6.1 Summary of Major Plans for the Future

A summary of XFD future plans is provided below, which includes both short-term initiatives and long-term strategic initiatives:

- Funds have been requested from the DOE to improve the performance of various components of major systems, such as insertion devices, front ends, PSS, EPS, etc., that are under XFD responsibility. Short-term needs will be supported to maintain the reliability of operations in order to deliver maximum beam time to the users. These tasks will receive the highest priority in XFD operations workload. The improvements will be performed using funds made available under the Accelerator Improvement Program.

- During FY 1998, the APS has set aside funds to design and build a liquid nitrogen distribution system on the experiment hall floor. The system will deliver liquid nitrogen to all the first optics enclosures on CAT beamlines to cool the optics. The system will be built during FY 1999.

- Effort and resources will be made available during FY 1999 to support the "top-up" mode at the APS. Implementation requires not only a close evaluation of the impact of the mode on user experiments but also provision for developing required systems to mitigate any difficulties encountered by the users in performing their experiments.

- SRI-CAT will be developing sector 4 for the use of polarized x-rays. The effort to deliver two independent x-ray beams from two undulators located on the same straight section to two independent beamlines poses new technical challenges. These will be addressed during FY 1999. The two radiation sources (undulator A and the CPU in a "dog-leg" configuration on straight-section 4 of the storage-ring), beamline front end, and the beamlines are planned for commissioning in early FY 2000. In the future, this type of dog-leg configuration can add an extra beamline in any sector of the APS by the installation of two undulator sources canted in the horizontal plane on the same straight section.

- The beamline, front end, and undulator for COM-CAT are funded by the State of Illinois. XFD staff are involved in completing the construction of this beamline during FY 1999.

- The APS Phase-2, which was described in the last XFD *Progress Report* 1996-97, has been submitted to the DOE. This Phase-2 initiative, in which the remaining sectors of the APS will be fully developed, is consistent with the recommendations of the BESAC Panel on DOE Synchrotron Sources and Science, November 1997 (chaired by R. J. Birgeneau and Z.-X. Shen). According to the plans included in the *DOE Basic Energy Sciences (BES) Facilities Roadmap* (July 1998, Fig. 6.1), this new initiative begins in FY 2000 and extends

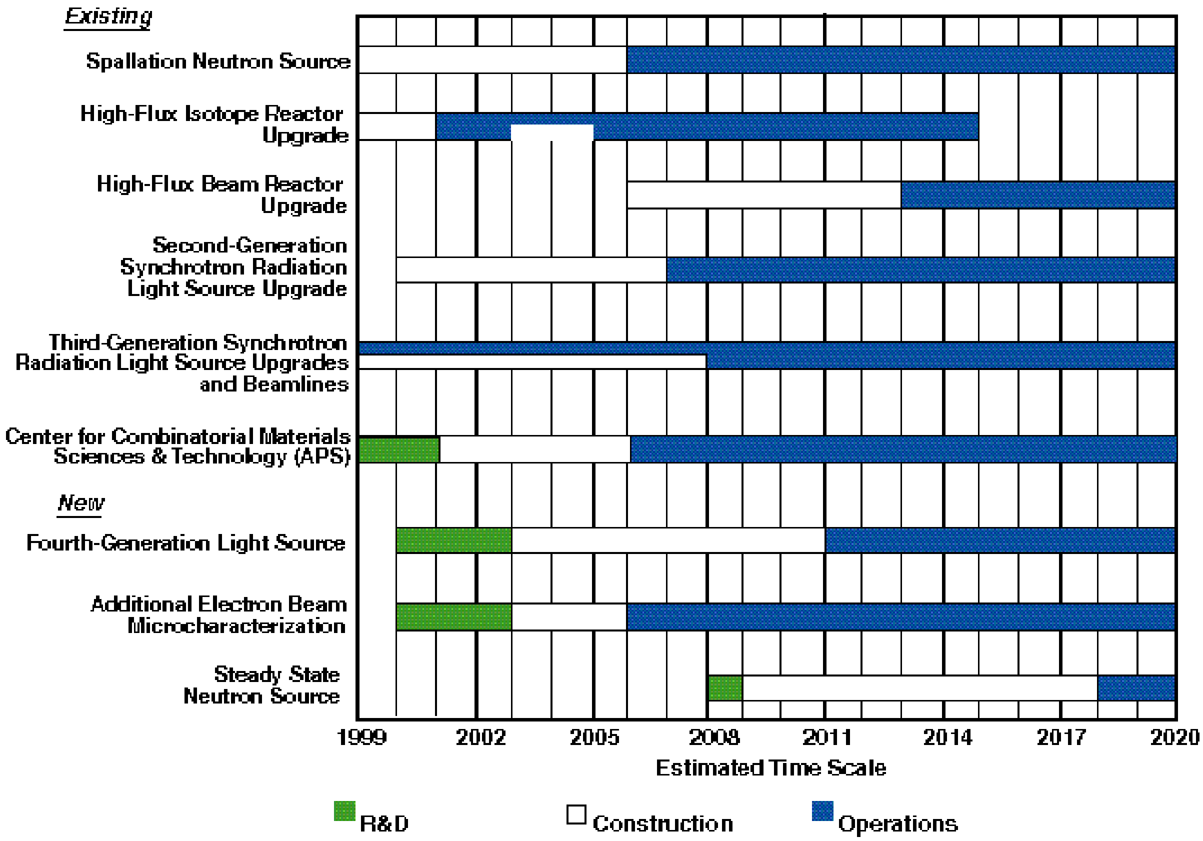

Fig. 6.1 DOE BES Facilities Roadmap

through FY 2008. A more detailed description of the proposal is provided in section 6.2.

- The fourth-generation light source concept has been a major area of R&D both in ASD and XFD in support of a laboratory initiative. Much effort has gone into the plan for an APS linac-based FEL in order to demonstrate the self-amplified spontaneous emission (SASE) concept in the UV wavelength range. XFD has the major responsibility to develop the undulators and associated particle and photon diagnostics required for the success of the project. Considerable progress in this initiative has been made. Major effort during the past years has gone into the development of a simulation code for the FEL, as well as defining the lattice and tolerances of various components, layout of the FEL undulator line, characteristics of the undulators required for FEL contrasting them with the needs of the APS, and the proposed optical diagnostics to monitor the performance of the FEL. These tasks (supported by LDRD funds) are described in detail in section 6.3. The current plans call for a demonstration of the SASE concept in the visible wavelength range during the summer of 1999 and in the UV range during the fall of 1999. The *DOE BES*

Facilities Roadmap (Fig. 6.1) includes a fourth-generation user facility with R&D funds for the facility starting in FY 2000.

- A major new initiative has been planned to develop a Center for Combinatorial Materials Science and Technology that will use beamlines in a sector at the APS. This proposal will involve staff from both XFD and the Materials Science Division (MSD) at ANL. The initial plan for this center (see section 6.4) was submitted to the DOE and has been well received; DOE has included this in the *DOE BES Facilities Roadmap* (Fig. 6.1). The center is expected to develop massively parallel techniques for complex materials synthesis using combinatorial methods and massively parallel physical characterization of the materials using microsensors developed using both deep-etch x-ray lithographic techniques and x-ray microprobes.

