TOWARD A FOURTH-GENERATION X-RAY SOURCE *

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Abstract

The field of synchrotron radiation research has grown rapidly over the last 25 years due to both the push of the accelerator and magnet technology that produces the x-ray beams and the pull of the extraordinary scientific research that is possible with them. Three successive generations of synchrotron radiation facilities have resulted in beam brilliances 11 to 12 orders of magnitude greater than the standard laboratory x-ray tube. However, greater advances can be easily imagined given the fact that x-ray beams from present-day facilities do not exhibit the coherence or time structure so familiar with the optical laser. Theoretical work over the last ten years or so has pointed to the possibility of generating hard x-ray beams with laser-like characteristics. The concept is based on self-amplified spontaneous emission (SASE) in free-electron lasers. A major facility of this type based upon a superconducting linac could produce a cost-effective facility that spans wavelengths from the ultraviolet to the hard x-ray regime, simultaneously servicing large numbers experimenters from a wide range of disciplines. As with each past generation of synchrotron facilities, immense new scientific opportunities would result from fourth-generation sources.

1 INTRODUCTION

The rapid growth in the field of synchrotron radiation research over the last 25 years has been the most exciting period in the history of x-rays since the period immediately after they were discovered by Röntgen over 100 years ago. The brilliance of x-ray beams versus time since their discovery in 1895 (Fig. 1) shows that the technology was unchanged for more than six decades. Remarkably, however, x-rays had unprecedented scientific impact. X-rays garnered the first Nobel Prize and some 20 more, all based on x-rays provided by only minor improvements of tubes that Röntgen used for his first experiments. From the first generation of parasitic synchrotron facilities that appeared in the 1970s through the second-generation facilities that were designed explicitly to produce synchrotron radiation, to the third generation that use an optimized magnet lattice and insertion devices, synchrotron x-ray research has enjoyed gains in beam brilliance that are 11 to 12 orders of magnitude greater than the standard laboratory x-ray tube. Given that this rate of improvement exceeds Moore's Law for semiconductors by approximately a factor of two, it is reasonable to ask, What could be a better source of x-rays than the insertion device (ID) upon which the Advanced Photon Source (APS) and other third-generation sources are based?

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2 SOURCE CHARACTERISTICS

An ID x-ray beam from a third-generation x-ray synchrotron radiation facility, while highly directional and monochromatic, does not have the full coherence of an optical laser. The transverse coherence length of radiation from an ID at the APS is ~10 µm, which is useful to condensed-matter physicists and others in understanding the dynamics of solids. However, the coherence length is small compared to the size of the source itself (170 mm), which means the source is only very weakly coherent. Making up for that shortfall represents an enormous opportunity. If the technology can be developed to make a source fully coherent, it would be orders of magnitude better than those existing today.

Another major opportunity to exceed the limits of existing x-ray sources lies with the time structure of the beam. Current machines produce bunch lengths in the 100-psec regime. This structure enables science well beyond the reach of steady-state x-ray tubes, and many experiments exploit this time dependence.

However, 100 psecs is longer than the time associated with many interesting physical phenomena. In the optical

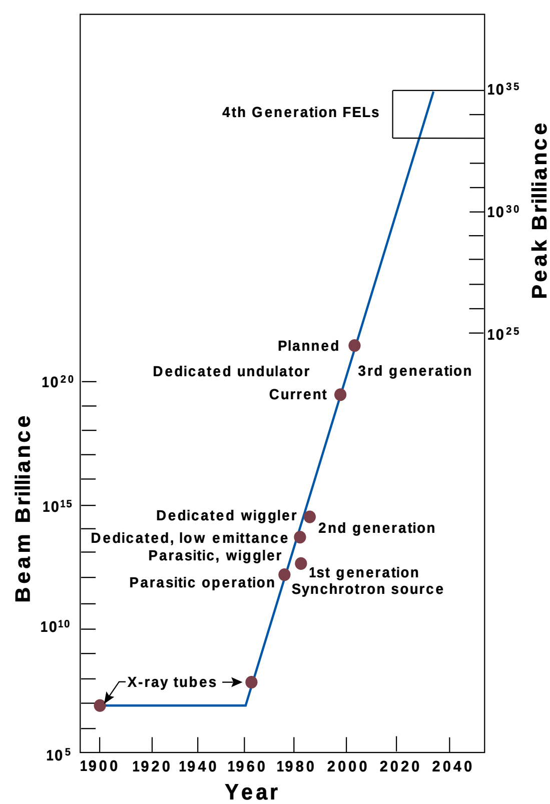

Fig. 1: History of (8-keV) x-ray sources, beam brilliance vs. time.

regime, femtosecond lasers have existed for quite some time and have made the first forays into this time domain. The ability to bring x-ray time scales down into the sub-picosecond regime is very compelling, since many of the most interesting physical phenomena cannot be studied with long-wavelength optical radiation.

