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A Program in Detector Development for the US Synchrotron Radiation Community

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A white paper based on a workshop held in Washington DC, Oct. 30 – 31st 2000

A Program in Detector Development for the US Synchrotron Radiation Community

Summary. There is a clear gulf between the capabilities of modern synchrotrons to deliver high photon fluxes, and the capabilities of detectors to measure the resulting photon, electron or ion signals. While a huge investment has been made in storage ring technology, there has not to date been a commensurate investment in detector systems. With appropriate detector technology, gains in data rates could be 3 to 4 orders of magnitude in some cases. The US community working in detector technology is under-funded and fragmented and works without the long term funding commitment required for development of the most advanced detector systems. It is becoming apparent that the US is falling behind its international competitors in provision of state-of-the-art detector technology for cutting edge synchrotron radiation based experiments.

There is thus an urgent need for a coordinated national program in detector research and development for synchrotron radiation research. Several new technologies are becoming available that could revolutionize the capabilities of detectors. One of the most important advances is the massive integration of parallel electronics into detectors on a pixel by pixel basis. Such detectors have the capability not only to work at very high rates, in some cases approaching 1 THz, but to include 'smart processing' of information on chip. Other important areas include the revolution in low temperature x-ray detectors capable of high energy resolution, and, if used in the form of arrays, potentially high counting rates. The science enabled by such detectors will be spread across the whole spectrum of synchrotron radiation research. For example, the study of the 3d structure of systems with short-range order using x-ray fluorescence holography (XFH), microsecond dynamics in polymers and magnetic systems studied using photon correlation spectroscopy, environmental chemistry studied using fluorescence yield micro-XAS, the study of chemical and electronic structure via photoemission and x-ray emission, and many more areas will be revolutionized by the use of advanced detectors.

The principle conclusions of a national Workshop on Detectors for Synchrotron Radiation held in Washington, DC, Oct. 30 – 31st 2000, were that:

- Funding of advanced detectors is the most cost effective way of increasing the effectiveness of both existing and planned future synchrotron facilities
- Funding agencies should make provision for use of the most advanced present-day detectors on existing facilities; there are examples of multi-million dollar 3rd generation beamline facilities with 1st generation detectors.
- There should be a nationally coordinated program to provide funding of long-range strategic research in a number of highlight areas.
- An organization modeled after the successful BioSync dealing with biological applications of synchrotron radiation, "DetectorSync" should be formed to coordinate the area of detector research, and to represent the communities needs to funding agencies.

In this document we point out general areas that should be targeted, and in coming months, these will be refined into definitions of specific programs with delineated targets. We urge that a major funding initiative and associated call for proposals be focused on these areas, with the aim of setting up large programs to serve the needs of the whole community. Key elements will be provision of information and resources to the research community, as well as wherever possible promotion of technology transfer to the industrial sectors associated with synchrotron radiation and other fields. A detailed cost estimate of such a program has not been made, but based on the expected number of areas of research and the size of each group required for an aggressive and efficient operation, an initial estimate would be approximately \$25M/yr.

1. Introduction

A general realization has emerged that there is a widening mismatch between the well-demonstrated ability of beamlines at synchrotron sources to deliver abundant photon fluxes and the only modest abilities of many detectors to record the results. Overall, the synchrotron facilities, each of which represents collective investments from funding agencies and user institutions ranging from many hundreds of millions to more than a billion dollars, are thus not being optimally utilized because of detector limitations. While this growing problem plagues facilities around the world, it is particularly acute in the United States, where detector research often has to ride on the coat tails of explicitly science-oriented projects, and long-range R&D in detectors is often difficult, if not impossible to carry out.

In addition to the lack of a well established tradition for supporting research specifically leading to advanced detectors, several factors are converging in today's fast-moving world that make it obligatory to transform detector development into a more focused activity with its own funding base. Many of these trends appeared first in the world of elementary particle physics, where detectors have long played a key role, and often represent 10 - 30% the cost of accelerator projects. The importance of detectors in this field is exemplified by the award to Georges Charpak (CERN) of the 1992 Nobel Prize in Physics "for his invention and development of particle detectors, in particular the multiwire proportional chamber". The synchrotron radiation community thus has much to learn from, and can in some instances take direct advantage of, detector development in high-energy physics.

Synchrotron radiation experiments are becoming ever more sophisticated, simultaneously demanding high count rate capabilities, high energy resolutions, and high spatial resolutions over large areas, for example. Developments in microelectronics technology that have played such a key role in particle tracking and other functions in the massive devices installed around colliding-beam storage rings built for studying elementary particles are now seen to be applicable to synchrotron-radiation detector systems, as well. As in the high energy physics field, this increasing complexity is outgrowing the ability of single investigators or small research groups to develop them, and a more coordinated approach involving teams of specialists looks certain to be the future mode of operation, at least for the most sophisticated systems. Finally, such systems will be expensive to produce, primarily due to the cost of research and development that will often span periods of 5-10 years.

