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Next-Generation Synchrotron Light Sources and Applications Using Their Coherent Properties

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A proposed energy recovery linac (ERL) source at the Photon Factory (PF) is briefly described. The PF-ERL source will not only produce round x-ray beams with an average brilliance of more than two orders of magnitude higher than the 3rd-generation synchrotron light sources, but also offer a high coherent flux and flux density. One of the most important applications of this highly coherent x-ray source is the structural analysis of non-periodic specimens by coherent scattering. We propose a novel method to generate density maps of particular elements in specimens using x-ray coherent scattering and anomalous dispersion near the absorption edges.

Key words: x-ray, synchrotron radiation, energy recovery linac, coherence, coherent scattering

1. INTRODUCTION

The upcoming linac-based synchrotron light sources are expected to have enormous impacts on physical, biological and materials science. These next-generation synchrotron light sources are classified into two categories: x-ray free-electron-lasers (XFELs) utilizing a self-amplified spontaneous emission process (SASE) [1-3] and energy recovery linacs (ERLs) [4,5]. For example, XFELs are now undergoing development at SLAC [1,2], DESY [3] and SPring-8, and ERLs are planned at CHESS [4,5], NSLS and Erlangen.

In 1982 the Photon Factory (PF) went into operation as a dedicated synchrotron light source in Japan. During the past two decades, the number of users per year has rapidly grown from 500 to 2600, and much effort has been directed towards upgrading the storage ring. Due to this effort, PF still has strong competitiveness in the world. There is, however, growing needs for a new light source to keep up with the rapid progress of SR science and technology. Therefore, in recent years, much discussion has been made on candidates for future light sources, and we have come to notice the excellent possibilities of ERL [6]. Although ERL is not as revolutionary as XFEL, ERL beams can be more intense and brilliant than the beams at storage rings. Another advantage of ERL is that we can build many undulators and beamlines at the transport loop section, and smoothly shift the current scientific activities to the new beamlines.

We have also investigated the scientific case for ERLs [6]. For example, time-resolved x-ray diffraction, x-ray photon-correlation spectroscopy (XPCS), x-ray Fourier spectroscopy, x-ray coherent scattering, and x-ray microscopy were considered. Among them, the structural analysis of non-periodic specimens by x-ray coherent scattering [7-10] has drawn much attention, since it has the potential to open up a new era of x-ray science. For example, if the structural analysis of a single molecule is realized, it will have an enormous impact on structural biology [10]. Since this innovative method is still in its infancy, there is much room for expansions and improvements. We have considered a novel method to generate density maps of particular elements in specimens using anomalous dispersion near the absorption edges.

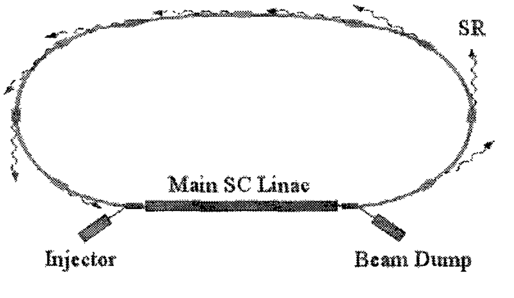

Fig. 1. Schematic diagram of a single-loop ERL consisting of an injector, a main superconducting linac, a transport loop and a beam dump.

Table I. Main parameters for the proposed PF-ERL.

Beam Energy	2.5 - 5.0 GeV
Beam Current	100 mA
Normalized Emittance	0.1 μmrad
Horizontal Emittance	10 pmrad at 5 GeV
Vertical Emittance	10 pmrad at 5 GeV
Bunch Length (rms)	1 ps - 100 fs
RF Frequency	1.3 GHz

Table II. Comparison between PF-ERL and SPring-8 at 8 keV.