3 TECHNOLOGICAL CHALLENGES

It now appears that substantial improvements in source characteristics can be achieved with the development of x-ray free-electron lasers (FELs). The technologies to produce FEL-based radiation for ultraviolet and shorter wavelengths have been under consideration for some time using different accelerator-FEL configurations. At this time, neither the optical cavity approach[1] nor the seeded amplifier concept[2] appears to be workable in the hard x-ray range, although future developments could change this situation. Recently, the concept[3,4,5,6] of self-amplified spontaneous emission (SASE) has captured the imagination of the synchrotron radiation community. The SASE concept eliminates the need for optical cavities or input seed radiation. The very stringent electron beam qualities required for SASE operation in the hard x-ray region can be met with the recently developed laser driven radio-frequency (rf) photocathode gun[7] and in the beam compression and linear acceleration technology in connection with the high-energy linear collider program.[8] Recent measurements by the University of California, Los Angeles group at Los Alamos National Laboratory[9] have shown the first convincing evidence of SASE gain at 16-μm wavelengths.

The Stanford Synchrotron Radiation Laboratory has developed a SASE-based concept[10] called the Linac Coherent Light Source, which would use the Stanford linac and theoretically produce a gain of 8 or 9 orders of magnitude over third-generation undulator beams in the hard x-ray range. This would be an excellent R&D project to supply the necessary experience for a new fourth-generation user facility. And it would be reasonably cost-effective since the linac already exists. However, it would not be sufficient to meet the needs of the synchrotron community at large, because the facility would only support a few experimental stations, at most. This limitation is due to the pulse rates associated with conventional linear accelerators.

A newer alternative, the superconducting linac, is in principle capable of supplying the pulse rate needed to support a farm of x-ray undulators, as shown in Fig. 2. This approach is based upon the anticipated maturity of the superconducting rf technology for the high-energy linear collider program. A group at the Deutsches Elektronen-Synchrotron[11] is pursuing the concept of a superconducting linac that can support the very high pulse rates necessary to feed a large number of SASE undulators for x-rays. Such a facility would also be able to produce ultraviolet beams either at lower energy points on the linac or by using spent electron beams after they have produced the SASE x-rays. Research and development is expected to go forward internationally over the next few years, yielding a decision on whether to proceed with such a facility in conjunction with a new high-energy physics linear collider.

At Argonne National Laboratory, we are installing a low-energy (750 MeV) undulator test line (LEUTL) (Fig. 3) on the APS linac.[12] The LEUTL is located in a 50-m-long extension of the linac tunnel that is configured to enable study of SASE in the 100-nm-wavelength range.

4 SCIENTIFIC RESEARCH

A fourth-generation light source will support a wide range of disciplines and a large number of individual experiments. It is therefore difficult to be specific about the scientific opportunities in a short article. To provide summary information, Figs. 4 and 5 attempt to simply characterize the advances from one generation of light source to the next in terms of our ability to extract spatial and temporal information from material systems, which is the essence of virtually all x-ray research. Focusing on spatial information to begin with in Fig. 4, we can see the