A disturbing trend is the increasing gap between the US and Europe in the amount of resources put into detector research. For example, the ESRF and Daresbury detector groups are each larger than the combined detector groups at all of the major U.S. x-ray synchrotron sources. Elettra also has an effort that is stronger than that at any single U.S. facility. The effect of this is an erosion of the capabilities of the US synchrotron radiation facilities with respect to their European counterparts, which ultimately will lead to a decrease in the scientific competitiveness of the US research community. To put this in budgetary perspective, the annual operating budget of the US synchrotron facilities is over \$200M. Although an accurate determination has not been carried out, it appears that only around 1% of this or \$2M is spend on development of new detectors. If one looks at the information rates in an experiment possible today by employing a combination of state-of-the-art detector and microelectronics techniques, gains as high as 10^3 - 10^4 are possible. It is interesting to note that this is as high as the brightness gain between 2nd and 3rd generation synchrotrons, a gain in the US bought with an investment of over \$ 1B. It is clear therefore that substantial investment in advanced detectors will allow maximum utilization of our expensive synchrotron facilities, and in addition, it will enable completely new areas of science to be explored.

These concerns of the community at large led to a two-day meeting in Washington DC, on Oct 30-31st 2000. The overwhelming view of the broad-based group assembled at this meeting was that now is the time for action. Emerging detector technologies, integration of microelectronics and the needs imposed by increasingly sophisticated experiments all mean that we have to aggressively react to these challenges or we will fall behind international competition, and indeed the potential of all of the sources in the world may not be fully realized.

2. Workshop on Detectors for Synchrotron Research, Washington DC, Oct 30-31st 2000

This white paper is based on presentations and discussions held at a 'Workshop on Detectors for Synchrotron Research', held in Washington DC, on October 30 – 31st 2000 and on discussions amongst the workshop organizers in the following weeks. One conclusion of this meeting was that a standing committee of synchrotron facility staff, users and detector experts should be formed, based on the successful BioSynch model, to advise agencies on policy in the areas of detectors development, to help coordinate programs, to disseminate information, and in general to carry on the work started at this recent workshop. One of the first roles of the "DetectorSync" organization will be to refine the strategy set out here, so that more concrete guidance can be given, particularly in relation to detector areas that need to be targeted, and for mechanisms for funding and reviewing a coordinated detector initiative. This document therefore represents a significant step toward a detailed roadmap for a coordinated US program in detector development for synchrotron sources.

The two-day Workshop on Detectors for Synchrotron Radiation in Washington was organized with the financial support of the U.S. Department of Energy, Office of Basic Energy Sciences, on behalf of the U.S. synchrotron radiation community by representatives from each of the US sources, Al Thompson (ALS), Denny Mills (Advanced Photon Source, APS), Steve Naday (Argonne National Laboratory), Josef Hormes (Center for Advanced Microstructures and Devices, CAMD), Sol Gruner (Cornell High Energy Synchrotron Source, CHESS), Peter Siddons (National Synchrotron Light Source, NSLS), John Arthur (Stanford Synchrotron Research Laboratory, SSRL), and Ralf Wehlitz (University of Wisconsin Synchrotron Research Center, SRC), with Franco Manfredi (University of Pavia) as an international member. Each organizer prior to the meeting was responsible for contacting the user base of his facility by e-mail to solicit input on the needs of the community. In addition several facilities organized meetings with user groups in advance of the national meeting, in the form of workshops, seminars and so forth. This information was presented during the meeting and ensured that all had an opportunity to contribute. The program of speakers was also chosen to span the full range of synchrotron radiation science, to include representatives from major international detector efforts, and to have representation from efforts in high energy physics.

The workshop agenda is attached. The overall format was organized so that the 1st morning had presentations on science, with an emphasis on the new science that could be enabled by new detectors, and the afternoon had presentations from international leaders in detector technology. On the 2nd day the workshop split into working groups for diffraction and scattering (Sol Gruner), spectroscopy (Peter Siddons), imaging (Mark Rivers), crystallography (Bob Sweet, Andy Howard and Ed Westbrook), timing (John Arthur) and infrared (Larry Carr). Each working group has produced a report and these will be published in due course

Although the output of each working group is specific to their own needs, there are many common threads that were identified;

1. *The best currently available detector technology needs to be installed on existing beamlines.* In a surprising number of cases, very expensive beamlines are limited by the inability to procure even

the best currently available detectors. This situation is especially true for beamlines that do not specialize in biological macromolecular crystallography. It makes no sense to limit beamline capabilities for the lack of funds for detectors that cost but a small fraction of the cost of the beamlines, much less the cost of the storage ring.

