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Feasibility of Single-Atom X-ray Fluorescence Imaging from an Energy Recovery Linac Source of Synchrotron Radiation

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Summary

We have researched the problem of using X-Ray Fluorescence to perform single-atom imaging and spectroscopy studies, both in free-standing samples and in detecting individual impurity atom dopants in wafers of silicon. Using numbers corresponding to currently available synchrotron radiation sources such as the ESRF, we found that it is all but impossible to presently image single-atom sized samples, with only one impurity fluorescent photon entering a detector every ten seconds, on average. The minimum mass-detection capacity of existing sources such as ESRF is calculated to be around 2.5×10^{-19} grams or about 1000 atoms with present day beamsizes of order 1 micron.

However, using predictions of a nanoprobe beam line on a possible Cornell University Energy Recovery Linac (ERL), with 1 nm beam size and an incident flux of 2.5×10^{12} x-rays/sec at 10 keV, we have calculated that the signal to a solid state detector from one single fluorescing Erbium impurity atom would be 2.6×10^{6} photons/second on top of a background of 3.2×10^{6} photons/second from Compton scattering from a 100 nm thick wafer. With these high count rates we believe it will be not only possible to spatially locate single impurity atoms in a relatively bulk portion of a silicon wafer to nm resolution, but also to spectroscopically examine their near neighbor environment with XANES or EXAFS and to determine whether they are electrically active or not. This may be very useful to researchers pushing the nanofabrication of circuits to the fundamental limit of an atom size.

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Introduction

X-ray fluorescence is a powerful tool for quantitative chemical analysis and spectroscopy. X-rays can be used to ionize the inner electrons of an atom in a material and when the atom returns to the ground state, it emits characteristic x-ray radiation characteristic of its atomic number and chemical state. With microbeams from present 3rd generation x-ray sources, the presence of as few as 1000 high-z atoms can be detected in a beam size of order 1 micron in diameter.

In this study we explore how much more the sensitivity can be improved when more powerful sources of microbeam x-rays are considered, such as from a Energy Recovery Linac source of synchrotron radiation when detected by a standard energy-dispersive solid-state detector.

To demonstrate the potential resolving power of high-intensity X-Ray sources through X-Ray fluorescence, we have undertaken a calculation below to demonstrate the theoretical detection limits with current X-Ray sources. To evaluate the practical consequences, we put in some of the parameters of the one of the premier microbeam stations of ID13 at the European Synchrotron Radiation Facility (Grenoble, France) and then extended the argument to the Energy Recovery Linac being proposed for Cornell University.

We have examined only the effects produced by the particular energy of radiation that will prove useful in the particular element that we are trying to image; the full brilliance curve of a particular synchrotron source will contain a distribution of energies with varying source intensities at different energies, but the energies very far from the particular absorption edge of our element of interest will not concern us much as we calculate the signal-to-background ratio for x-ray sources after a single-crystal or multilayer monochromator to try to better optimize the excitation of fluorescence. Since the limiting quantity in any fluorescence-detection experiment is ultimately the photon flux at our detector, we proceed below to calculate the photon flux through to a detector with assumed parameters from a microbeam x-ray source and apply it to ESRF and ERL situations.

Mass-Detection Limits

Let us say that we have an incident beam which has a flux of I_o photons/second through a area, A, on the surface of our sample. The quantity of flux that is lost as the beam goes through a certain thickness of the sample is proportional to the depth into the sample:

$$dI/dx = -\mu x \qquad (1)$$

I is the flux through a plane at depth x into the sample, and μ is a constant called the photon attenuation coefficient. μ is, in general, a function of the energy of the incident radiation and the element that is being subjected to the radiation. Equ. (1) is a simple first-order differential equation, with the general solution:

