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A BEAM LINE FOR EXPERIMENTS WITH COHERENT SOFT X-RAYS

M.R. Howells*, J. Kirz** and S. Krinsky*

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INTRODUCTION

The ultimate limitation on the perfection of an imaging system is diffraction. For example, if a system has a circular aperture of diameter x , then wavefronts which geometrically should converge to a point, in fact are subject to angular smears x' due to diffraction which cause the point to be imaged as an Airy Function where

$$x' = \frac{2.44 \lambda}{x} \quad (1)$$

(x' is the angular full width of the first dark ring.)

If the system contained only the circular aperture the same angular blurring would occur. In particular a perfect plane wave confined to pass through the circular aperture would also be subject to the angular blurring given by (1). We are thus lead to the following theorem:

$$\epsilon_x \equiv xx' \gtrsim 2.44 \lambda, \quad (2)$$

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where ϵ_x is the x plane emittance of the beam of waves. 2.44λ is thus the smallest emittance beam allowed by diffraction. It is also the largest emittance beam which is coherent within a certain tolerance. For these reasons we are often obliged to use beams of emittance about 2.44λ . Another way to state the situation is that a diffraction limited optical system can only utilize the flux emitted into the coherence angle: usually given as $2\lambda/x$.

For most x-ray applications this is not a limitation because the acceptance of x-ray spectrometers (angular x spatial) is normally much larger than 2.44λ so that much higher emittance beams can be accepted without loss. However, for a certain class of experiments which depend on the creation of very small spots (microprobes¹) or diffraction limited spots (microscopy, holography and soft x-ray diffraction) the limitation is extreme. An example will make this clear. Suppose we wish to make a diffraction limited spot with $30 \text{ \AA}$ x-rays. Equation (2) gives the value of ϵ_x we need as

$$\epsilon_x \approx 72 \text{ \AA} \cdot \text{rad} \equiv 7.2 \text{ mr} \cdot \mu\text{m}.$$

We conclude that for a 300μ source our collection angle $= 7.2/300 =$ 0.024 milliradians! For such small collection angles the extra brightness provided by undulators is crucial.

In this report we address the scientific motivation for this type of beam line, the nature of the source required and the general design of the beam line and its optical system.

SCIENTIFIC MOTIVATION

What we know about biological structures comes partly from morphological, and partly from biochemical evidence. For features too small to resolve optically, ($<2500 \text{ \AA}$), our main source of morphological information is the electron microscope. This instrument has superb instrumental resolution; however, for the study of biological specimens, it presents a number of problems.

1. Because the electron column must be under vacuum the specimen must be dehydrated, freeze-dried, or kept in a complex environmental chamber.²

2. Most biological specimens have low inherent contrast under the electron beam. Therefore, they are commonly treated with heavy metal stains to bring out features of interest. This staining process may introduce artifacts, and may complicate the interpretation of electron micrographs.³

3. The electron microscope is not suited for the examination of specimens more than a few μm thick.⁴

4. Radiation damage to the specimen due to the electron beam often leads to destruction of the feature to be observed before the observation is completed. Careful analysis of the electron microscopy of unfixed specimens identifies radiation damage as the ultimate limitation on obtaining high resolution.⁵ In fact, few such specimens yield detail finer than $1000 \text{ \AA}$.

It seems clear, therefore, that a less damaging probe is highly desirable, especially if it would not require vacuum or dehydration, could provide contrast without stains, and allowed flexibility with respect to specimen thickness.

Soft x-rays promise all this.⁶ In particular, the wavelength band between the oxygen and carbon absorption edges is particularly suitable for image formation by differential absorption. The characteristic absorption length is typically 0.5 μm in organic matter, about six times longer in water, and several mm in air or helium at 1 atmosphere. Contact microscopy and zone plate microscopy have already demonstrated the power of soft x-rays in imaging biological specimens. Radiation damage to the specimen can be kept to a minimum if the x-rays incident on the specimen are fully utilized. Optimum utilization is achieved in the scanning geometry, where a flow proportional counter detects practically all transmitted quanta. This is the method presently used by the x-ray microscope on beam line U15. Its resolution is limited by the smallest x-ray spot that can be formed.