2. *The funding agencies should support enhanced cooperation between detector groups in the U.S. and abroad.* The Europeans especially are making a number of advances in many detector technologies. More cooperation and collaboration would benefit everyone involved, especially since the funding resources come from distinct pools. Cooperation may take many forms: joint workshops, visitor exchange programs, web publication of details of detector advances not suitable for journal publication, and cooperative agreements which allow access to integrated circuit libraries and software.
3. *Mechanisms are needed to allow duplication of detector advances in which the market is too small to attract industry.* The explosion of research based on biomacromolecular crystallography was enabled by the availability of image plate and CCD detectors. In this case, the market for a single kind of diffraction experiment was large enough to attract industry, with the result that a steady stream of incremental advances are now proceeding with little need for government intervention. However, few synchrotron radiation research areas are able to boast of such a market; rather, the needs are large, but the specific methods are diverse. Detectors suitable for many of these needs are often developed by individual groups, but these groups are ill-suited to duplicate and provide the detectors to other groups. In the absence of industrial participation, there is no effective mechanism to make these detector advances available to the larger community.
4. *The number and size of detector groups in the U.S. needs to be dramatically increased, both at the synchrotron sources and in the universities.* Detector groups are needed both to assist users in full detector utilization (both in hardware and software aspects) and for the development of new detector technology. The absence of in-house detector groups to assist users at the sources will limit the effective utilization of detector technology, even if this technology were to become available, because detector expertise is required to integrate state-of-the-art detectors into experiments. Due to lack of funds, detector groups, both at the sources and elsewhere, have shrunk both in size and number. An infusion of funds is desperately needed to reverse this situation. New detector advances have historically come from many different sectors: universities, national labs and industry have all played key roles. Therefore, it is important that funds for detectors be made available based solely on competitive merit of the proposals, and not simply by the location or sector. Another important factor is that funding needs to be coordinated so that key technologies receive adequate support. However, as a different issue, funding also needs to be stable enough on 5-10 year timescales that sophisticated new systems can actually be developed and brought on line.
5. *Detector research support needs to balance shorter term needs with long term basic research.* Incremental improvements on, for example, high energy or high resolution CCD phosphors, would have an enormous impact on the utilization of existing CCD detector technology. These are likely to be short-term projects. On the other hand, very promising future technologies, such as Pixel Array Detectors (PADs), active matrix pixel detectors, superconducting detectors, etc. will require gestation periods of 5 – 10 years. There is a need to fund both short-term application needs and more speculative longer term research.

6. *A standing detector advisory committee should be formed to identify opportunities and to suggest ways in which detector development might advance.* Detector developments take a very long time - frequently decades - before reaching fruition. While a few-year major Detector Initiative would be welcome, especially in terms of providing existing technology, sustained long-term support is required if detector advances are to continue. A standing committee should be formed to advise the agencies of detector areas in need of attention. This advice might include things like suggestions of detector opportunities for Requests For Proposals (RFPs), suggestions for workshops and exchange programs to promote international cooperation, and suggestions for leveraging synergy with other communities with related technological problems (e.g., the high energy physics community or medical radiology groups). Our proposal would be to model this organization on Bio-Synch, an institution that has been successful in representing the needs of the biology community with agencies. As a working model we therefore will form DetectorSync, to continue the work started at the Washington workshop.

3. Science enabled by next generation detectors

The application of new advanced detector technology will affect almost all aspects of synchrotron radiation science. It is therefore difficult to give a comprehensive description of scientific areas that would benefit, but rather here we give a few brief examples to illustrate the wide range of new science that will be enabled by development of next generation detector technology. We group these by scientific topic, but clearly most of the detectors described could be equally well applied to many other scientific areas.

Biological Sciences: The study of biological systems has been revolutionized by the application of the tools of crystallography to the determination of protein structures. The pace of development has accelerated in the last few years due to the advent of multiple wavelength anomalous diffraction (MAD) phasing techniques, fast computers for solution and refinement, higher intensity sources and better detectors. But the need for even faster data collection and structural solution is now even higher, with the ongoing revolution in genomics and structure-based drug design requiring an increase in throughput of perhaps 100 times over current capabilities in the next few years. In addition, there is a trend towards higher resolution data collection through the use of robotic crystal screening using x-rays. While x-ray CCD cameras have been a major step forward, they now represent one of the bottlenecks to more rapid and more accurate data collection. Ideally, in monochromatic oscillation crystallography one wishes to record the diffraction from a given Bragg reflection only when the corresponding reciprocal lattice point is passing through the Ewald sphere, i.e., when it is in a diffracting condition. The optimum signal-to-noise ratio is then achieved by subtracting the time-normalized background signal immediately before and after the spot passes through the Ewald sphere. This procedure automatically takes into account slowly changing background levels and helps to remove detector flat-field variations. This is the essence of the so-called phi- or fine-slicing method. By contrast, CCD or image plate detectors operate in integrate/readout cycles which, in practical terms, means that the user selects an oscillation range and records all reflections over that range. Since different spots pass through the Ewald sphere at different times, any fixed oscillation range will necessarily involve the recording of reflections which are only partially through the Ewald sphere at the ends of the oscillation range. The scaling and merging of these partials often limit the quality of the data, so the user is forced to compromise between a wider oscillation range, which reduces the fraction of partials, and a fine oscillation range, which can approach more ideal fine-slicing. In addition CCD based detectors have a relatively wide point spread function, resulting in signal in high intensity reflections ‘bleeding’ into adjacent areas, reducing the signal-to-background ratio of nearby weak reflections. A better approach would be to develop Pixel Array Detectors (PADs) or other photon counting detectors which record the data into user-selectable,

arbitrarily short time-bins which may vary asynchronously across the face of the detector. Such detectors do not now exist, at least at the requisite count-rates, but are clearly possible.