		PF-ERL undulator @ 5 GeV		SPring-8 undulator @ 8 GeV	
Beam current		100 mA	100 mA	100 mA	100 mA
Undulator length		30 m	5 m	25 m	5 m
Source size (μm)	horizontal	37.8	18.2	892	892
	vertical	37.8	18.2	22.8	10.6
Source div. (μrad)	horizontal	4.1	9.8	37.4	38.4
	vertical	4.1	9.8	4.3	10
Beam size @ 50m (μm)	horizontal	244	510	2761	2813
	vertical	244	510	236	509
Brilliance ($ph/s/0.1\%/mm^2/mr^2$)		6.0×10^{23}	7.6×10^{22}	2.2×10^{21}	5.0×10^{20}
Flux (ph/s/0.1%)		1.9×10^{16}	3.1×10^{15}	9.0×10^{15}	2.4×10^{15}
Coherent flux (ph/s/0.1%)		3.6×10^{15}	4.6×10^{14}	1.3×10^{13}	3.0×10^{12}
% beam coherence		19	15	0.14	0.13

In this paper, we briefly describe the proposed PF-ERL source, and show a novel method for element-specific structural analysis.

2. PROPOSED PF-ERL SOURCE

Figure 1 schematically shows a simple, single-loop ERL source, consisting of an injector, a main superconducting linac, a transport loop and a beam dump. An electron bunch from a low-emittance electron source is injected into the superconducting linac, and accelerated to high energy (2.5 – 5 GeV). Next, the electron bunch is guided into the transport loop consisting of a series of undulators, which produce very brilliant, high flux beams. The electron bunch is then guided back into the superconducting linac at the decelerating phase (180° out of accelerating phase), and discarded into the beam dump. Due to this one-pass nature of the ERL source, both transverse and longitudinal emittances can be made smaller than those at storage rings. From this basic nature stem the two distinctive advantages of the ERL source: (i) high coherence in both transverse directions and (ii) short x-ray pulses on the order of 100 femtoseconds.

To date, various designs have been proposed for ERL sources. At PF two designs were considered [6]: multi-pass type (Multi-turn Accelerator Recuperator Source, MARS) and one-pass type. The basic machine parameters for the one-pass type PF-ERL are listed in Table I (several parameters are not yet finalized). Table II gives a comparison between PF-ERL and SPring-8 at 8 keV. For calculations, the parameters for the PF-ERL were set at E = 5 GeV and $\varepsilon_x = \varepsilon_y = 10$ pmrad. The parameters for the 30m-undulator were $\lambda_u = 1.6$ cm, N = 1875 and $\beta_x = \beta_y = 20$ m, and those for 5m-undulator were $\lambda_u = 1.6$ cm, N = 312 and $\beta_x = \beta_y = 5$ m. As can be seen from Table II, the ERL source would produce round x-ray beams with an average brilliance of more than two orders of magnitude higher than SPring-8.

The ERL source offers a high coherent flux and flux density in the hard x-ray region (Fig.2). Compared to SPring-8, the average coherent flux per unit area from the ERL source can be 10^2 – 10^3 times higher. Compared to the XFEL sources, such as LCLS and TESLA, the ERL source provides competitive coherent flux densities.

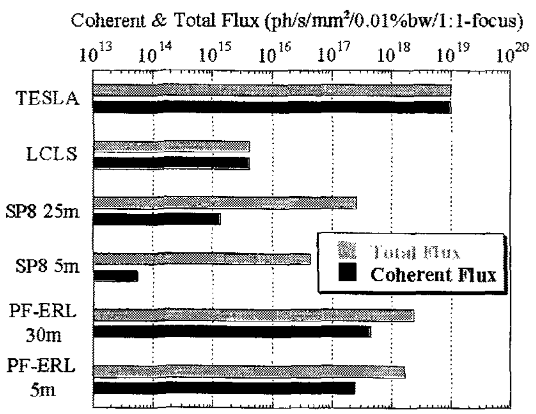

Fig. 2. Coherent and total flux density from various x-ray sources under the 1:1 perfect focusing condition.