The U15 microscope is the first of its kind, and is soon expected to demonstrate high resolution imaging with bending magnet radiation. However, as the resolution improves, the time required to make a micrograph of a given specimen area increases with the inverse square of the resolution. With undulator radiation the microscope will gather high quality biological information about three orders of magnitude more rapidly, and there is little doubt that in that case high resolution microscopy would become a matter of routine. We must now ask what will then be the limit on the morphological information obtained and what should be the next step?

The primary limitation of the scanning x-ray microscope (shared by all transmission x-ray and electron microscopes) is that it measures a two-dimensional projection of a three-dimensional density distribution. This is limiting enough at low resolution where it is at least possible to maintain the sample thickness at about one or a few pixels and try to cut serial sections to get some three-dimensional information. As resolution improves

this strategy rapidly loses its effectiveness and one faces a serious loss of structural information due to the fundamentally two dimensional nature of the image. The natural response to this is to turn to three-dimensional imaging techniques such as holography.⁹⁻¹² This is particularly compelling for x-ray microscopy since for the very large f numbers involved in x-ray optical systems one does not have the option of utilizing very short depths of focus as can be done in the visible.⁸ The advantage of holography is that all layers in the sample are simultaneously imaged onto the two-dimensional detector and one can extract the information layer-by-layer during the reconstruction process. Not all holographic geometries are equally good in this respect and a great deal of study has been given to choosing the best arrangement.¹³ Present indications are that the best approach will eventually turn out to be Fourier Transform Holography. However, we expect that our policy on an undulator beam line will be guided by experiences on U15 and it is not our purpose to discuss this in detail here. However, we do note that recording a hologram is fundamentally more difficult than recording a two-dimensional micrograph of the same spatial resolution because of the increase in the number of pixels and the introduction of coherence length requirements.

An alternative approach to three-dimensional imaging has been proposed by D. Sayre.¹⁹ In his scheme a crystallographic approach is used. The entire sample is considered to be the unit cell and diffracted rays are detected over essentially the entire 4π solid angle. Various methods are under study for determining the phases of the diffracted waves. Once this is done the diffraction pattern is readily inverted by the standard computational procedures of crystallography to give the three dimensional "optical density" distribution of the sample.

OPTICAL REQUIREMENTS

These may be stated as follows:

Scanned Image X-Ray Microscopy

- Wavelength range 15-50 Å with 30 Å running very popular.
- Monochromator resolving power ~ 100 .
- X-ray focal spot produced by a zone plate "lens". Spot size determines resolution. Goal is few hundred Å. Zone plate must be coherently illuminated thus a beam of emittance $\sim 2.44 \lambda$ is required.

X-Ray Holography (Fourier Transform Geometry)

- Same as scanned image microscope except resolving power needs to be high - goal of 2000-3000.

X-Ray Holography (In Line Fraunhofer Geometry)

- Same wavelength range and resolving power as Fourier Transform case.
- Small spot not necessary if high resolution detector (e.g. resist) is used.

Soft X-Ray Diffraction

- Same wavelength and coherence requirements as holography.
- Small spot not necessary.