Time resolved crystallography using Laue diffraction techniques is now being used to probe the dynamics of protein motion. At present the technique is usually performed by laser initiation of a process followed at a set time interval by interrogation of the structure by recording of a Laue pattern. The time course of a process is built up by repeating the process for a series of time intervals, and typically this can involve the use of many crystals. This therefore is a laborious process that can be prone to error. A significant improvement in the technique could be made if the time course could be measured in one continuous recording. In conventional time resolved Laue measurements the data are recorded on a conventional x-ray CCD camera, and time resolution is obtained by mechanically shuttering one x-ray pulse; the time resolution is in principle then just given by the bunch length. In a continuous recording the time resolution is given by the time resolution of the detector. Using PAD technology in which there is parallel transfer to on-chip storage, it should be possible to achieve time resolutions of a fraction of a microsecond. The problems of variability from crystal to crystal would be solved, and data quality should be considerably improved. The use of continuous recording would be a major step forward in the use of Laue diffraction for the study of time dependent processes.

The same type of detectors could also be employed in time-resolved small angle scattering studies of molecular function and assembly, for example in recording the action of muscle during activation. PADs not only would be capable of much better time resolution than present day wire detectors, they could allow completely new acquisition methods. For example, many systems undergo oscillatory structural changes, or can be made to do so in synchrony with a periodic signal, such as stretch-activated insect flight muscle. In many of these cases, the x-ray diffraction differences of interest during different parts of the oscillatory cycle are very small and the acquisition of accurate data requires signal averaging over many cycles. Many samples exhibit slow fatigue, drift, radiation damage or large sample-to-sample variations (e.g., due to absorption) which complicate or limit the ability to integrate low noise diffraction from different parts of the oscillatory cycle or from multiple samples for later subtraction to uncover the small fractional differences. In other cases, the frequency of oscillation is simply too high for ready isolation of a small part of the oscillatory diffraction. For single point signals, the time-honored way to deal with such low-level signals is to use phase sensitive lock-in amplifier methods. It is entirely feasible to develop x-ray detectors in which each pixel over a 2-dimensional surface effectively acts as a lock-in amplifier. For example, pixel array detectors can be designed in which the signal from each pixel is successively either added into or subtracted from an in-pixel integrating capacitor in synchrony with an external electronic clocking signal. It is even possible to put several integrating capacitors into each pixel to divide the oscillatory cycle into small segments. Such analog PADs can have effectively long integration times to extract very small differences over an enormous number of cycles, even if the count rates are very high. Alternatively, for lower count rates (MHz /pixel) digital PADs can directly bin the counts in-pixel into externally phase-locked bins. The availability of such point-by-point area lock-in x-ray detectors would substantially expand the feasibility of many kinds of very low-level difference experiments.

Materials Science: The high brightnesses of third generation sources and in the future fourth generation sources provide several new avenues for studying materials properties. Of note here is that detectors must be developed for both photons and electrons.

Photoemission spectroscopy is one of the most powerful tools in the study of the electronic structure of materials, as well as of their surfaces and interfaces, and this is becoming evermore important in various aspects of nanoscience. As one example of its power, by measuring the direction and energy of valence electrons leaving a crystalline material, the electronic bandstructure can be mapped in exquisite detail.

This technique has been applied to almost all classes of crystalline materials, but in the last few years it has been applied with particular success to the study of correlated electronic systems, examples of which are high temperature superconductors and materials that exhibit giant magneto-resistive properties. In discussing the origin of high temperature superconductivity, a now famous quote of solid state physics Nobel laureate Phillip Anderson is that “..angle resolved photoelectron spectroscopy will provide the smoking gun” for the ultimate understanding of the theory of the electronic properties of these materials. In studying all correlated electronic systems, it is critically important to study in very fine resolution the details of the electronic structure near the Fermi level, if possible also with resolution of the spin of the emitted electrons. In traditional photoelectron spectrometers, a single channel detector was used to record electron intensity and the analyzing energy was swept through the energy window defined by the detector. In more modern systems, this single channel detector is replaced by microchannel plates and a variety of imaging detectors. In one direction the energy of the electrons is dispersed, and in the orthogonal direction the angular distribution is imaged. For some applications, one desires simply to integrate over angle so as to derive 1D energy distributions in the most rapid manner; in others a simultaneous 2D detection in both energy and angle is desired. None of the present day detectors come close to dealing with the enormous data rates present (which can rise to the GHz level over the full detector), and typically many orders of magnitude in signal are wasted. The intrinsic advantage of energy and angle dispersion is very significantly diluted by the absence of an adequate detector. One and two dimensional multi-anode pixel array detectors could revolutionize this situation, enormously speeding data acquisition. This will improve data quality, but it will allow much more subtle details of the electronic structure to be resolved. The same types of detectors could be used in many other types of photoemission experiments. For example, the study of surface chemical reactions could be extended to the time domain, with spectra being accumulated in as little as 1 ms, with time scales for surface diffusion and reaction often being much longer than this. Many surface reactions are relatively slow and further are inhomogeneous, occurring in waves rather than uniformly across the surface. The combination of time resolved photoemission with imaging would be an extremely powerful tool in the study of surface chemical reaction dynamics. Finally, being able to rapidly accumulate full-hemisphere photoelectron datasets at various photon energies should permit developing photoelectron diffraction and holography into more routine probes of surface atomic structure, including the time dependence of structures.