- Another major new laboratory initiative that addresses structural genomics is called the "Illuminator Project" and involves staff from XFD and the Center for Mechanistic Biology and Biotechnology (CMB) at Argonne. In understanding the "blue-print" of life, the knowledge of DNA sequence coding for thousands of proteins is a prerequisite. While the genome project has made considerable progress towards this goal, the information is insufficient for full understanding of human and other living systems. The knowledge of 3–D protein structures and their folding patterns is an essential next step to make greater strides in this field. In this quest, there are two major bottlenecks in which XFD staff plan to contribute: (a) production of thousands of purified crystals for structural analysis, and (b) measurement of these structures using an APS beamline. Neither can be performed in a time efficient way with existing capabilities. Both these bottlenecks can be overcome through the development of robotics capabilities for crystal growth and operation of "smart" beamlines. In anticipation of funding support for the Illuminator Project, the Laboratory is providing LDRD funds starting in FY 1999 to CMB and XFD to jointly pursue these tasks (see section 6.5). The benefit of this R&D is expected to influence all disciplines represented by the APS user community in performing research in a more efficient fashion.

Strategic planning has been performed by XFD to develop new initiatives included in the above list to meet future APS goals. This planning has resulted in four major new initiatives: 1) a Phase-2 plan to develop the remaining beamlines at the APS, 2) a SASE FEL, 3) a proposed Center for Combinatorial Material Science and Technology, and 4) the Illuminator Project. The DOE BES Roadmap, shown in Fig. 6.1, includes three of the above initiatives. In the following sections, brief technical descriptions of these four initiatives are provided.

6.2 Phase-2 Initiative

6.2.1 Background

In the completed phase (Phase-1) of the APS Project, 40 of the 68 possible x-ray sources have been readied for use. Within the scope of Phase-1 construction, IDs and beamline FEs were built and installed by XFD so that the users could build 40 beamlines on the experiment hall floor to perform research. The 40 x-ray sources to be completed in Phase-1 have already been committed to their full use through this century by the scientific and technological users. Two more sectors have recently been awarded (SRI-CAT sector 4 and COM-CAT sector 32), which leaves 12 more sectors available for the development of Phase-2 beamlines. Demand for beamlines spanning a wide variety of scientific disciplines continues to increase. Many of the new users are also proposing technique-specific beamlines to be developed at the APS to support national communities of users. The concept of technique-specific beamlines is also endorsed by the Birgeneau-Shen committee in their report. These new beamline facilities will be targeted for the most important science/technology goals of the U.S. research community and will be available on a peer-review or proprietary basis to all researchers from universities, federal laboratories, and industry.

In this APS Phase-2 Initiative, 2.5-m-long and 5-m-long ID x-ray sources will be built on 12 straight sections of the APS storage ring, and an additional 12 BM sources will also be put in use. The beamline FEs for these 24 x-ray sources will be built to contain and safeguard access to these bright x-ray beams. In addition, funds will be provided to build an additional six state-of-the-art technique-specific beamlines to meet scientific and technological research demands well into the next century. These include, for example, the demands of the biotechnology, medical imaging, environmental science, microprobe, and high-energy x-ray scattering communities.

The APS Phase-2 Initiative also proposes to build two laboratory-office modules for the users. These modules are similar to the six included in the Phase-1 construction project. In addition, a specialized laboratory will be added to meet specific scientific goals of the users performing research in the areas of combinatorial materials research (see section 6.4) and biotechnology (see section 6.5).

6.2.2 Beamline Plan in the APS Phase-2 Initiative

In the APS Phase-2 Initiative, the plan is to prepare an additional 12 sectors (or 24 beamlines) of the APS. There will be 12 straight sections of the APS storage ring that can accommodate IDs. It is proposed that the IDs in six of these straight sections will be undulators similar to those built in the current phase. Such sectors are referred to as Type A sectors. On the remaining six straight sections of the storage ring, IDs to meet the specific needs of unique scientific and technological research communities will be built. These technique-specific sectors are referred to as Type B sectors and will also include the beamlines to be constructed by the APS staff. Details of the current user status are given in Table 6.1.

In this new initiative, the six Type A sectors will be completed to meet the demand of the

Table 6.1 Status of Collaborative Access Teams (CATs) and Scope of Phase-1 and Phase-2 (October 1998)

APS Sectors[a] Operational in Phase-1	20
New APS Sectors Assigned (SRI-CAT and COM-CAT)	2
Sectors Requested by the New Proposals for Phase-2	4
Sectors Approved for Phase-2 by the PEB (October 98)	2
Sectors Waiting for PEB Approval	2
Type A Sectors to be Instrumented behind the Shield Wall in Phase-2	6
Type B Sectors and Beamlines to be Instrumented in Phase-2	6
Technique-Specific Beamlines on Type-B Sectors in Phase-2[b]	6
Laboratory/Office Modules Built in Phase-1	6
Laboratory/Office Modules in Phase-2	2

a) A sector at the APS provides two beamlines: one for the ID source and the other for the BM source.

b) Includes two sectors for strategic initiatives described in sections 6.4 and 6.5.

CATs approved by the PEB. Simultaneously, attention will be given to the special purpose beamlines that will occupy the six Type-B sectors. The technical subjects for beamlines in these sectors will not be decided at this time. However, ten possible subjects for such beamlines have been identified. As the new initiative matures, a decision will be made on the special purpose beamlines using the best expertise from the scientific and technological user community of the APS and the PEB, as recommended by the Birgeneau-Shen Committee. The list of these beamlines includes the following: structural genomics, medical imaging, very high energy x-ray scattering, sub-nanosecond temporal resolution studies, coherence and interference techniques, three-dimensional imaging, microcomponent fabrication, archaeology and archaeometallurgy, radiation therapy, x-ray microprobes (microfluorescence, microimaging and microdiffraction), and combinatorial materials science. Many of the LDRD programs in FY 1998 (see section 1.10) support this initiative.

6.3 FEL Project

The recent success of third-generation synchrotron radiation sources around the world laid the groundwork for exploring new levels of brightness for VUV and x-ray sources. In the past few years, there have been a number of scientific and technical workshops on the next generation of synchrotron radiation sources. One important outcome of these meetings is the technically well-supported conclusion that a linac-based self-amplified spontaneous-emission free-electron laser (SASE FEL) could represent a future fourth-generation synchrotron radiation source.

Several laboratories around the world, including the APS, recently started construction of SASE FELs for the VUV/x-ray wavelength range. The APS SASE FEL would consist of two major parts: the 600-MeV linac equipped with a small-emittance electron gun, and a set of twelve undulators that would generate and finally lase VUV radiation. Initially, operations will be at a lower energy in order to produce light at a visible wavelength. This relaxes requirements for the electron beam, undulator, and diagnostics. After experience is gained at 510 nm, the linac energy will be increased to achieve SASE operation at 120 nm. This entire project is supported by LDRD funds.

XFD is responsible for the design, construction and commissioning of the undulator line of the APS SASE FEL, while ASD is responsible for delivering the electron beam. For the XFD staff, the SASE FEL project is a very natural continuation of the ID development process that has been quite extensive during the entire APS project. As of summer 1998, there are 22 IDs installed in the APS storage ring, as described in section 5.1 of this report. The uniquely equipped ID Magnetic Measurement Facility and innovative methods of magnetic tuning provide a solid base of support for the state-of-the-art performance of APS IDs. Also, x-ray diagnostic techniques developed and implemented at the APS permit independent verification and confirmation of ID performance. All this expertise is essential in beginning development of a new generation of synchrotron radiation sources.

The main difference between the development of IDs for the APS storage ring and for the FEL is the integration process. While IDs for the APS storage ring must be integrated into the existing magnetic lattice of the machine, the FEL IDs themselves *are* the lattice, and therefore the choice of lattice, in most cases, lies in the hands of the ID developers. With this choice comes the responsibility for justifying the lattice and the ID specifications. In order to accomplish this task, new codes for the simulation of SASE FEL performance have been written and extensively tested, and the results were found to agree with results from previous SASE FEL codes.