SOURCE PARAMETERS

It is proposed that an undulator with the following parameters be used:

PROPOSED UNDULATOR PARAMETERS

Period	7.5 cm
Number of Periods	40
(Total Length)	(3 m)
Range of K Values	0.5 - 1.4
Tuning Range of First Harmonic	17.6 - 30.9 Å
Gap	Adjustable, always > 4 cm
Magnetic Field	0.7 - 2.0 kG
Magnetic Materials	Rare Earth Cobalt Plus Iron
Mechanical Layout	External to Vacuum Vessel, Always Outside Beam "Stay Clear Region"
Character of Source Region	Low Beta
e- Beam Parameters at Source Center	$2\sigma_x = 0.6 \text{ mm}$ $2\sigma_y < 0.10 \text{ mm}$ $2\sigma_x' = 0.48 \text{ mr}$ $2\sigma_y' = 0.1 \text{ mr}$
Effective Source Size Allowing for "Depth Broadening"	$2\sigma_x = 1.0 \text{ mm}$ $2\sigma_y = 0.20 \text{ mm}$
Approximate Angular Width of Source output	Horiz: $2\sigma_x' \sim 0.5 \text{ mr}$ Vert: $1/\gamma \sim 0.2 \text{ mr}$

The detailed mechanical and magnetic design are presently under study but it is possible to make some general statements. First, the NSLS x-ray ring lends itself very easily to the operation of soft x-ray undulators. No stringent requirements are imposed on the beam nor is any difficult magnet or vacuum technology involved. Second, an undulator on a storage ring is by far the brightest soft x-ray source presently available. Eventually, one may have lasers which are superior in time structure and in both transverse and longitudinal coherence. However, these are not conveniently available at present.

Figure 1 shows the angle integrated spectral output of the proposed undulator for various K values. Although the intended beam line geometry will certainly not integrate over angle, the observed output will be similar to Fig. 1 because of the spectral smearing caused by the spread of directions in the electron beam at a low beta insertion. This apparently deleterious effect does not, in fact, cause a loss of brightness as compared to a high beta insertion.¹⁴

To get an idea of the suitability of this source for producing a diffraction limited beam, we show in Fig. 2 the coherent power¹⁵ (power emitted into the coherence angle) as a function of wavelength for this and various competitive sources. We see that the new source will supply four orders of magnitude more coherent power than a VUV ring bending magnet for equivalent levels of storage ring performance. In addition, assuming the source plus beam line are working at the same percentage of ideal performance that U15 now is, we find that we have seven orders of magnitude more coherent power than was used in making the best x-ray holograms so far achieved! This is certainly cause for optimism.

BEAM LINE DESIGN

The design rules for creating a diffraction limited beam are considerably different than for a normal beam. Generally speaking this is helpful and combined with our modest needs with regard to wavelength coverage should lead to a beam line design which is at once, simple, inexpensive and reliable. The most challenging aspect is to achieve a resolving power such that the coherence length $\ell_c (= \lambda^2 / \Delta\lambda)$ will be sufficient to coherently illuminate an interesting biological structure. It is generally agreed⁹ that ℓ_c should be about 5-10 μ . For $\lambda = 30 \text{ \AA}$ this requires a resolving power of 2000-3000.

The general strategy will be to use a conventional diffraction grating system for the high resolution part and conical diffraction¹⁶ for the low resolution part. This realizes a greater gain in intensity than just the enlargement of the band pass. A diffraction limited beam in the soft x-ray region can be collimated to a high degree whilst still maintaining a small spatial extent. This suggests the use of monochromator designs which depend on collimation for their spectral selectivity. A suitable type is the double grating design described by Hunter¹⁷ and by Howells.¹⁸ The simplest form of this using only pinholes as collimators and focussing elements is shown in Fig. 3 for a standard replica grating. Some performance parameters for this configuration are displayed in Table 1. Because of the narrow beam one can design a single axis rotation system that would enable this monochromator to be engineered very simply. This is shown in Fig. 4. We see that the scheme is well matched to the size of zone plate that one would probably want to illuminate and shows promising resolving power. Some further study is needed to try to reduce the overall length and increase the number of illuminated grooves.