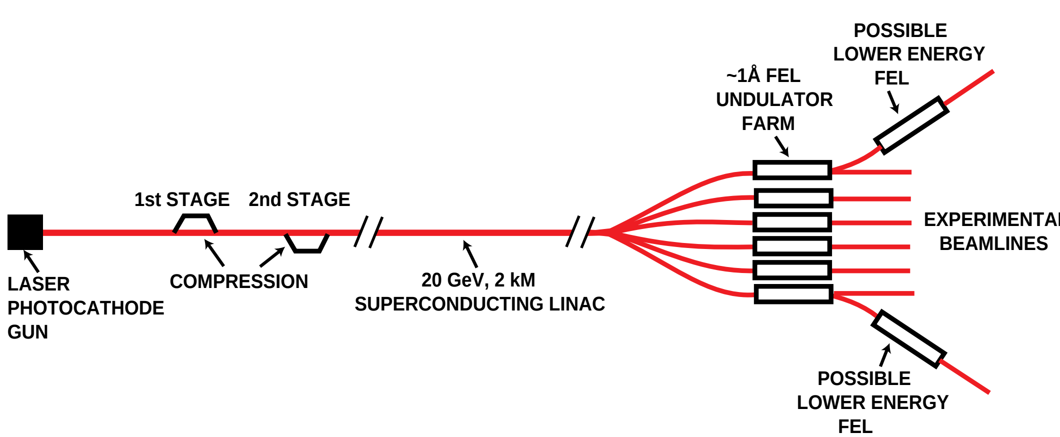

Fig. 2: Diagram of a possible fourth-generation synchrotron facility using self-amplified spontaneous emission free-electron lasers.

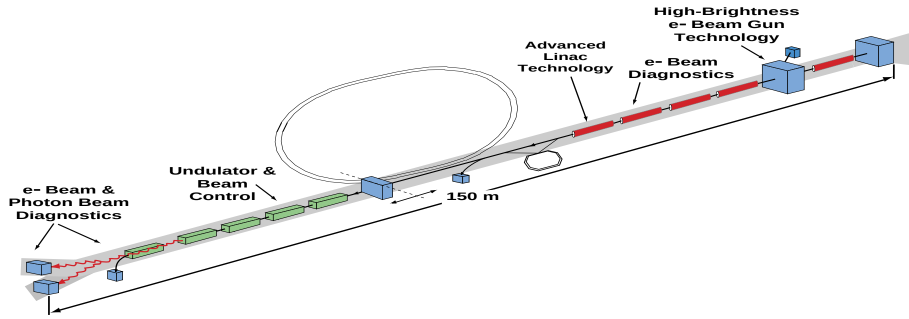

Fig. 3: Drawing of the low-energy undulator test line at Argonne National Laboratory.

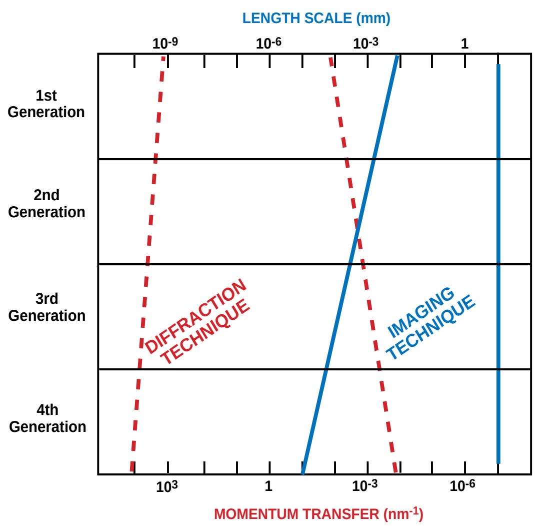

Fig. 4: Research opportunities with synchrotron radiation: spatial structure.

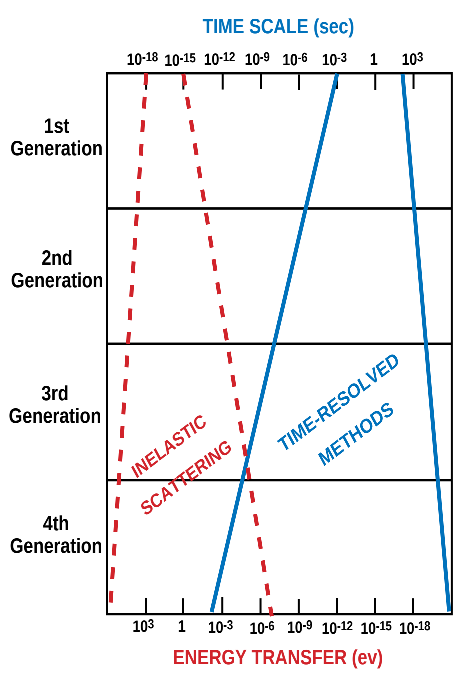

Fig. 5: Research opportunities with synchrotron radiation: temporal structure.

general evolution of imaging methods in direct space or diffraction methods in momentum or reciprocal space. Generally, information on the structure of materials is extracted over a length scale from 1 mm to atomic dimensions. As the brilliance of x-ray beams has improved, higher fluxes, coupled with much higher degrees of collimation, have expanded the boundaries of various diffraction and imaging techniques.