$$I = I_o \exp(-\mu x) \qquad (2)$$

I_o is the flux impinging on the surface of the sample and exp(x) is the natural exponential function. Equ. (2) describes the flux at any depth into the sample. However, we are not interested in the flux at any point in the sample; we are more interested in the quantity of x-rays that *do not make it* to that particular point in the sample. The x-rays that do not make it to a particular point in the sample those that are either absorbed by the sample through photoelectric interactions, or scattered by the matter via Compton and Rayleigh scattering effects. Scattering effects may be neglected when we are considering the amount of photon flux (i.e. useful signal) produced at the detector, but they are very important when we begin to examine the background noise that makes its way to the detector. For this derivation, however, we shall ignore scattering effects and shall at the end supply a separate calculation (see Appendix A) of the relative strength of Compton scattering.

The quantity of light that is absorbed through photoelectric absorption into the sample (and therefore the number of atoms that are put into an excited state), therefore, is equal to:

$$I = I_o(1-\exp(-\mu x)) \qquad (3)$$

. Not all of these excited atoms will yield fluorescent photons; some will yield free electrons and thus not contribute to our useful signal in a solid-state detector. The proportion of excited atoms that yield fluorescent photons is a unit less ratio called the photoelectric yield , denoted by ϖ (where $0<\varpi<1$).

$$I_f = I_o\varpi(1-\exp(-\mu x)) \qquad (4)$$

Equ. (4) describes the total number of fluorescent photons emitted by our sample per unit time. However, a detector of entrance area A2 that is a distance R away from the samplest will never be able to capture all of these liberated fluorescent photons. The the fraction of them intercepted is proportional to Ω, the ratio of the surface area of the detector. The fraction of the fluorescence intercepted is this solid angle divided by4π Thus the flux of fluorescent photons to the detector is:

$$I_d = I_o\varpi^*(\Omega/4\pi)^*(1-\exp(-\mu x)) \qquad (5)$$

Now, to determine our detecting limits, we assume that we have some sort of minimum count rate at the detector I_m, below which our detector cannot effectively obtain data. Then we can solve for the "thickness" x of the sample that will give us something useful in terms of flux through the detector and thus we will have a practical mass-detection limit. We know the area of the beam impinging on the sample, and we know the density of the material that we are trying to image (presumably), so we can find the minimum mass (since mass is equal to density times volume, or density times area times thickness) that can be resolved through this method. To facilitate the extraction of the thickness x through this, we can make a simplifying assumption that (μx) is a *small* quantity for thin samples. Therefore, by Taylor's theorem:

$$\exp(-\mu x) \cong 1 - \mu x \ldots \qquad (6)$$

and plugging (6) back into (5), we finally have:

$$I_d = I_o\varpi^*(\Omega/4\pi)^*(\mu x) \qquad (7)$$

Rearranging and solving for x gives us:

$$x = 4\pi I_d/(I_o \varpi \Omega \mu) \quad (8)$$

The mass-detection limit(MDL), therefore, will be equal to:

$$MDL = 4\pi I_d A\rho/(I_o \varpi \Omega \mu) \quad (9)$$

where A is the area illuminated by the beam (the beam spot size) and ρ is the density of the material being studied. Note that the parameters over which the experimenter has control is that of the incident beamsize, incident beam intensity, and the detector solid angle.

As a direct example to show the range of mass detection possible even with current technology, let alone future x-ray sources such as the Energy Recovery Linac, we have below done a direct calculation with currently available x-ray source brilliances (as available at beam ID13 of the ESRF).

The particular element that we wanted to examine was Erbium (atomic number 68, with fluorescence in the 6.9 to 9.0 keV range), which, for now, I will assume is a freestanding sample . The necessary parameters for this particular calculation are the incident intensity $I_o = 10^{10}$ photons/sec, the beam size A = 1 μm^2, ρ = 9.066 g/cm^3, and an assumed minimum detector intensity I_d = 10 photons/sec. Erbium has it's L-absorption edge (that is, the highest energy which will excite electrons out of the L-shell) at 9.75 keV[1], so a good energy to choose for our incident radiation is 10 keV. The mass-attenuation coefficient at this energy is $(\mu/\rho) = 269.4\ cm^2/g^2$. Erbium's fluorescent yield for its L-shell electrons is $\varpi = .2410$[3]. The particular detector that was employed subtended a solid angle of $\pi/4$ steradians (detector had a circular face of 5 mm diameter located at a 10 mm distance from the sample).