Once the new codes were validated, their efficiency and flexibility were used to determine that the magnetic lattice for the APS SASE FEL could be based on a separated functions approach, i.e., the undulators and quadrupole lenses do not need to be combined in the same magnetic element. The calculated FEL output power is not affected significantly by the choice of combined or separated focusing functions in the magnetic lattice. This crucial result brings extremely critical simplifications to the FEL undulator design, in that the well-developed and well-proven approach used in the design and construction of the APS IDs can be applied to the SASE FEL. In addition, conventional beam diagnostics can be placed along with the quadrupoles in the breaks between separated IDs.

6.3.1 FEL Computer Code

A computer code was developed to investigate important design considerations for the APS FEL. For example, the possibility of the horizontal focusing being separate from the undulator was studied, and, more recently, mechanical tolerances have been determined. The code numerically integrates the equation derived by Vinokurov (1996) to determine the electron distribution function in a high-gain FEL. The ability to handle longitudinally inhomogeneous magnetic systems, such as separated undulator segments with quadrupole focusing lenses inserted in the breaks between undulators, was specifically built into the code. For the case of a continuous undulator, verifications against semianalytical expressions and other codes, such as GINGER and TDA3D, have been performed, with very good agreement in all cases.

The results of calculations that looked at the difference between a continuous undulator and separated undulator segments with horizontally focusing quadrupoles between the segments are shown in Fig. 6.2. The power output of the FEL is proportional to the modulus, squared, of the electron bunch peak current density. This quantity is expected to grow exponentially for a perfect continuous undulator, with horizontal focusing provided by shaping of the pole tips. The dotted line in the top panel of Fig. 6.2 is indeed a straight line, as expected for a log plot. The solid line shows the result of the simulation for the planned APS FEL design. The amplification is reduced due to the breaks between undulators, but the reduction of $\ln(|J|^2)$ is the ratio of the break length to the cell (i.e., undulator plus break) length. Thus, the electron bunch peak current density is not adversely affected by a lattice with separate function elements. No extra undulator magnetic structure length is needed to compensate for loss of gain in the breaks. The lower panel of Fig. 6.2 shows the scaling factor F, which is inversely proportional to the power gain length. The integral of F is also proportional to $\ln(|J|^2)$.

The calculations were performed at a beam energy of 220 MeV for a beam emittance of 2.50×10^{-8} m-rad (for both the horizontal and vertical directions), and a beam energy spread (s.d.) of 0.15%. The undulator period length was 3.30 cm, and the total length of one undulator segment was 2.3265 m (70.5 periods). The break length was fixed at 36.5 cm with a single horizontally focusing quadrupole (off-centered longitudinally by 8.0 cm, and focal length 1.00 m) in each break. The undulator K values were 3.10. These parameters give a fundamental harmonic in the visible light range (5168 Å). (This differs slightly from the plan for the APS FEL, which is to adjust the beam energy slightly away from 220 MeV in order to have a fundamental harmonic of 5100 Å.) The undulators were perfectly aligned, the incident beam was centered, and matched beam parameters at the entrance were used.

We have also examined beam and mechanical tolerances and were able to determine the full set of necessary specifications. The misalignments of one undulator with respect to adjacent undulators were simulated, and the sensitivity to unmatched beam parameters (the Twiss parameters α and β) at the entrance and to a noncentered incident beam (x_o, x_o', y_o, y_o') were checked (for a full report see Dejus and Vasserman, 1998). The calculated tolerances given in Table 6.2 are based on requiring that the power output not change more than approximately 10% for a given parameter.

Table 6.2 Acceptable tolerances

Parameter	with centered quadrupoles, f=2.39 m	with quads 8.0 cm off-center, f=1.00 m [a]
Longitudinal undulator displacement	1.0 mm	1.0 mm
Vertical undulator displacement [b]	50 μm	<50 μm preferred
Horizontal alpha function, α_x	0.20	0.20
Vertical alpha function, α_y	0.20	0.20
Horizontal beta function, β_x	0.50 m	0.40 m
Vertical beta function, β_y	0.20 m	0.15 m
Horizontal incident beam coordinate, x_o	200 μm	100 μm
Vertical incident beam coordinate, y_o	50 μm	< 50 μm preferred
Horizontal incident beam angle, x_o'	100 μrad	50 μrad
Vertical incident beam angle, y_o'	50 μrad	< 50 μrad preferred

a) These additional simulations were done after Dejus and Vasserman (1998), for other conditions being considered for the APS FEL.

b) Horizontal displacement much more relaxed: use 1.0 mm.

6.3.2 The FEL line

The simulations confirmed that a separated-undulator approach was reasonable. This approach gives greater flexibility in the diagnostics and allows us to build on our existing undulator expertise. The FEL line will consist of a series of identical cells, where each cell includes an undulator, a diagnostics section, and a quadrupole singlet. The quadrupole and diagnostics section will be located in the gap between consecutive undulators. A total of 12 cells is planned.

The length of the gap between successive undulators must be carefully chosen so as to maintain the proper phasing between undulators. The length of the section also depends on the strength of the undulator magnetic field. The undulators will be adjusted to a K of 3.1, corresponding to an effective magnetic field of 10.061 kG. The length of the break between undulators will be 36.5 cm from the last full-field pole (the next-to-last pole) of one undulator to the first full-field pole (the second pole) of the next undulator. This break can accommodate the quadrupole and the optical diagnostics. When the length of the full-field region of the undulator is included, the cell length becomes 269.15 cm.

The undulator magnetic field itself provides vertical focusing of the particle beam. Horizontal focusing is provided in the space between undulators by the quadrupole magnet. The FEL simulation codes were used to evaluate a variety of different lattices. Configurations with a single quadrupole, a doublet, or a triplet placed in the break between undulators were considered. The singlet was found to give the best particle beam bunching. The codes were also used to optimize the strength of the quadrupole so as to maintain the best bunching within the particle beam. Once the strength of the quadrupole was chosen, the