Detecting electron spin is also crucial to studies of magnetic, as well as strongly correlated, systems. This is now almost universally done via the time-consuming method of single-energy-channel Mott scattering, with an attendant loss in efficiency of 10^3 - 10^4 . This inefficiency has held back progress in such studies, and needs a concerted R&D effort to try to develop a more efficient, multi-channel methodology. One promising approach for this is the use of spin-selective scattering in the transmission of low-energy electrons through ferromagnetic films of nanometer-scale thickness.

Beyond such photon in-electron out experiments are several classes of photon in-photon out experiments that would benefit from advanced detectors, with a recent DOE-sponsored workshop having explored these possibilities in great detail [Pikeville workshop March 2000: Publ. Oak Ridge National Lab]. As a first example, soft x-ray emission has experienced a renaissance due to third-generation beamline brightnesses, and various aspects of it involving what can be viewed as both elastic and inelastic x-ray scattering in both resonant and non-resonant conditions offer exciting new probes of bulk, buried interface, and surface properties. But the effects here can be very weak, such that higher energy resolution and much higher throughput is needed from detectors to make such developments possible.

High-brightness third-generation sources can also be used to probe time dependent fluctuations in materials properties with nanoscale spatial resolution using the x-ray and soft x-ray analogs of dynamic

laser light scattering. Pioneering experiments have been performed looking at the dynamics of magnetic domain motion, colloidal motion, and liquid crystal ordering. A major limitation, however, is that the brightness of third generation sources is orders of magnitude lower than that of a laser, while the time structure of fourth generation sources is far from optimal. Both of these limitations might be addressed by improved detector technology. We confine our comments here to improved detectors for dynamic scattering experiments at third generation sources. In a dynamic light scattering measurement, one a) prepares a transversely coherent photon beam, b) probes a particular length scale by selecting the appropriate scattering wave vector, and c) forms a temporal autocorrelation function for the scattered signal. The experiment is typically repeated at many different wave vectors by changing the experimental geometry. The figure of merit is the count rate per speckle (scattered coherence solid angle), since this determines how long one needs to count to achieve satisfactory statistics at a given time resolution. By this measure, most dynamic x-ray and soft x-ray experiments are very count-rate-limited. A single wavevector and hence length scale can be probed in principle at high time resolution, but then must be repeated for a range of wavevectors making the process slow. On the other hand a range of wavevectors can be probed using an imaging detector, but the serial nature of the readout of conventional CCDs makes the effective time resolution very poor. These problems could be largely circumvented by developing an array detector with each element having a temporal autocorrelator. In this case, one could measure a large range of scattering wave vectors simultaneously, speeding acquisition times by many orders of magnitude. The parallel detection over a range of desired length scales would make today's pioneering experiments routine, and open up the range of applications to a much wider class of materials.

X-ray diffraction probes the structure of systems with long-range order giving 3D information of atom locations, and x-ray absorption spectroscopy (EXAFS) probes systems that need have only short-range order but reduces information to primarily 1D inter-atomic spacing information. However, there are many materials which exhibit only short-range order but for which 3D information is essential to their understanding. Among these one could list dopants in glasses and semiconductors, clusters, ions in solution and many more. The recent advent of X-ray Fluorescence Holography (XFH) has opened the possibility of studying important classes of materials that exhibit only short-range order, but where 3D information on atom locations is essential. XFH can be carried out in two ways. The first is the direct method wherein fluorescence from a source atom is scattered by adjacent atoms before being detected in the far field. The intensity distribution in angle is the result of direct fluorescence from the source (the reference wave in a holographic sense) and its interference with the scattered photons (the object waves in a holographic sense), and so encodes amplitude and phase so that holographic reconstruction can be performed. As the scattering processes are rather weak, the modulation of intensity in the far field is superimposed on a large background, with effects in the 0.1% range being typical. In the inverse method, the incoming x-ray beam is used as the reference wave, with the source atom becoming a detector which indicates the local intensity of direct and scattered waves through its fluorescence intensity. In this case the total fluorescent intensity is monitored as a function of the orientation of sample and incident beam. In both methods the intrinsic resolution is set by the size of the source or detector respectively, ie. the size of an atom. While both methods have been applied to bulk crystalline samples with spectacular results, application to real systems awaits development of advanced detectors. The problem lies in the small signal-to-background ratio inherent in these experiments, and to the huge overall data rate. As an illustration, if we look at the direct method and realize that signal-to-background ratios are typically less than 1 part in 1000, a huge number of photons have to be recorded for each pixel and for as wide an angle range as possible. In addition, fluorescence from other atoms and for other scattering processes have to be filtered out, and so ideally an ultra-fast area detector with reasonable energy resolution of ~ 100 eV is required. For this reason, the inverse method is typically used, but this again has problems of data rate, the need to integrate over one whole hemisphere ideally and the need to mechanically scan the sample in angle. Many of these problems could be solved by development of a

pixellated detector with high counting rate capability, with each pixel having energy resolving capability. With such systems not only could holograms be taken in seconds, opening up the possibility of time resolved experiments, but the technique could be applied to ultra-dilute systems such as dopants in a wide class of materials. The integration of analog to digital convertors into the structure of a PAD will be a significant challenge, but no fundamental barriers are present. Such energy resolving pixellated detectors would be widely used in many branches of synchrotron radiation research.