Therefore, the thickness limit obtained was 2.718×10^{-11} cm. The area illuminated was 1 μm^2, or $10^{-8}\ cm^2$. The volume limit on the sample, therefore, is $2.718 \times 10^{-19}\ cm^3$. Multiplying this by the density gives us the mass-detection limit, or 2.46×10^{-19} g.

To find out how many atoms this corresponds to, we can merely divide this mass by the mass of an individual Erbium atom. The mass of an individual Erbium atom, in grams, is obtained by taking the mass of one mole of Erbium (167.26 g) and dividing by Avogadro's Number ($N_A = 6.022 \times 10^{23}$). Performing the calculations allows us to obtain the number of atoms that can be resolved by this method as being 8.8×10^3 atoms.

If we were to try and decrease the resolving limits, one of the first and easiest things to do would be merely to increase the solid angle of the detector. If we were to have a detector that completely encompassed one side of the sample, it would subtend a solid angle of 2π steradians. This would be an increase in Ω by a factor of 8, or therefore a corresponding decrease in mass-sensitivity and atom-sensitivity by the same factor of 8. The atom-sensitivity would now decrease to 1.1×10^3 atoms. This is quite small.

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[1] Various Authors, X-Ray Data Booklet, (2001), < http://xdb.lbl.gov/ >, Section 1.2

[2] Hubbell, J.M. and S.M. Seltzer, Tables of X-Ray Mass Attenuation Coefficients and Mass-Energy Absorption Coefficients, (1996), < http://physics.nist.gov/PhysRefData/XrayMassCoef/cover.html >

[3] Table of Fluorescence Yields, < http://www.seismo.berkeley.edu/geology/labs/epma/fluoresc.htm >

Further decrease of the detection limits would easily be accomplished by examining what will directly be possible with the proposed Energy Recovery Linac. With data from Appendix B, we can see that, with the ERL as our x-ray source, we can now create beams with 2.5×10^{12} photons/second with a spot size of 1 nm^2. With such a source (and a 2π steradian detector solid angle), we can achieve mass detection limits of 7.70×10^{-27} grams. This is actually well below the mass of one Erbium atom (which is of the order 10^{-22} grams), so the fluorescent x-ray flux received from a single atom with the ERL source would be more than enough to get a decent image.

Single-Atom Dopant Imaging

In a recent AEP seminar (February, 2002), Dr. Paul Voyles from Bell Laboratories gave a talk about imaging the location of a single Sb atom in a 20 Angsgrom layer of silicon (work being written up for publication) with an electron beam. It caused us to ask if we could do the same thing with x-rays, but now in a more bulk-like situation when we have have a "thicker" sample and all the tools that have been developed in during the last 100 years of x-ray science.

As we will see below, it may not only be possible to image the location of a single atom, but also to perform spectroscopy on a single atom to determine its local chemical environment (from the near edge XANES and the extended EXAFS region of the absorption curve). This has interesting consequences for semiconductor electronics circuits, for instance, that are pushed to the ultimate nm dimension. We will have the spectroscopy tools to diagnose which dopants are electrically active and which are not - thus an ERL x-ray nanoprobe may open new opportunities in this arena of semiconductor research.