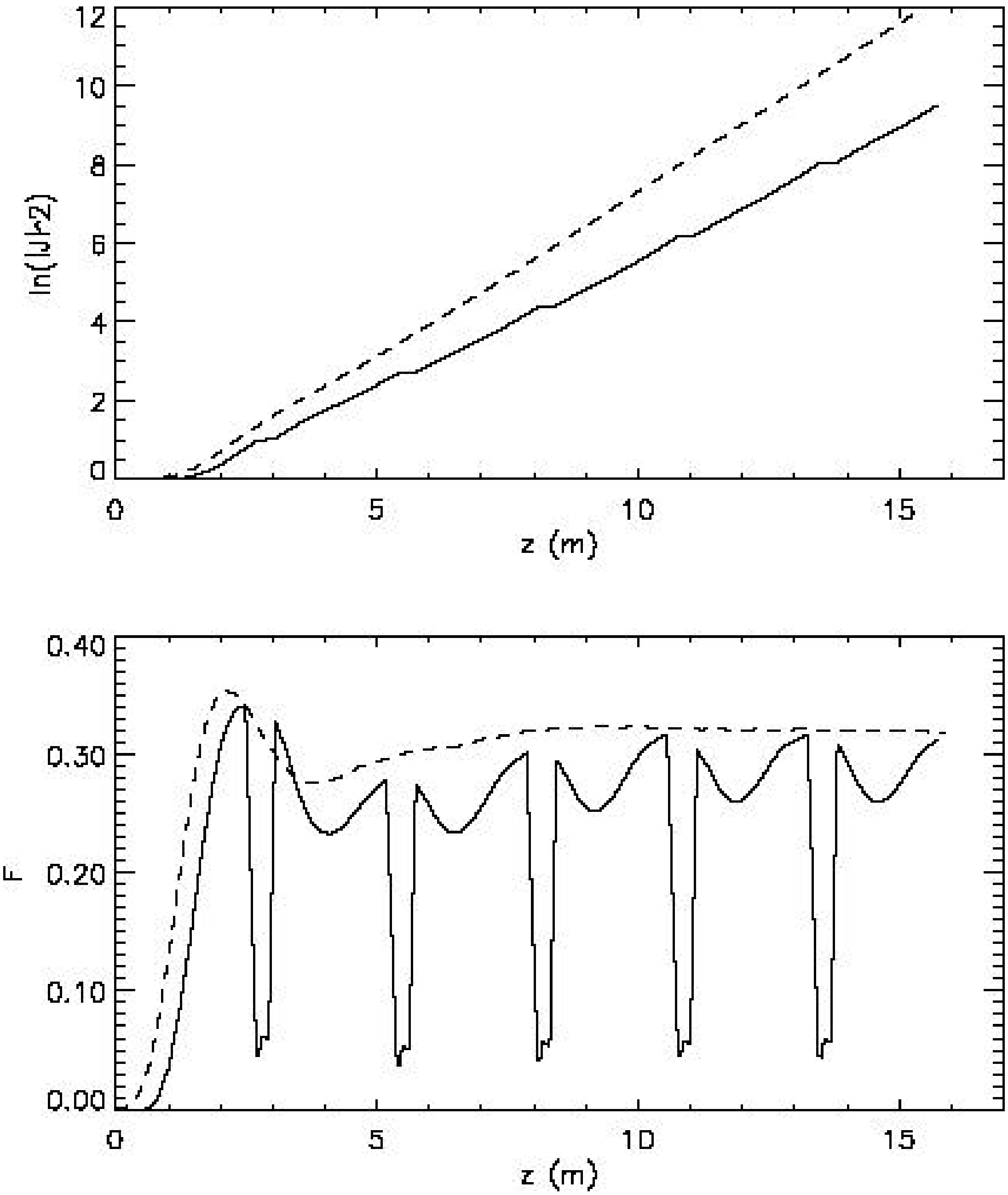

Fig. 6.2 (top) Natural logarithm of the modulus squared of the electron bunch peak current density for a continuous undulator (dashed) and the APS FEL design with break sections (solid). (bottom) The dimensionless scaling factor F for the continuous undulator (dashed) and the APS FEL (solid).

beta function for an undulator cell could be calculated. The result is shown in Fig. 6.3.

The first quadrupole magnet has been assembled and characterized. In addition to providing the quadrupole field to focus the particle beam horizontally, this magnet has windings to allow it to serve as a dipole correction magnet, steering the beam vertically and horizontally. Much attention has been paid to precision in the fabrication of the magnet components, in order to keep the geometric and magnetic axes of the magnet coincident. The aperture of the magnet will be 12 mm.

6.3.3 Characteristics of the FEL Undulator

The period length of the undulators for the FEL is 33 mm. Simulations were carried out of the expected gain using period lengths as short as 27 mm, but the results show very little sensitivity to changes in the period. Therefore, the decision was made to proceed with the 33-mm-period undulator that is

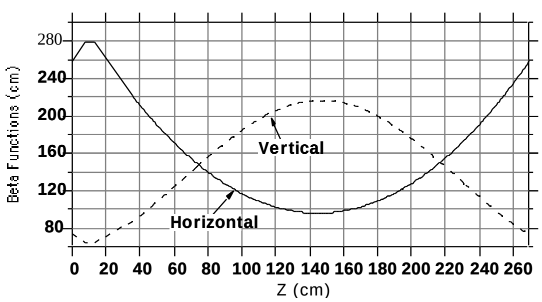

Fig. 6.3 The beta function for a cell of the FEL lattice. The cell consists of: a 7.785-cm break, followed by a 5-cm quadrupole, then a 22.665-cm break for optical diagnostics, and finally a 233.7-cm undulator (not including the end poles).

already well-understood at APS, and the design for the FEL magnetic structure will be identical to that of the standard APS undulator A. A photo of one of these magnetic structures, mounted as it will be in the FEL tunnel, is shown in Fig. 6.4. The undulator A and FEL magnetic structures are mechanically identical, and the magnetic structures for the FEL will be built by STI Optronics.

Some of the magnetic tuning requirements for FEL undulators are more demanding than those for a storage ring undulator. For an FEL, it is critically important that the particle beam path coincide with the axis of the emitted radiation and that the coincidence extend not just over the length of one undulator but through the entire series of undulators. This means that the trajectory of the particle beam must stay straight through the undulator end regions as well as through the full-field regions. This requirement translates into the requirement that the second field integral (averaged over each period) remain less than 3300 G-cm^2 through the entire length of the undulators, including the end sections. For a beam energy of 220 MeV, this would correspond to a trajectory displacement of 45 µm. (The corresponding requirement for a storage ring undulator is that the second field integral through the full-field region be below 10^5 G-cm^2 for all gaps, with no special requirement for the ends.)

Another requirement for the FEL undulators is that the effective magnetic field strengths for each undulator must be nearly identical so that the light produced by one undulator is at the resonant wavelength for the next. Simulations are being carried out with different field strengths assigned to different undulators. An initial guess is to require that the wavelengths from different undulators

Fig. 6.4 One of the undulators, mounted as it will be in the FEL tunnel.

must be the same to within 5% of the width of the first harmonic peak from one gain length's worth of undulator. This results in the requirement that the undulator parameters K be the same to within 1.5 parts in 1000, which translates into the requirement that the effective magnetic fields of the undulators be the same to within 15 G. This error in the magnetic field would result if the gap of the undulator were mis-set by 16 µm. In order to achieve the magnetic field values needed for a K of 3.1, the undulator gap will be near 9.3 mm, but the gap of each undulator will be adjusted individually to ensure field strength uniformity between undulators.

Other FEL requirements are less demanding than the corresponding requirements for storage ring undulators. Because the FEL undulators will operate at a single fixed gap, magnetic tuning only needs to be done at that one gap. Also, a small phase error is important for a storage ring undulator to ensure high brightness in higher order harmonics, whereas FEL operation only relies on the first harmonic radiation being bright. Since the brightness of the first harmonic is much less affected by phase errors than the brightness of higher harmonics, the rms phase error requirement is less demanding for an FEL undulator. The criterion used for the FEL is that the first harmonic intensity should not decrease by more than 5% due to phase errors. This leads to the requirement that the rms phase error be less than 10°.

6.3.4 The Optical Diagnostics

The diagnostics serve two purposes: 1) to monitor and maintain the alignment between the particle beam and the undulator radiation, and 2) to evaluate the characteristics of the light that is produced by the FEL.

A schematic of the diagnostics section that will be located between the undulators is shown in Fig. 6.5. Since it is critical that the particle beam and the axis of the emitted light beam coincide through the entire series of undulators, three different and complementary monitors of the particle beam position have been included. The capacitive button BPM, or beam position monitor, is the same as the BPMs used at the ends of the insertion device straight sections in the APS storage ring. The relative positions of the buttons are different than in the storage ring; however, because the FEL vacuum chamber has a smaller vertical aperture than the usual storage ring ID vacuum chamber, the buttons will be vertically closer. They will also be closer transversely in order to improve their sensitivity. The wire BPM is an absolute position monitor that consists of two perpendicular sets of four parallel wires. The wires are spaced 0.5 mm apart and have a diameter of 15 µm. The current to individual wires is monitored as the particle beam is steered to strike the wires. The beam can be centered vertically and horizontally by determining where it hits the wires on opposite sides of the beam center line and splitting the difference. During normal operation the beam will not strike the wires because the spacing between wires will be a few times the beam size. The third beam position monitor is the YAG scintillator crystal. The optics that will be used to image the YAG crystal will give a 1:1-sized image of the YAG crystal on a CCD camera, so that the 6.5 × 6.25 µm pixel size will be the resolution at the crystal. Therefore, the optical resolution will be comparable to the 10 µm resolution reported for the YAG crystal itself (Safranek and Stefan, 1996).