This progress is very tangible now at the APS, where imaging and diffraction methods overlap to cover the entire range of spatial length scales, from the atomic up to the macroscopic, particularly in the 1-μm regime. That is the very important length scale on which information is stored in the human gene, as well as in integrated circuits. For example, protein crystallography is arguably the most challenging area of x-ray diffraction today. Two years ago, the first protein crystal structure solved with the APS was a complex, 100,000-atom molecule.[13] Data sets for proteins of this complexity can now be obtained at the APS in less than an hour, and in some cases less than 15 minutes. With the APS operating 5000 hrs/yr, the possibility of achieving within a decade a storehouse of comprehensive data on all proteins that are important to life seems realistic.

As one looks at the region of Fig. 4 that pertains to fourth-generation sources, there is growing overlap between imaging and diffraction methods. In practice, this overlap actually represents the emergence of integrated imaging and diffraction approaches, which are only possible with highly coherent sources. As an example of what may be possible with the enormous increase in coherence from x-ray FELs, consider how we now obtain information on the structure of complex molecules. The major prerequisite to an x-ray diffraction experiment of the type mentioned above is a crystal in which some 10^{18} copies of the molecule are arranged in a nearly perfect crystalline array. The need for this form of the sample is a consequence, in principle, of the relative weakness of the source of x-rays and the associated scattering cross-section. Furthermore, it is a tremendous burden to the researcher interested in the structure to be required to have such a sample of the molecule of interest. It is now the most significant limitation in the rate of protein structure determination. One of the most compelling aspects of the x-ray FEL source is the possibility to eliminate the need for this form of the sample and to be able to extract molecular structure, using new x-ray holographic methods,[14] from a single molecule or a relatively small number of identical molecules in solution. One cannot underestimate the impact of this evolution on biology and chemistry. It is beyond the scope of this paper to discuss this method further, but this will be the subject of upcoming fourth-generation scientific workshops in the next few years.

The other complementary aspect of x-rays is the ability to extract information on the dynamic structure of materials. Figure 5 shows how information is extracted using direct time-resolved x-ray studies and the reciprocal method known as inelastic x-ray scattering. On early storage-ring sources, these two techniques were separated by many orders of magnitude and their ability to extract information in the very important intermediate regime (millivolts or picoseconds) was essentially non-existent. With better beam sources, this gap has narrowed. On third-generation sources, phonon dispersion curves[15] are studied in order to conduct inelastic experiments that have millivolt energy resolution. Time-resolved experiments are moving into the sub-nanosecond region. Investigations of complex materials, such as proteins, are benefiting from third-generation sources, which allow imaging a high-quality diffraction pattern in the time of a single intense pulse—about 100 psecs.

We now proceed to the area of the Fig. 5 that relates to the fourth-generation sources. Here it is anticipated that the improvements in source characteristics made possible by x-ray FELs will finally lead to the closure of the "dynamics gap" shown in the figure. While this appears to be only a quantitative improvement in the range of the two principal methods, it is actually much more than that because it allows access to the energy range in which most phenomena of interest in chemistry, biology, and the physics of technologically-relevant materials occur. It is not yet clear specifically how experimental methods will evolve to permit the anticipated extensions of resolution. Like x-ray holographic methods discussed briefly above, which are a blend of imaging and diffraction methods, we expect that new approaches will be devised to take advantage of the extraordinary time-structure and peak brilliance of the source. The objective will be to provide movie-like representations of molecular motion at the sub-picosecond level. It is critically important that these new methods provide information in direct space where motion is more naturally related to function, as in catalytic reactions or biological processes. In traditional crystalline solid-state systems where crystal momentum is a good quantum number, inelastic methods are very powerful. But in complex a-periodic systems, real-space methods for elucidating dynamics will be much more readily interpreted. If this challenge can be met, fourth-generation sources will have immense impact.

5 CONCLUSION

One can easily imagine that extraordinary science would result from the use of x-ray sources based on FELs. The higher coherence and greater spatial resolution afforded by FELs, together with a two- or three-order-of-magnitude improvement in time resolution to the 100-fsec range would prove invaluable for determining molecular structures and watching atomic and molecular processes. Furthermore, beyond the examples mentioned above, the high intensities in these short pulses would provide intriguing opportunities for non-linear physics, and perhaps offer powerful new opportunities for applications in microscopy.

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