Environmental Science: The realization that the study of many environmental issues requires a very detailed knowledge of local chemical and structural information has emerged over the last few years, and has indeed given rise to the naming of a new scientific discipline, Molecular Environmental Science (MES). MES will be important in many areas such as remediation of contaminated sites and the understanding of transport of toxic materials in both soils and plants. A key challenge is understanding how contaminants react with the minerals and clay materials in soils, often via surface-mediated processes, so that sequestration or transport of materials can be predicted and perhaps altered. These studies are for example important in remediation of sites damaged by nuclear and industrial waste. Such studies require measurement of the reactivity of the heterogeneous clay and mineral materials in soils, and for this a combination of photoemission spectroscopy and x-ray absorption spectroscopy to identify chemical species and diffraction to identify mineral phases is ideal. However, the heterogeneous nature of the materials means that a huge quantity of data must be measured to have any hope of understanding such a complex system. On a grain by grain basis over wide areas, usually at the micron level, XAS and XRD data must be taken to build a statistical picture of reactivity. Whereas in a conventional experiment on a single crystal sample a single data set would be taken, here tens of thousands or perhaps up to a million 'samples' must be probed. The 3rd generation sources have given us the photon brightness required to in principle do such complex experiments, but good detectors are wholly lacking. The energy resolving pixel array detectors described above would be a good solution, or as a stepping stone to such complex technology, many-element-array solid-state detectors could be used, possibly employing drift diode technology due to their superior noise and speed characteristics together with integrated electronics. It should be noted that unlike say biological systems where one may be measuring the presence of one metallic element in a metalloprotein, it is critical to maintain measurement of a wide range of elements simultaneously in the mixed heterogeneous environment of MES samples. This restricts the usefulness of diffractive schemes for energy selection.

One of the principle problems in many systems is the diluteness of the element of interest relative to a matrix. It is however these low concentrations that are critical in many cases in determining reactivity and transport properties. The diluteness one can measure is determined by absolute signal, but also by signal-to-background ratio. With conventional fluorescence detectors there is a fundamental mismatch between the energy resolution of the detector, and the usually two orders of magnitude smaller fluorescence line width. In principle therefore having a detector with much better energy resolution would allow much more dilute samples to be measured, if they still had high rate capability. Cryogenic detectors using microcalorimeter and superconducting tunnel junction technology can now achieve a few eV resolution, but have very low count rate capability and have small areas. In order to improve area and rate capability, several groups are now investigating the possibility of array detectors. It appears possible that arrays with thousand or even tens of thousands of elements would be possible with significant R&D, revolutionizing the capabilities of energy resolving detectors throughout synchrotron radiation research.

4. A national detector development program

One of the roles of DetectorSync will be to develop a detailed roadmap of a national detector development program. We here offer some overall guidelines that could be used in the initial establishment of such a program.

Selection of key strategic areas: There are many detector systems and many competing technologies. Considering the complexity of many detector systems, in order to be effective, a program will have to concentrate resources in relatively few key areas. Assessment of these areas should be done in collaboration with the US community, and benchmarked against international competition. From the efforts in the US to date, several core areas already stand out as essential, although this list should be refined as we move forward.

The widespread availability of microelectronic design and manufacturing capability for specialized electronics is driving a trend for the integration of microelectronics directly into detectors. One example is the silicon Pixel Array Detector (PAD), in which a photodiode array is bump bonded to an Application Specific Integrated Circuit (ASIC), in which microelectronics directly reads and encodes the output from each array element in a parallel fashion. This should be contrasted with current state of the art x-ray CCD detectors in which data is segmented into perhaps 16 channels, rather than the 1 million or more of a PAD. PADs can also work with analog back end electronics so that the energy of a photon can be recorded. Using this technology, the count rate limitations of conventional Ge and Si(Li) detectors can be overcome, by making a massively parallel system. The count rate capability of such systems will be several orders of magnitude higher than the best system using discrete detectors and electronics. The same PAD technology can be used without the bonded photodiode to directly record electrons, usually generated from a microchannel plate amplifier. Projects in the US and elsewhere are already attempting to integrate ASICs directly into 1D and 2D designs, but more development is needed to make these fully workable. Again, PAD and ASIC technology will take counting rates from the MHz to the GHz regime, opening up many new avenues of research. Not only can data-rates be vastly higher, but on chip processing can enable experiments not possible using conventional systems. These include time stamping of each event, auto and cross-correlation, or programmed time sequence framing. PADs and ASICs will be a core area, with several key detector technologies being developed in parallel.