Upstream of the undulators, there will be a chicane for the particle beam. The synchrotron radiation produced at its bends will be monitored as a means of characterizing the particle beam, and it will also provide a place for an alignment laser to be inserted. The alignment laser will be directed down the inside of the vacuum chamber and will be used to define the desired straight-line beam path. Since the alignment laser light will travel through the same optical systems as the FEL light and the light from the YAG crystal, the desired position of the light on the CCD arrays can be defined.

In order to relate the overlap between the particle and emitted light beams inside the undulators to where it is measured between the undulators, it is convenient to require that the particle beam stay in a straight line, with no displacements or deflections, through the ends of the undulators. (The particle beam needs to be straight through the length of the full-field region of the undulators in any case.) Because no position monitors will be located inside the undulators themselves, careful magnetic characterization and tuning of the undulators will ensure the straightness of the trajectory through the ends as well as through the full-

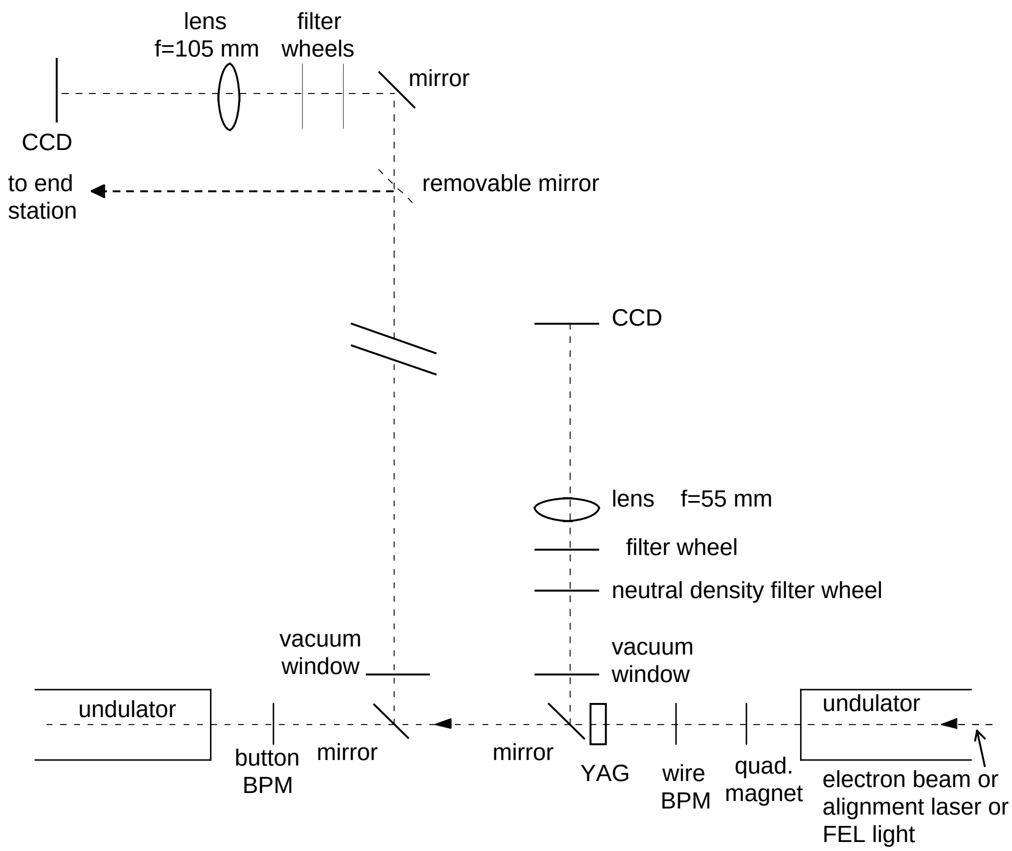

Fig. 6.5 Schematic of the diagnostics section (not to scale)

field regions. The allowed limits for displacement and deflection are a fraction of the size of the particle beam and of the opening angle of the radiation, respectively.

It should be possible to be able to confirm that the trajectory inside the undulator is as expected, despite the absence of position monitors there. The optical systems will provide this ability. The lens and CCD in the upper left of Fig. 6.5 will be used to check the angular deflection inside the undulators. The CCD will be placed at the focal distance from the lens, so that all the light that is incident parallel to a particular angle will be imaged to the same point on the CCD. In this configuration, all position information about the incoming light is lost and the image on the CCD will reflect the distribution in angle of the incoming light. If there is an angular deflection between undulators or a trajectory kick within an undulator, the CCD image will show an apparent displacement.

There are two filter wheels in the upper left of Fig. 6.5. One of them will carry bandpass filters. The other filter wheel will carry a variety of neutral-density filters so that the light levels can be adjusted to suit the CCD.

Another way in which the lens and CCD in the upper left of Fig. 6.5 will be used is with an adjustable distance between the lens and CCD. The CCD will not always be at the focal distance from the lens. Instead, the focus of the optical system will be adjustable so it can fall at different distances along the undulator (or undulators). When the optics are used in this way, the positions of the emitted light at different positions along the undulator will be monitored.

For the purposes described thus far, the bandpass filter used will be one that passes the on-axis FEL light. A different bandpass filter, one that passes light that is slightly red-shifted from the on-axis light, can be used instead. The red-shifted, off-axis light that will be passed by this filter will be in the shape of a cone around the axis, and the angle between the cone and the axis will depend on the wavelength passed by the filter. Although the resolution of the optical system is no different when viewing red-shifted vs. on-axis light, using the red-shifted light to guide adjustments of the relative trajectories through two consecutive undulators may allow more accurate adjustments. The red-shifted light appears as a ring, and two rings may be easier to align than two spots. Also, the width of the annulus of red-shifted light is smaller than the size of the on-axis spot, so the difference is between aligning two sharp rings as opposed to two broader spots.

As shown in Fig. 6.5, a mirror is inserted into the particle (and light) beam path in order to reflect the FEL or alignment laser light into the optics at the upper left of the figure. This mirror will have three positions: one where the mirror is removed from the beam path, one where the mirror completely blocks the beam and reflects all the light, and one with a hole in the center so that there is nothing directly in the path of the particle beam but any light at more than 0.2 mm from the axis will be reflected into the optical system. Demanding requirements have been placed on the motion of this mirror so that the position of the light on the CCD is repeatable to within a pixel despite the approximately 1-m-long distance between this mirror and the next mirror in the light path. In order to more readily achieve this repeatability, the direction of motion of the mirror between its different positions is parallel to the plane of the mirror face.

Another use for the optics in the upper left of Fig. 6.5 is as a diagnostic for the light produced by the FEL. Each set of these optics will be calibrated for absolute intensity. They will then be used to measure the intensity from each undulator individually, as follows. The mirror in the particle beam path after the first undulator will be positioned so that the 400-μm hole allows the particle beam to pass unobstructed. A small fraction of the undulator light will also pass through the hole, but most of it will be reflected into the optics where the absolute intensity of the light from the first undulator will be measured. The small amount of light that passes through the hole is important because it is the light that will interact with the particle beam in the second undulator to induce the bunching needed for lasing. When the light is viewed after the second undulator, the contribution from the first undulator will be a small portion of the total intensity; almost all the intensity will be from the second undulator. If no lasing is occurring in the second undulator, then the absolute intensity seen in the optics after that undulator will be the same as the intensity after the first undulator. This comparison of intensities will be made along the entire line of undulators.

