on this topic would be appropriate soon after such a facility is authorized. Although bend magnet ports will be available for exploitation, users believed that adequate models for the allocation of such ports exist at operating synchrotron radiation facilities.

The Working Group on Materials, Interface, and Surface Science addressed the issue of proper allocation of high-performance beamlines in their report. They wrote that high-performance beamlines alone

> "...will not really address the problem of synchrotron radiation availability to a large community of users, unless users form teams and cooperate in both beamlines and individual experiments. This is an entirely new, and perhaps not very satisfactory, sociology for the materials science community. However, if truly new and exciting scientific results are to come out of a new ring, the combined expertise and resources of several different researchers will almost certainly be required in assembling the experimental apparatus.
>
> Perhaps the most important point to realize is that the amount of time made available to any one experiment may and probably should increase over that presently available at the existing rings. This will be necessary in order to encourage high potential but high risk experiments. Simply making more photons available will not qualitatively change the type of science performed at a new ring if many individual experiments are scheduled for short amounts of time each--the experiments that will be done will simply be those that are safe quantitative improvements of present work.
>
> In terms of the instrumentation of a new ring, the most ideal situation would be for the ring to be funded as an entire unit, i.e., including insertion devices, monochromators, and end

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This section was compiled by K. Berkner and R. Johnson.

> stations. However, rather than have the host institution build the beamlines, they should enter into cooperative arrangements with Insertion Device Teams in order to make certain that the needs of the most desirable experimental programs are met. The materials, interfaces, and surfaces research community by itself could make strong arguments for taking up seven or more beamlines at a new insertion-device ring. Since the total user community of such a new ring includes many other groups, each of which may have very different insertion device and monochromator requirements, the decision on how to instrument the beamlines may have to be done on a proposal basis."

The Beamlines Working Group also addressed the question of high-performance beamline allocation:

> "There is a spectrum of styles by which one can make synchrotron radiation available to users. At one end is the "participating research team" (PRT) approach, exemplified by the Brookhaven policy for bending magnet sources. At the other is the system whereby the facility staff operate all beamlines, which are time-shared by the users on a proposal basis. This approach is used for example on most SSRL beamlines. The PRT system is most natural for cases where there is a large number of nominally identical sources. The proposal system is most natural for cases where a few highly unique sources are available and their monopolization by a single institution would be inappropriate.
>
> For a machine that addresses itself primarily to insertion devices, one expects to be nearer the "proposal" end of the spectrum since it is expected that most of the insertion devices would be unique. A disadvantage of the proposal system is that it is hard for expertise and material resources to be drawn in from a wide community.
>
> In the light of these considerations we recommend that multi-institution groups of users be formed for each insertion device (similar to the Brookhaven "insertion device teams"). These groups would have the mission of providing technical input on the nature of the beamline(s) and contributing a negotiable fraction of the needed resources under the overall project management of the facility staff. Willingness to make a large financial contribution should not be the dominant consideration in selecting these teams. For bending magnets we recommend that the maximum number of beam ports be provided within the practical limits set by exploitation of the insertion devices as a first priority. We recommend that assignment to single institution PRTs be allowed as one of the modes of bending magnet beamline development."

The Beamlines Working Group also addressed general purpose computing. Their comments on this subject follow.

> "The host institution for the new facility should take responsibility for both beamline control and general purpose experimental computers. In particular this recommendation is meant to apply to both control and data acquisition software. In most experiments data acquisition and beamline control are inseparable, requiring a unified approach to both computer hardware and software. Wherever

> possible, labwide hardware and software should both possess the following characteristics: 1) High-level modularity (e.g., CAMAC hardware level, and Fortran-callable subroutine software level); 2) labwide uniformity; 3) transparent use, well documented; 4) In-house support for both maintenance and reconfiguration to changing needs. Therefore we recommend that the overall light source project computer group should include hardware and software professionals to implement these recommendations. To ensure that performance is planned and obtained which truly meets the community's needs, we further recommend the formation of a user's software advisory/oversight committee. This committee would be composed of knowledgeable outside users and would, in conjunction with the appropriate host institution personnel, be empowered to set software development priorities and critically monitor progress in attaining them."

The Materials Group had points to make about the design and operation of the new ring. They would like to see the following characteristics:

> "The machine physicists should attempt to design a machine in which the users are as well isolated from each other as possible. In particular, provision should be made for researchers to change the gap of an undulator with stored beam in the ring without disturbing other users. It will also be desirable to scan an undulator and a monochromator synchronously, for absorption-type measurements. The ring should definitely be designed for high brilliance, but it must also be flexible to enable it to meet the requirements of a diverse community of users. For instance, for experiments with high flux requirements, i.e., x-ray absorption, a running mode with high current and long lifetimes (i.e., 6 hours) is essential, but medium brilliance is acceptable. For experiments with high resolution requirements, the high brilliance mode is necessary. Refer to Table 9-1 for a listing of the requirements for the various techniques.
>
> Sufficient floor space in which to perform experiments is also a critical concern. Room should be available for large sample preparation chambers, such as molecular beam epitaxy, and for making measurements complementary to synchrotron radiation experiments. Facilities for sample handling and preparation prior to performing experiments must also be available. A clean laboratory with fume hoods and proper facilities for preparing and disposing acids and organic solvents is essential. Most materials will require some sort of chemical etching or cleaning before being installed in a vacuum chamber. The requirements for handling special materials should also be considered. In particular, the handling of the actinide elements, most of which are radioactive, is a matter of concern. Perhaps an entire beamline and a section of the building would have to be dedicated to experiments involving such materials.
>
> The availability of a first class facility for studying materials will also require that the materials to be studied be of the highest quality. This will require that those members of the