A second revolution is occurring in the area of energy resolving detectors. The PAD systems described above can be used in an energy resolving mode, but the intrinsic energy resolution is set by the characteristics of the semiconductor photodiode used to convert photons into electrons, and this typically leads to a resolution of 150 eV for a cooled germanium detector. Going beyond this requires a greater number of particles to be created in the conversion process, and the route to this is to use superconducting sensor technology. Two classes of detectors have been developed, micro-calorimeters (MCs) and superconducting tunnel junctions (STJs), both of which operate at temperatures around 0.1 K. MCs measure the x-ray induced temperature rise of an ultra-sensitive thermistor, typically a superconducting transition edge sensor, or a doped semiconductor. MCs offer high energy resolution, presently as high as 2 eV, but this comes at the expense of a low count rate typically 500 Hz, due to the intrinsically long time to bring the system back into thermal equilibrium. STJs can operate one order of magnitude faster, but have typical resolutions of 5 – 10 eV. The desired new technology that is now emerging is in more routine low temperature cryogenics, in improved speed and resolution, and in making arrays of such sensors to speed up their rate capability and overall solid angle of collection. Arrays of a few elements have now been constructed, and in the longer term, it appears feasible to produce arrays with tens of thousands of channels. If this can be done, then we will have detectors with comparable rate capability to conventional semiconductor arrays, but with almost two orders of magnitude better energy resolution. This resolution capability would be used in many areas from

enhancing sensitivity in x-ray absorption spectroscopy through a better match of detector bandpass to fluorescence emission width to direct detection of chemical state information from the fluorescence spectrum to state-resolved fluorescence holography.

A combination of new technologies is also coming together to revolutionize what might be viewed as traditional x-ray detector technologies based on gas amplification. The multiwire detector has been in existence for several decades and is still the workhorse of many x-ray experiments. These systems have many excellent characteristics including large area, shapes tailored to specific scattering geometries, and single photon counting. However the spatial resolution and rate capability are limited. To a large extent these limitations can be removed using micro-gap or even array electrode constructions, and in combination with on-detector microelectronics, they can in principle achieve extremely high performance. Obvious applications include increased time resolution in biological small angle scattering applied to the study of assembly dynamics of macromolecules to small and wide angle scattering studies of polymer dynamics during synthesis and processing.

Definition of funded projects. The aim is to have a nationally coordinated program in detector development. A fundamental point is to avoid the waste of over-duplication, and to avoid the waste incurred in funding many small sub-critical efforts. As stated above, with a limited budget it will be essential to focus on a few selected areas. A call for proposals resulting from a detector development initiative will therefore have to define quite specifically the type of program required, rather than being an open call for the funding of a broad range of detector technology. In a sense, the call would define a contract for the provision of detector technology with defined goals in terms of timescale and performance. In this way, funding will be focused in an efficient manner on the most pressing problems. The definition of the projects would be the responsibility of the community, through the DetectorSync organization in collaboration with DOE and other agencies. Due to the scale of some of these projects, it would be natural to think of some of these as being consortia of several groups with different expertise, involving national labs, universities and industry.

Promotion of technology transfer. It is apparent that a considerable amount of technology remains locked within individual groups due to the sometimes significant cost of technology transfer. Some mechanisms exist, for example through CRADAs, SBIRs etc., and while these provide a useful mechanism they are insufficient to unlock the tremendous store of information locked in individual labs. As part of any funded project, provision should be made for transfer of technology to the general community, and where appropriate to industry, either for its own use or for development as products to be sold to other research scientists. Not only would funded groups be responsible for production of specific detectors, but they would be responsible for the dissemination of information so that other groups could use the technology, or if there was a market, so that industry could commercialize the technology.

International collaboration. The problem of providing detectors matched to the capabilities of modern synchrotrons is a world wide problem. Very large economies could be made if collaborations could be formed with leading foreign groups, either to work as part of a team, or to simply exchange technology. Collaboration or technology exchange require that similar resources are put in from each side, but with the present limitations on detector funding in the US this has not happened.

Peer review of proposals and progress. Proposals should be reviewed by an international panel of synchrotron users and detector specialists. Assessment should be on the basis of competitive merit only, mapped onto the specific goals of the individual call for proposals. Clearly for the large scale programs that are envisaged, both the expertise and past track record for executing significant programs on time and budget must be important considerations. A similar review process would be used to assess progress towards the goals stated in the call and in the proposals.

Standing advisory committee. An organization modelled on Bio-sync, DetectorSync, should be created to guide the program forward. It would aid in national coordination of the overall program between funding agencies, provide a conduit from the community to agencies, and assist in provision of information on detector issues to the whole community. The latter would include for example provision of centralized information on the program projects, and a centralized source for information interchange.