A second diagnostic of the FEL light will be located in an end station, downstream of the line of undulators. A Paschen-Runge-type spectrograph will be placed on the low-radiation side of a shielding wall at the downstream end of the undulator line. A schematic of the spectrograph is shown in Fig. 6.6. It will be used for high-resolution spectral measurements near the first harmonic, and, since the goal is to measure the spectral structure in the SASE light, each pulse from the linac will be individually measurable. Light sent to this station will have been picked off after any one of the undulators (including after the last undulator), using the removable mirror shown in the upper left of Fig. 6.5. It will pass through a hole in the shielding wall and be sent to the spectrograph. The slit size will be changeable; for a 20-μm slit width the spectral resolving power will be $\lambda/\Delta\lambda$ = 13900. After cooling the CCD to reduce the dark current and noise level, the light per incident electron bunch and per pixel from a single undulator with no FEL amplification is expected to be at least 20x higher than the background per pixel. The charge collected in all the pixels in a column will be added together to make the signal-to-noise ratio even more favorable.

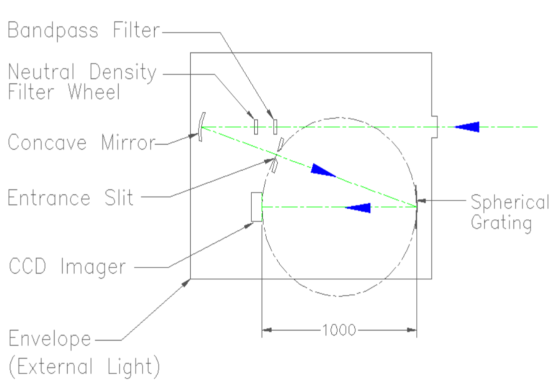

Fig. 6.6 A top view of the Paschen-Runge-type spectrometer that will analyze the light from the SASE FEL.

6.4 Center for Combinatorial Materials Science and Technology

In 1997, the National Research Council completed a study on the subject "The Physics of Materials: How Science Improves Our Lives." The complete study will be published later in 1998. It emphasizes the fact that many of the discoveries in materials science during the present century have had a major impact on the technologies of modern times, on our powerful economy and, as a result, on human well-being. Examples include the discovery of transistors, which led to modern silicon technologies, the discovery of fiber optics has led to the communication revolution, the discovery of compound semiconductors has miniaturized communication hardware, the discovery of superconductivity has led to numerous scientific instruments including the MRI, the discovery of liquid crystals has provided the bread-and-butter to the photoconductive display industries, and so on. The materials involved in all these applications are simple and are truly materials of the past. Recently, materials scientist have focused their attention to "complex materials"—materials containing many elements that show complex ternary, quaternary, or higher order phases. They also demonstrate a complex mix of new and rich properties. They exhibit new physics involving strong coupling between electron-, phonon-, and spin-orderings.

Their synthesis, discovery, and characterization however cannot be carried out in the traditional methods used in this century involving a trial-and-error approach, which is both inefficient and time consuming when systems are complex.

Hence one requires a new approach based on systematic and massively parallel synthesis and characterization. The development of new tools to search for complex materials will lead to a revolution in materials science and technology in the next century.

A combinatorial approach to materials synthesis is a new field (Xiang et al., 1995). The method lends itself as an efficient, systematic, and massively parallel process to synthesize an as-yet-unexplored universe of complex materials made up of ternary, quaternary, and higher order materials libraries. An example of producing combinatorial materials is shown in Fig. 6.7. While the technology of producing combinatorial libraries of 100 to 10,000 differing materials is becoming feasible, the limitation in the discovery process for materials with new and unique properties is the ability to measure the physical properties of such libraries quickly and efficiently in a massively parallel process. Thus high-throughput microtechniques must be developed to measure the physical properties of materials libraries if progress is to be made. Figures 6.8-6.10 show examples of a few microtechniques that could be used to measure various properties of combinatorial samples. Having measured

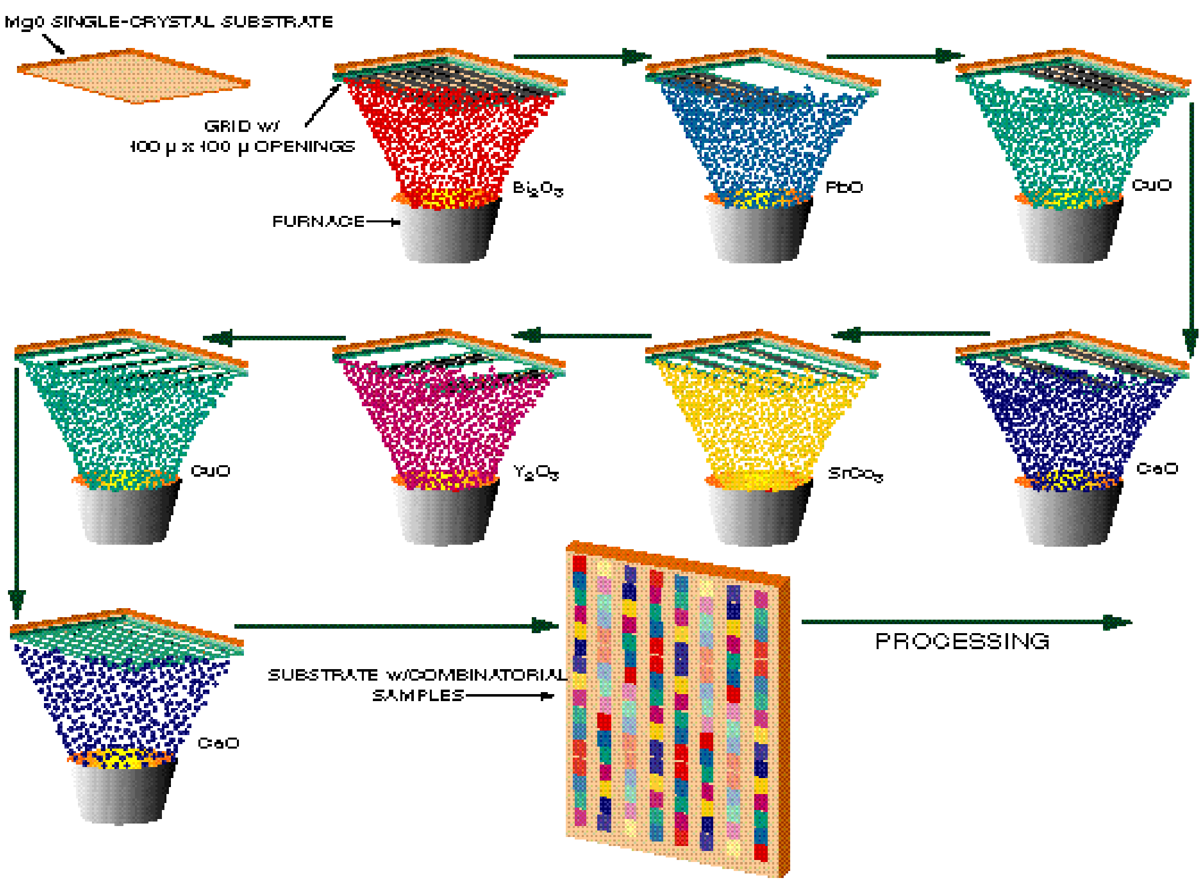

Fig. 6.7 Combinatorial synthesis of pseudo-ternary compounds (Bi, Y)-(Sr, Co)-(Pb, Cu)-O.