To focus in on single atom image, let us now take another example, somewhat distinct from the general case of the first that was discussed above. Let us assume that we have a single Erbium atom embedded in a thousand-angstrom thick layer of Silicon. What will be the fluorescent output flux? Now, we have a situation that is more easily analyzed somewhat differently than the analysis shown above. If we have a single atom and we are shining light of a particular color onto it, then the amount of flux that is absorbed through any particular interaction (for example, the photoelectric interaction) is given by the product between the incident *intensity* (defined as flux per unit area, general units of energy or photons/unit area/unit time) and the *cross-section* of the atom for that particular interaction. Therefore, the amount of flux that is absorbed by a single atom via the photoelectric interaction, let us say, is given by the incident flux times the *photoelectric cross section* of that particular atom at that particular energy. The total cross section (photoelectric + scattering) can, of course, be obtained from the photon attenuation coefficient and vice versa (this will be discussed later as necessary). Now, our expression for the fluoresced intensity changes somewhat. I will state the new formulation below and discuss the ramifications of the change and how it makes things easier to discuss things in this new notation. The fluorescent flux is given by:

$$I_f = I_o \varpi \sigma_{pe} / A \qquad (10)$$

In this formulation, however, I_f and I_o are the fluoresced and incident *flux*, and A is the size of the beam (thus, I_o/A is the *intensity* of the incident beam), and σ_{pe} is the photoelectric cross-section of the particular atom that is being studied. ϖ, the fluorescent yield, plays the same role that it played before, as a factor describing the number of fluorescent photons produced per excited atom. Now, since this atom of Erbium will be embedded in a layer of silicon, the intensity at the atom will be attenuated beyond the intensity at the surface. This attenuation can merely be factored in using a factor of $\exp(-\mu x)$, just as was derived in equations (1) and (2). However, the μ is the pho-

ton attenuation coefficient for Silicon, *not* the coefficient for Erbium, since the intensity is being attenuated through the Silicon substrate, not through the Erbium. The total path length of light from the point of entry into the silicon layer to fluorescing at the Erbium atom to leaving the silicon layer, will be (on average) equal to a little more than the thickness of the layer. Therefore, we can say that the total output flux from the sample will be:

$$I = I_o \varpi \sigma_{pe} \exp(-\mu t)/A \qquad (11)$$

Once again, to find the amount at the detector, we multiply by the factor incorporating the solid angle of the detector:

$$I_d = I_o \varpi^* (\Omega/4\pi)^* \sigma_{pe} \exp(-\mu t)/A \qquad (12)$$

With the source figures given above, $I_o = 10^{10}$ photons/sec, $(\Omega/4\pi) = ½$, $\varpi = .2410$, $A = 10^{-8}$ cm^2, $t = 10^{-5}$ cm, μ (Si) = 78.9637 cm^{-1}, and σ_{pe} (Er) = 8.58×10^{-20} cm^2. (All figures are for an energy of 10 keV). The obtained I_d here is .01, which is well below one photon per second. However, the useful information that can be shown from this is that, ignoring effects from background, a thousand fold increase in intensity will enable us to successfully perform single photon imaging (since we need an I_d of 10 cps). This supports the assertions found by the first calculation performed above, which seemed to indicate that we could resolve objects as small as 1000 atoms with the ESRF source intensities that we were using above.

Employing the ERL source figures that are calculated in Appendix B, with $I_o = 2.5 \times 10^{12}$ photons/sec, $A = 10^{-14}$ cm^2(a 1 nm beamsize created with assumed perfect optics), and all other factors the same, we obtain the photon count per second at the detector $I_d = 2.58 \times 10^6$ photons/second. As you can see, this will easily be more than enough flux to get an excellent image quickly. The criterion that had been stated before was a 10 photon per second signal at the detector to get an image in a reasonable time. In Appendix A (please reorder the Appendicies as you have B coming before A) the Compton scattered count rate from the 100 nm silicon thickness is almost identical to the fluorescent count rate.. (This is not a problem, just count for a slightly longer time). Thus we conclude that it is within the realm of possibility to do x-ray fluorescence imaging and spectroscopy on a single Er atom impurity in a 100 nm thick silicon crystal.