Scale of a national program. As pointed out previously, perhaps 1% of the national budget in synchrotron radiation research gets spent annually on detector development, even though detectors, not sources or beamlines are the limitation in most of today's cutting edge experiments. Provision of state-of-the-art technology available today is an important 1st step in solving this problem. However, in order to stay internationally competitive, a national program has to involve sustained and substantial long-term funding. How large would this funding have to be to allow the US community to first catch up and then to provide the innovations needed in the next decade? Without a complete definition of program projects, any assessment will naturally be a rough approximation, but we can make an estimate by comparison with some of the leading European laboratories, and by extrapolation of the known costs of the existing US programs. The European labs that have invested heavily in detector development are Daresbury and ESRF, although Elettra also has made a significant contribution in this area. The first two labs have developed complementary strengths, for example solid state arrays and wire detectors at Daresbury, fast CCDs and high resolution imaging amongst others at ESRF. Other European labs such as Trieste have expertise in fast electron detectors, and SLS has an ambitious pixel project for 1D and 2D arrays. If we sum the number of staff working in these core areas, we come to a number of around 75 - 100 people. These numbers are then augmented by significant research efforts at, for example, the Max Planck Institutes and universities. If we try to assess the number of people required based on existing projects we come to a similar number. For example, integrated over 1D and 2D pixel array detector projects at LBNL, typically 3 staff have been on average involved with the projects at any one time, but usually on a parttime basis. However, these projects have progressed very slowly due to limitations of funding. In order to make serious advances in this field in a reasonable time scale, as well as to satisfy the above needs for technology transfer, information dissemination and the requirement to provide technology for the community, we estimate that around 8 – 10 fulltime staff would be required. Multiplying by the 8-10 or so program projects that would be the core of a national laboratory/university/industry-based detector program, we reach a similar requirement for staff in the vicinity of 100 people. Averaging over the salary ranges of scientists, engineers, technicians, and computer programmers needed on such projects and including overhead gives a budget of around \$ 20M/yr in operations. Although the majority of costs will be operational, significant capital would be required, especially for the projects involving use of microelectronic foundries. Again based on existing experience this would be typically 20 – 25 % of the operational total, giving a total annual cost of \$25M, or about 12% of the present total budget for operating synchrotron facilities in the US.

We have used here the example of several European labs in our model for what a US program should look like. This is however a simplification, and it is clear that even at the laboratories quoted, the capabilities of the sources in many cases far outrun the capabilities of detectors. The development of

detectors is also too slow, with the latest generation of detectors taking up to a decade to develop, a significant fraction of the lifetime of a synchrotron facility. This is in general not limited by technology, but simply by the limited staff involved with a single project. In basing our estimates to some extent on the successes of the European laboratories, we should recognize that they are affected by the same problems as the US laboratories, and also need enhanced investment to make full use of the powerful synchrotron sources we have available today.

Workshop on Detectors for Synchrotron Research

Courtyard Marriott Embassy Row, "General Scott" Room
Washington, DC, October 30-31, 2000

MONDAY, OCTOBER 30, 2000

8:00 Registration, Continental Breakfast served

8:30 Introduction - Al Thompson (LBNL)

8:45 DOE perspective – to be confirmed

Morning Sessions: Requirements for Improved Detectors in Different Research Areas

Session Chairman - Peter Siddons (NSLS)

9:00 Spectroscopy and atomic structure determinations with soft and hard x-rays

Chuck Fadley, UC Davis/LBNL

9:20 Materials science characterization using diffraction techniques - Sean Brennan, SSRL

9:40 Studying the heterogeneous world using x-ray microscopy - Mark Rivers, Chicago

10:00 Structural measurements using EXAFS - Steve Heald, PNCC Cat at APS

10:20 Coffee

Session Chairman – Grant Bunker (APS)

10:40 Ultra fast dynamics in solids - Roger Falcone, UCB

11:00 Science and detector requirements for fourth generation synchrotrons - John Arthur, SSRL

11:20 Infrared research - Larry Carr, NSLS

11:40 Macromolecular crystallography - Bob Sweet, BNL

12:00 Characterization using x-ray scattering and fluorescence - Chi Chang Kao, NSLS

12:20 Lunch

Afternoon Sessions: Advanced Detectors for Synchrotron Research

Session Chairman - Franco Manfredi, University of Pavia

1:00 Overview of detector research areas - Rob Lewis, Daresbury

1:30 Gas detectors - Graham Smith, BNL

1:50 High energy resolution superconducting bolometer arrays - Kent Irwin, NIST

2:10 CCD Detectors for Crystallography - Steve Naday, APS

2:30 Coffee

Session Chairman – Veljko Radeka (BNL)

Silicon Pixel Detectors for Crystallography and Other Applications

2:50 Analog systems - Sol Gruner (CHESS)

3:10 Digital systems - Christian Broennimann (Swiss Light Source)

3:30 Integrated systems - Jacques Millaud (LBNL)

3:50 High Energy/Synchrotron Perspective - Erik Heijne (CERN)

Other detectors

4:10 Multi-element Si(Li), Ge and CdTe detectors for EXAFS - Gareth Derbyshire

4:25 Silicon drift detectors - Pavel Rehak (BNL)

4:40 Avalanche photo diodes - Alfred Baron (Spring 8)

4:55 Sub-picosecond streak cameras – Jean-Claude Kieffer (INRS Univ du Quebec)

5:10 Reports on detector needs by synchrotron representatives (5-10 min/speaker)

5:25 Formation of working groups

7:00 - 9:00 - Dinner

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**Courtyard Marriott Embassy Row, "General Scott" Room
Washington, DC, October 30-31, 2000**

TUESDAY, OCTOBER 31, 2000

8:15 Continental Breakfast

Morning Session: Discussion and Writing of Working Group Recommendations

Session Chairman - Al Thompson

8:45 Charge to Working Groups

9:00 First Meeting of Working Groups

10:30 Coffee/cookies Available

10:45 Working Groups continue writing their contribution to roadmap

12:00 Lunch

Afternoon Session "Refining and Discussion of SR Detector Road Map Report"

Session Chairman - Al Thompson

1:00 Brief summary of working group progress - 10 min/group

2:00 Refining of contributions by Working Groups

3:00 Coffee

4:00 Workshop closeout

4:30 End of workshop