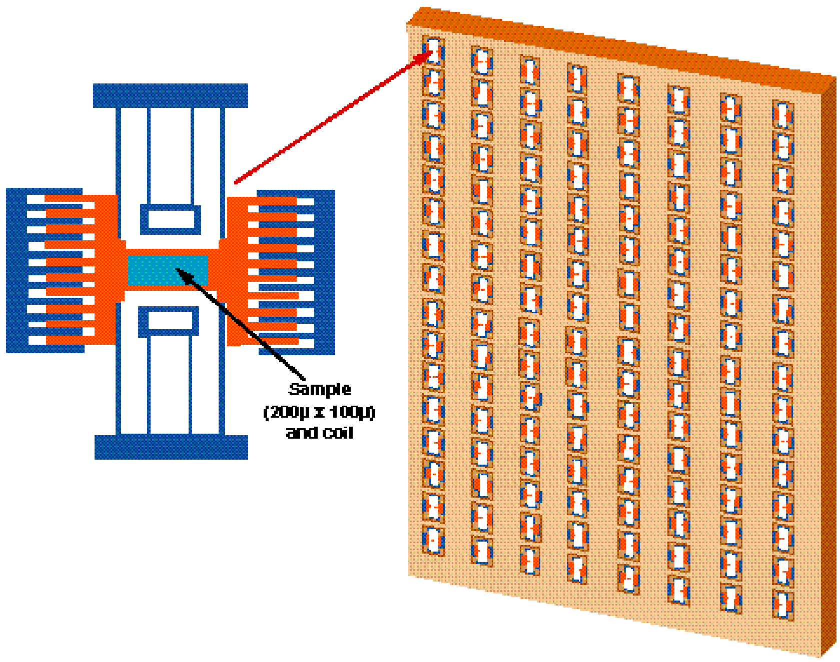

Fig. 6.8 Microsensors for the determination of magnetic properties using the principle of a vibrating coil magnetometer.

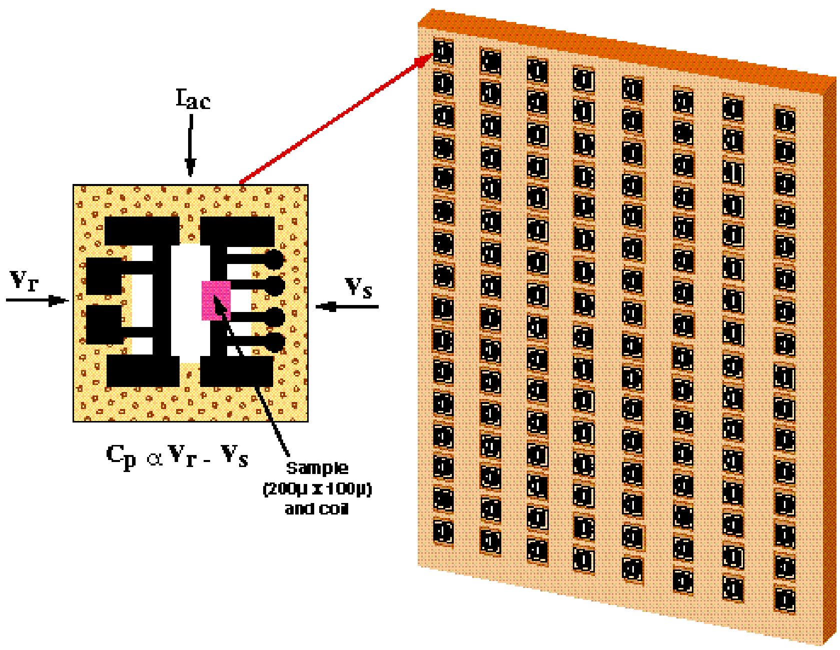

Fig. 6.9 Microsensors for the measurement of heat capacity based on a differential calorimeter.

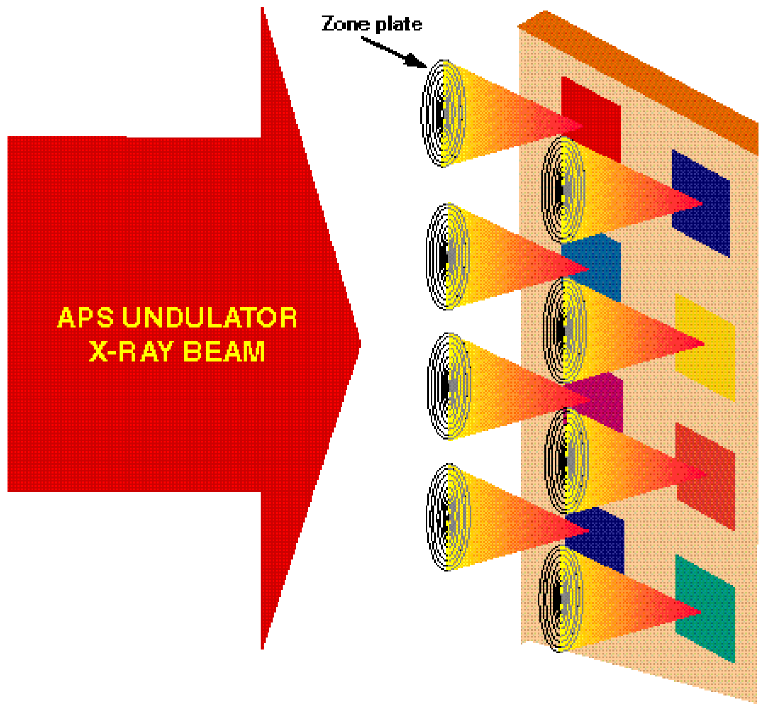

Fig. 6.10 Multiple microbeam materials analysis of combinatorial samples to obtain phase and structural information.

the physical properties, it is then necessary to interpret and understand this vast amount of information. The primary requirement for making progress in this area is to determine the combinatorial possibilities of atomic configurations in a new material in the library. Second, an evaluation of the local structure of materials in the library is also important in interpreting the measured properties of these materials. This process is summarized in Fig. 6.11.

The proposed APS Center for Combinatorial Materials Science and Technology will use the unique capabilities of the APS x-ray beams. The goal of the Center is to develop high-throughput micromeasurement tools and techniques using the high-brightness x-rays from the APS in conjunction with combinatorial processes, which will lead to an efficient and optimized process for the discovery of new materials required for new technologies. The masks for production of both bulk- and nano-phase combinatorial material libraries will be fabricated at the Center using micromachining capabilities now being developed at the APS. The same micromachining fabrication technology will be used to develop microtechniques to measure mechanical, thermal, electrical, magnetic, and optical properties of material libraries with extremely high speed. The final part of physical measurements will involve use of submicron x-ray beams already being produced at the APS to map three-dimensional atomic/molecular configurations in combinatorial material libraries and the local chemical and

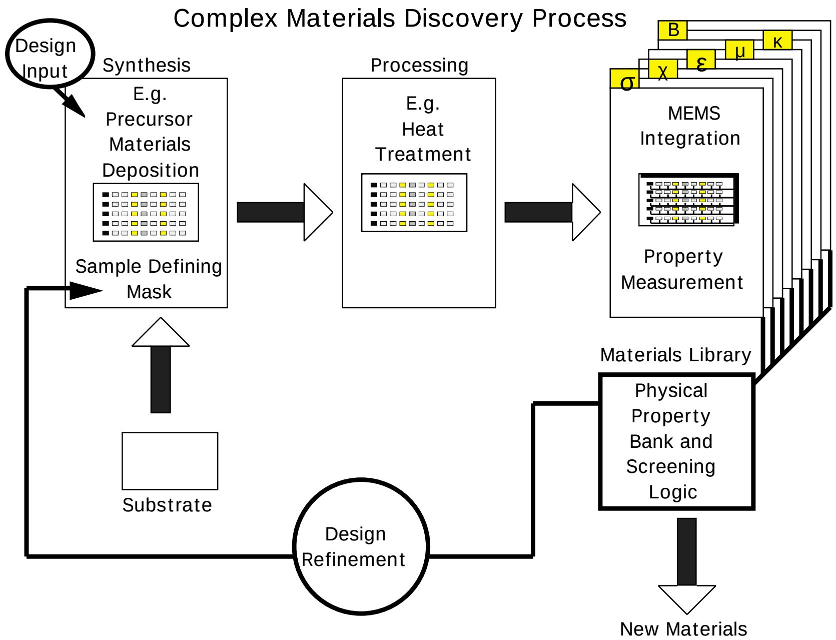

Fig. 6.11 A laboratory on chips.

magnetic structure in these systems. The high brightness of the APS x-ray beams is essential for fabrication of apparatus for the microtechniques required to measure both physical and structural properties. The present plans call for the measurement and understanding of the physical properties of both hard and soft combinatorial material libraries of interest to materials scientists, chemists, and biologists.