Acknowledgements: This report summarizes some of the independent study (with Don Bilderback and Rong Huang) for an Applied and Engineering Physics 490 course taken by Soumendra Banerjeee during the Spring semester, 2002.

Appendix A. Quantitative Estimate of Background Due to Compton Scattering

Quite possibly the most important factor demonstrating the validity and usefulness of any experimental technique is the effective amount of information yielded by the experiment in a unit time. Above, we have stated that the amount of information that is derived from the X-Ray Fluorescence setup for imaging a dopant in a silicon lattice is equivalent to the number of fluorescent X-Rays that make it to the detector in a given amount of time. However, this is not exactly the full story. This would be true if the only X-Rays that impinged upon the detector at any given time with energy equal to the L-emission energy of Erbium were, in fact, fluorescent X-Rays. However, the effects of inelastic (Compton) scattering can shift the energies of incident photons to near the energy of the fluorescent photons, to such a degree that the fluorescent photons cannot be distinguished from the incident photons. If this were to happen, then it would be significantly more difficult to detect the actual substance within the substrate. Also just as important is the count rate that the solid state detector must count. In most situations, the detector must count all the x-rays (fluorescent + Compton). The detectors have count rate limitation so the minimum detectable limit is determined not only by the count rate of the desired signal, but also by the count rate of the Compton scattering.

In this appendix, we first review the process of Compton scattering and then estimate the Compton count rate in the detector to the desired fluorescent count rate for the ERL situation where one erbium atom is located in a 1 nm diameter microbeam crossing a 100 nm thick pure silicon wafer.

Inelastic scattering, also known as the Compton effect, is caused when photons strike "free electrons" in a piece of matter. Electrons that are reasonably far away from the nucleus, or have reasonably low binding energies compared to the energy of a given incident photon, can essentially be thought of as free electrons in space. It is assumed that these electrons are, essentially, at rest before being struck by the incident photons. Therefore, when a photon collides with one of these electrons, the collision will obey the familiar laws of mechanics: conservation of momentum and conservation of energy. Employing the DeBroglie relations for the momentum and energy of a photon:

$$|\mathbf{p}| = h/\lambda \qquad (13.1)$$

$$E = h\nu = hc/\lambda = |\mathbf{p}|c \qquad (13.2)$$

and, of course, the familiar (non-relativistic) expressions for Kinetic energy and momentum of the electron:

$$\mathbf{p} = m\mathbf{v} \qquad (14.1)$$

$$E = \tfrac{1}{2}m|\mathbf{v}|^2 \qquad (14.2)$$

it is possible to derive the Compton equation:

$$\lambda_2 - \lambda_1 = (h/mc) \times (1 - \cos\varphi) \qquad (15)[4]$$

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[4] Evans, The Atomic Nucleus, 675-676 (1955)