Table 9-1.

	hν (eV)	ΔE (meV)	Lifetime (hr)	Spot (mm)	Pulse (psec)	Flux	Comments	Optimize
Core level								
PES	→ 1000 eV	100	—	<.5	—	10^{11}		Brightness
Ultrahigh resolution								
PES	→ 150 eV	10	—	<.5	—	10^{12}	More flux → higher ΔE, Δτ	Brightness
SEXAFS	→ 2500	2000	≥ 6	1	—	$>10^{14}$	More flux → higher dilution	Lifetime, photons/fill
NEXAFS	→ 2500	100	≥ 6	1	—			
Time resolved								
PES(a)	→ 1000	100	—	<.5	—	$>10^{13}$	More flux → better Δt	Brightness
TRPES(na)	→ 100	50	—	<.5	20	$>10^{14}$	Pulse stability < 5 psec	
Spin-resolved								
PES	→ 150	50	—	<.5	—	10^{14}	Raw flux	Brightness
Photoelectron microscopy	→ 1000	500	≥ 6	<.1	1000	$>10^{14}$	Stable sources long lifetime to form an image	Lifetime, flux

> materials science community who prepare those materials are integrated into the experimental efforts at the new ring and are suitably rewarded for their efforts."

Members of the Working Group on Biology and Medicine want strong user support, especially the availability of modular beamline components that can be readily assembled for one-of-a-kind experiments. They reported as follows.

> "Biologists have special problems in using a synchrotron radiation source that should be addressed. They perform a variety of experiments to solve each specific problem, and a new set of experiments with each new problem. Thus it is not reasonable for each experimenter to have on hand all the necessary components for utilizing a beamline. Rather, components (monochromators, detectors, windows) should be available to the user to assemble for a particular experiment.
>
> Biological samples are often fragile and can not be made to order. Blocks of time on the ring should be available on call to accommodate experiments on fickle samples that have finally been successfully prepared."

The Working Group on Industrial Research and Technology raised the following user issues in their report.

> "A synchrotron facility for industrial research needs to satisfy several organizational and technical requirements. The facility has to allow for proprietary research. This was not viewed as a problem by the working group. The procedure established at the NSLS could be readily adapted. More importantly, the facility has to allow repetitive access. It is recognized that industrial development work can only be successful if it is possible to complete the necessary iteration steps without excessive delays. The beam time allocation procedure has to account for this need. In order to be successful, the synchrotron facility has to provide technical support in key areas. The existence alone of a beamline would not guarantee its efficient use. Sample preparation and inspection capabilities need to be available and supported by the facility. X-ray lithography in particular requires the construction of a cleanroom of class 10 or better around the exposure station including a full resist processing line and optical and SEM inspection tools operated and maintained by facility personnel. The working group feels that the local academic community should recognize the excellent opportunity to collaborate with industrial research groups in areas of need of technological advancement. It is therefore recommended that a local mask fabrication process be established to provide at least the pattern definition and transfer onto prefabricated mask substrates. This effort would enable the local community to develop expertise in this key area of advanced lithography. At the same time it would provide a modest supply of masks needed to support the work at the lithography beamline."

Other user-related items that must be considered in laying out a new facility are:

- Storage space for users.
- Office space and parking for users.
- Inexpensive housing, especially for graduate students.
- User access to host laboratory infrastructure - shops, engineers, technician support.

Some of the users felt that three-shift/day operation would be counterproductive, especially for small groups who do not have the personnel to staff around-the-clock support.

The forefront experiments discussed during the workshop would require the highest possible brightness over a broad spectral range. For some experiments, broad undulator tunability at ~ 1 keV would be ideal. For other experiments, high intesity down to ~ 4 eV is needed.

Facility parameters that would best meet the sometimes conflicting needs identified by the various scientific working groups were consolidated on the last afternoon of the workshop at a joint meeting of the organizing committee and the chairmen of the working groups. Consensus was reached on machine parameters that appear to satisfy this range of needs: nominally 1.5-GeV electron-beam energy with a current of 400 mA, 12 straight sections in the ring, pulses as short as 20 to 50 psec, with minimum jitter, and a horizontal emittance below 10^{-8} π m-rad. Undulator tuning should be possible during operation; position and angular stability of the beam should be a small fraction of nominal values of these quantities; beam lifetime should exceed 6 hours; and considerable floor space should be made available for experimental apparatus. The ring design should be flexible enough to permit routine operation at higher energies (up to ~ 1.9 GeV) for materials, biomedical, and other applications and at lower energies ($\leq$ 1 GeV) so as not to preclude the future development of a free electron laser operating mode.

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