A recent National Academy Report concludes that: "*Increasingly sophisticated equipment has become necessary for scientific innovation, from electron-beam instruments to giant x-ray synchrotrons.*" Consistent with this statement, the DOE has included a center for combinatorial materials science and technology in the *DOE BES Facilities Roadmap* (Fig. 6.1).

Our proposal would involve construction of a set of laboratories occupying approximately a 30,000 sq. ft. area adjacent to the APS. These laboratories will be equipped with chemical and physical tools for the production of combinatorial material libraries in various forms, from amorphous materials to single crystals. A specialized laboratory will be dedicated to micromachining technology to support deep-x-ray lithography and conventional microfabrication for the development of analytical tools for high-speed micro-electromechanical systems (MEMS). An additional laboratory will be dedicated to chemical and biological work. Four beamlines will be dedicated to the Center, one for micromachining, the second for microimaging, the third for microdiffraction, and the fourth for micro-XAS. The synchrotron techniques required to scan libraries with as many as 10,000 materials in a very short period with robotics manipulation of the samples will be developed. The operations of the Center will be the joint responsibility of the APS

Experimental Facilities Division and the Material Science Division at Argonne National Laboratory.

6.5 Structural Genomics Project

A structural genomics initiative is being jointly developed under the leadership of the Center for Mechanistic Biology and Biotechnology (CMB) and XFD. The initiative will focus on the concept of using genomic data as the basis for the selection of proteins for which determination of structure will provide new knowledge of the relationship between amino acid sequence and three-dimensional structure identifying unique folding motifs. It is suggested that approximately 5000 key structural homology groups emerging from the results of Human Genome project represent a viable irreducible set that could eventually provide a virtually complete “almanac” of natural protein structures. Under an optimal scenario where all the required crystals are readily available and the beamline on an APS undulator is capable of uncovering structures without any bottleneck, the structural almanac will conservatively take 5 to 10 years. The reality is far from this optimal situation. The initiative will hence address the two key bottlenecks in accomplishing this task. The known bottlenecks are the following: 1) conventional technologies cannot deliver 1000 crystals of proteins desired per year, and 2) the sample delivery (mounting, aligning and cooling the single crystals) to a beamline, data collection, and structure analysis of 1000 crystals per year cannot be achieved with present day experimental techniques.

The strategy to be used to generate high-throughput production of protein crystals may be thought of as a parallel and iterative production and expression (PIPE) approach. We assume that in order to achieve 5000 crystals, all of which represent new proteins, we must attempt to crystallize 50,000 proteins. The critical step in the crystallization process is growth monitoring. A detailed analysis indicates that over a thousand examinations have to be performed per day using polarized light, which interrogates the reflectance and/or transmittance of the crystallization chamber. The design of an interrogation robot will be the responsibility of XFD.

The other limitation in reaching the target goals of this initiative in structure determination is the current capability of an APS beamline. The target goal is governed by the need to determine the structure of a large number of crystal protein samples. The following additional constraints increase the number of samples. They are (1) short exposures to x-rays in order to reduce the crystal damage from radiation, thus increasing the number of samples of one kind to be studied, and (2) additional data sets to be collected for each structure with different contrast agent (such as Se, Br, Eu, Re, Os, Ir, Pt, Au, Hg, U) and at least two x-ray energies above and two below the absorption edge for a complete MAD analysis. The bottleneck for collecting data sets on each sample is the constant need to change and realign each single-crystal sample. This task currently is both manpower intensive and time consuming. The principal part of this initiative is to develop robotics technique in order to increase the efficiency of sample delivery to the APS undulator beam. This involves automation of the crystal changing procedure, which includes the following:

(a) an automatic or semi-automatic mounting tool that will retrieve the crystal from a crystallization droplet to a mounting device, (b) a micron-precision crystal pre-alignment station outside the experiment station, (c) a micron-precision crystal mounting goniometer, (d) a liquid nitrogen compatible sample transport system that will permit transfer of the pre-aligned sample into the experiment station, (e) a multiple-sample mounting system or cartridge that will permit automatic sample change, and (f) new alignment tools and procedures. The goal here is to reduce the frequency of experiment station access and to reduce the time taken to align the sample. The challenge is to maintain the samples at cryogenic temperatures throughout the process from crystal mounting to alignment to the actual exposure to x-rays during data collection. A proposed multiple-sample mounting stage is shown in Fig. 6.12.

This initiative will receive LDRD support starting in FY 1999 for a period of three years. The success of the developments in this initiative can be transferred to many of the APS beamlines to optimally utilize the beam time when ever possible.

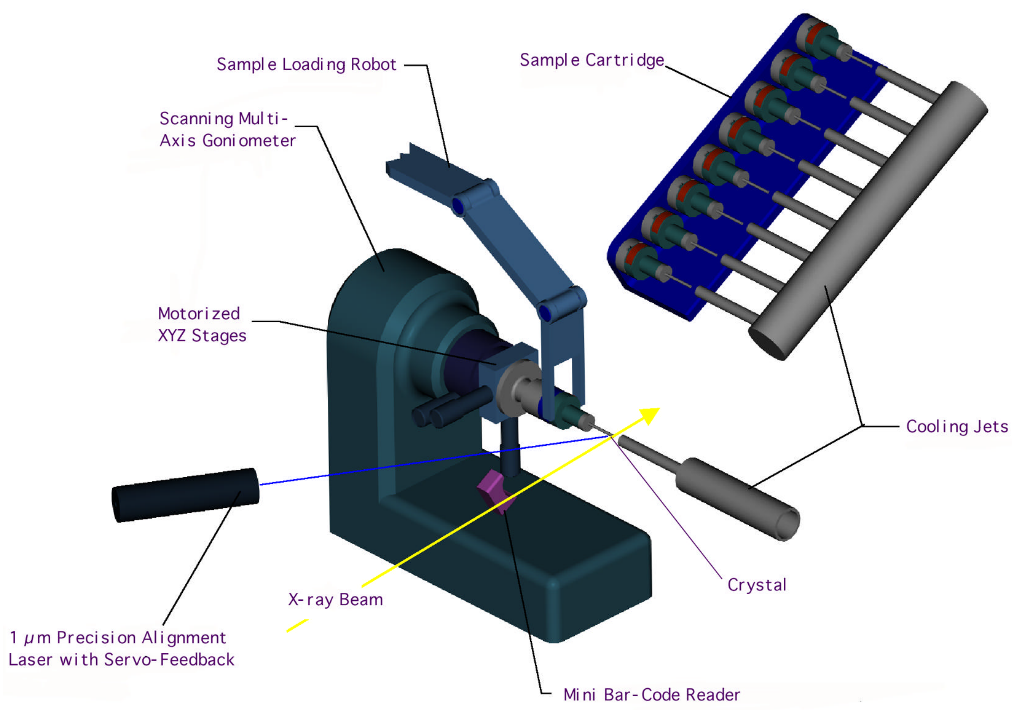

Fig. 6.12 Multiple sample mounting stage.

6.6 References

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