3. ELEMENT-SPECIFIC STRUCTUAL ANALYSIS BY X-RAY COHERENT SCATTERING

When a finite specimen is illuminated by coherent x-rays, the scattered x-ray photons produce a continuous diffraction pattern in the far field. By measuring the intensity of this pattern at a spacing finer than the Nyquist frequency, we can recover phase information and reconstruct the specimen image using an iterative algorithm [7-10]. Figure 3 shows an example of a 2D image reconstruction. The pixel-size of the original image shown in Fig.3(a) is 185 x 125, and that of the surrounding zero-valued region is 512 x 512. The oversampling ratio, therefore, is 11.3. Figure 3(b) shows the calculated Fourier transform (oversampled diffraction pattern) of the image. For 2D image reconstruction, an iteration algorithm developed by Gerchberg, Saxton and Fineup (GSF algorithm) [11,12]

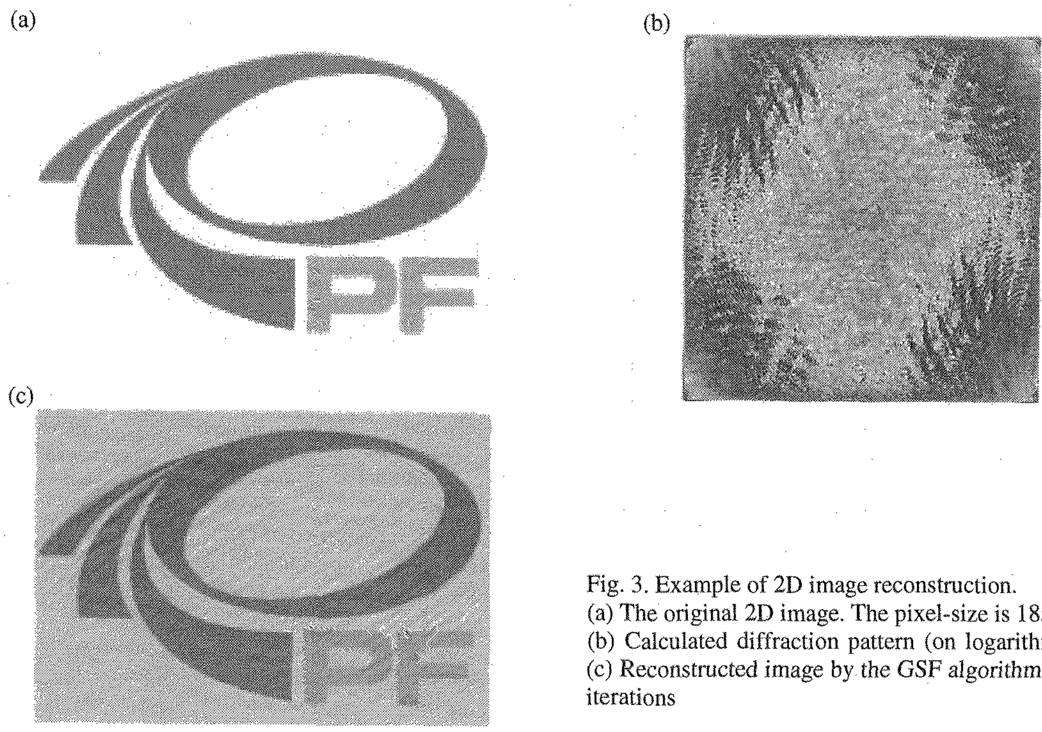

Fig. 3. Example of 2D image reconstruction.
(a) The original 2D image. The pixel-size is 185 x 125.
(b) Calculated diffraction pattern (on logarithmic scale).
(c) Reconstructed image by the GSF algorithm after 3000 iterations