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TABLE 1

PARAMETERS OF DOUBLE GRATING MONOCHROMATOR, TELESCOPIC CONFIGURATION

 PINHOLE WIDTH= .1 MM
 DIVERGENCE= .02 MR
 P' HOLE/GRATING DIST= 5000 MM
 EXIT APERTURE WIDTH= .2 MM
 EXIT APERTURE DIST= 10000 MM
 GRATING BLAZE= 1 DEG
 GROOVE DENSITY= 1200 GR/MM

λ (A) E(EV) α (DEG) δ (DEG) DISP
(A/MM)

10	1240	89.0298	87.0298	.011
12	1033	88.6356	86.6356	.014
14	886	88.2412	86.2412	.017
16	775	87.8468	85.8468	.021
18	689	87.4521	85.4521	.024
20	620	87.0573	85.0573	.027
22	564	86.6623	84.6623	.030
24	517	86.2671	84.2671	.033
26	477	85.8717	83.8717	.036
28	443	85.4761	83.4761	.039
30	413	85.0801	83.0801	.042
32	387	84.6839	82.6839	.045
34	365	84.2874	82.2874	.048
36	344	83.8905	81.8905	.051
38	326	83.4934	81.4934	.053
40	310	83.0958	81.0958	.056
42	295	82.6979	80.6979	.059
44	282	82.2996	80.2996	.062
46	270	81.9008	79.9008	.065
48	258	81.5016	79.5016	.068

λ (A) $\cos^2 \alpha$ WIDTH WIDTH ANGLE
 ----- EXPO- NEEDED TO
 $\cos^2 \delta$ SED MM HORIZ(2 σ)
 MM (DEG)

10	.1068	5.91	.58	3.940
12	.1646	4.20	.80	4.729
14	.2192	3.26	.99	5.518
16	.2691	2.66	1.15	6.306
18	.3143	2.25	1.27	7.096
20	.3550	1.95	1.38	7.885
22	.3917	1.72	1.46	8.675
24	.4248	1.54	1.53	9.466
26	.4547	1.39	1.59	10.257
28	.4819	1.27	1.63	11.048
30	.5067	1.17	1.67	11.840
32	.5293	1.08	1.70	12.632
34	.5501	1.00	1.73	13.425
36	.5692	.94	1.75	14.219
38	.5868	.88	1.77	15.013
40	.6032	.83	1.79	15.808
42	.6183	.79	1.80	16.604
44	.6324	.75	1.81	17.401
46	.6455	.71	1.82	18.198
48	.6578	.68	1.83	18.997

λ (A) BEAM RES'N RES
 WIDTH (ANG) POW'R
 (MM)

10	1.3396	.014247	702
12	.8827	.012459	963
14	.6769	.011792	1187
16	.5648	.011644	1374
18	.4964	.011783	1528
20	.4514	.012100	1653
22	.4201	.012536	1755
24	.3976	.013058	1838
26	.3808	.013643	1906
28	.3680	.014276	1961
30	.3580	.014947	2007
32	.3501	.015648	2045
34	.3438	.016373	2077
36	.3387	.017119	2103
38	.3344	.017883	2125
40	.3309	.018660	2144
42	.3280	.019450	2159
44	.3256	.020251	2173
46	.3235	.021061	2184
48	.3218	.021879	2194

Suggested undulator for microscopy/holography/ soft x-ray diffraction

FIG 1

PRESENTLY PROPOSED UNDULATOR WITH $K=1$

FIG 2

Fig 3.

Grating pair in two positions

(a) $\lambda = 15 \text{ \AA}$ $\theta \sim 4^\circ$: RAY arrowed grating pair dotted

(b) $\lambda = 45 \text{ \AA}$ $\theta \sim 10^\circ$: RAY not arrowed grating pair not dotted.

Gratings are rigidly fixed to each other and rotation is about O
One can show that:

$$S = 2D \cos \theta$$

For the case shown ($D = 10 \text{ mm}$)

$$S(45^\circ) - S(15^\circ) = \Delta S = 255 \text{ \mu m}.$$

which is quite small and can be made smaller by considering lower values of D and smaller ranges of wavelength

Fig 4.