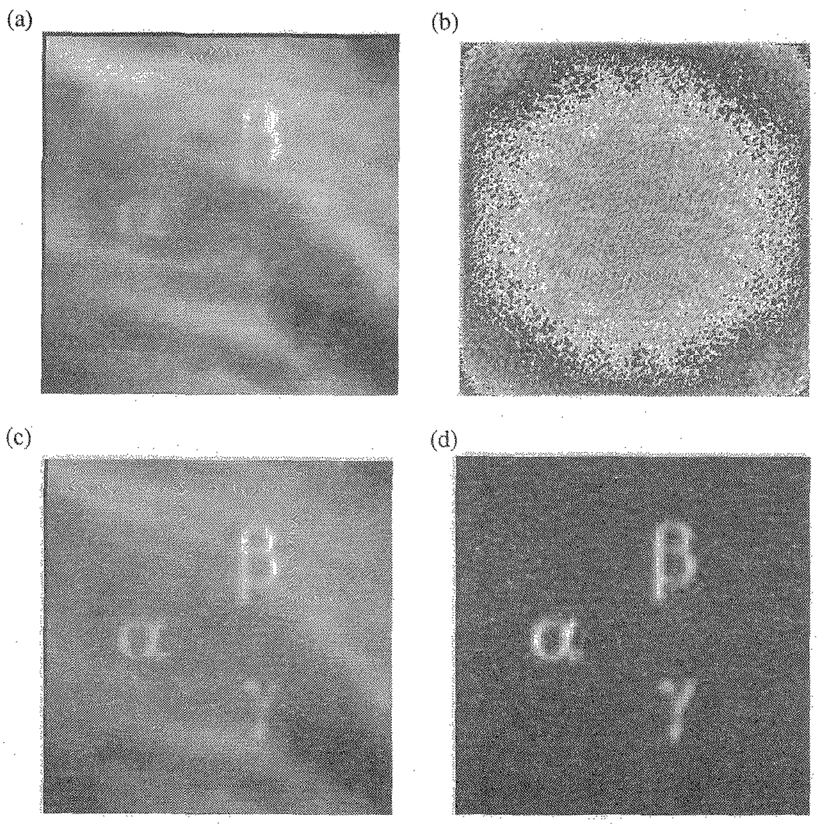

Fig. 4. Example of density reconstruction of a particular element in a specimen. (a) Map of the atomic density in a specimen. The letters "α", "β" and "γ" are composed of gold atoms and the other part is composed of silicon atoms.
(b) Calculated diffraction pattern at 2091 eV (on logarithmic scale). (c) Reconstructed image by the GSF algorithm after 1000 iterations. (d) Density map of the gold atoms obtained from the reconstructed images at 2091 eV and 2194 eV.

was used. After 3000 iterations, a perfect reconstruction was obtained as shown in Fig.3(c). The computing time for 3000 iterations was about 20 minutes on an Athlon XP 2400+ PC.

It is well known that the atomic scattering factor of an element changes around its absorption edges. This opens up a new possibility for generating density maps not only of whole electrons, but also of particular elements. The process of this element-specific structural analysis involves generating electron-density maps at several x-ray energies. The presence of particular elements is indicated by sudden large density changes at absorption-edge energies. Figure 4 shows an example of the density reconstruction of a particular element. In Fig.4(a) the letters "α", "β" and "γ" are composed of gold atoms, and the other part is composed of silicon atoms. The calculated diffraction pattern at 2091 eV (near the Au $M\alpha_1$ absorption edge) is shown in Fig.4(b). Figure 4(c) is the reconstructed image by the GSF algorithm after 1000 iterations. By comparing the reconstructed images at 2091 eV and 2194 eV, the density of the gold atoms was obtained as shown in Fig.4(d). This simulation clearly shows the validity of this method.

4. SUMMARY

In this paper, we briefly described the proposed PF-ERL source, which will offer a high coherent flux and flux density in the hard x-ray region. One of the most important applications of this highly coherent source is the structural analysis of non-periodic specimens by x-ray coherent scattering. Currently, various efforts have been made towards the structural analysis of a single biological molecule. Although there are many problems, such as radiation damage and sample handling, if this ultimate goal is achieved, it will have an enormous impact on structural biology. As a novel application of x-ray coherent scattering, we have proposed an element-specific structural analysis which produces density maps of particular elements in specimens. This method will find applications, for example, in nano-technolgy research.

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