In the above equations, h is Planck's constant (6.63×10^{-34} J·s), c is the speed of light (3.00×10^{8} m/s), m is the mass of an electron (9.11×10^{-31} kg), **v** is the velocity acquired by the electron after being struck by the incident photon, λ_2 is the wavelength (in meters) of the scattered photon, λ_1 is the wavelength of the incident photon, and φ is the angle between the direction of the incident photon and the direction of the scattered photon. If we make the assumption that the Compton-scattered radiation (in the non-relativistic limit, again) is essentially isotropic, we can easily see that there is a very narrow spectrum of radiation produced from a single collision. The order of magnitude of the (1-cos φ) term will be at most of order unity, and (h/mc) has the value 2.43×10^{-12} m. Given that our incident radiation will have wavelengths of order 10^{-10} m, the corrections and dispersion of the radiation by the Compton scattering will be negligible. The Compton-scattered spectrum from each atom, then, will be roughly evenly distributed between the maximum possible energy of the scattered photons (equal to the incident energy, here assumed to be 10 keV) and the minimum possible energy. The minimum possible energy will have the highest wavelength (which would be the wavelength found when $\varphi = \pi/2$, if we look only at "forward" scattered photons and "forward" fluoresced photons). $\lambda_{max} = \lambda_0 + \lambda_{shift}$, where $\lambda_0 = 1.24 \times 10^{-10}$ m (10 keV), and $\lambda_{shift} = 2.43 \times 10^{-12}$ m, $\lambda_{max} = 1.26 \times 10^{-10}$ m, and thus $E_{min} = 1.57 \times 10^{-15}$ J = 9.81 keV. Thus, the Compton scattered energy distribution, which, in the non-relativistic limit, is relatively spherical, will have a spread between the 10 keV incident beam and the 9.81 keV "sidescatter" beam. Repeated collisions (scattering of scattered photons) will further reduce the bottom limit on the energy, but the "peak" of the Compton-scattered spectrum will lie between 10 keV and 9.81 keV, with decreasing numbers of photons at lower energies. The full Compton spectrum will extend all the way down to photons of near-zero energy as their wavelengths are progressively increased through repeated collisions. However, the number of photons will actually decrease as we look at lower-energy Compton photons, and so there will be a diminishing energy distribution all the way down to photons of near zero energy.

The best means to determine the total number of Compton-scattered photons that enter the detector is by employing the Compton-scattering cross-section of the substrate. In our case, the substrate is silicon, so the Compton-scattering cross-section is 5.04×10^{-24} cm^2/atom[5] (at 10 keV). The relationship between the scattering cross-section and μ_s, the linear scattering coefficient, is:

$$\mu_s = \sigma\varrho/\mu A \qquad (16)^6$$

where σ is the Compton-scattering cross-section of the atom, ϱ is the density, μ is the atomic mass unit ($1.6605402 \times 10^{-24}$ g/Dalton), and A is the atomic mass in Daltons of the atom of interest. The atomic mass of silicon is 28.0855, and the density of silicon at room temperature is 2.329 g/cm^3. The attenuation coefficient, therefore, is .2517 cm^{-1}. Using our prior assumption that we can approximate (1-exp(-μt)) as being just (μt), we can say that the total Compton scattering into a half-sphere (solid angle of 2π) as being:

$$I = I_O(\mu t)/2 \qquad (17)$$

which would imply that the total Compton scattering into our 2π solid angle detector is about 2.5×10^2 photons per second with an ESRF source. Employing source data for the ERL, however, our

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[5] Veigle, W.M., Atomic Data Tables, 5, pp. 51-111 (1973)

[6] Hubbell and Seltzer, Section 2. < http://physics.nist.gov/PhysRefData/XrayMassCoef/chap2.html >

scattering count jumps up to 3.15×10^6 photons/sec. However, despite the fact that this number is actually a little larger than our signal intensity with the ERL source, we recognize the fact that this number reflects a number of photons scattered into a rather wide spectrum of different energies. The portion of this total number that actually contributes to effective noise is at most one tenth of the total number of scattered photons, since it is not likely that much more than this number will come out of the sample with an energy close to the energy of the fluorescent photons from the Erbium. While the rest of the photons *do* go into the detector, we will obviously be able to discard them as noise in the data set. However, photons at energies near the fluorescent energy (roughly 9.75 keV, for Erbium's L absorption edge) will not be easily discernible, and thus only these will factor into our experimental measurement as noise. Therefore, although there will be quite a bit of background noise, the effective amount that we need worry about will not be more than 3.15×10^5 photons/sec, which is about a factor of eight less than the signal strength obtained, 2.58×10^6 photons/sec. This number is also virtually a worst-case scenario; if the scattering had been a real problem, it would be quite possible to increase the energy of the incident radiation slightly such that the bulk of the Compton-scattered spectrum would be further away from the energy of the fluoresced photons to reduce the effective noise even further.

Appendix B: Flux estimation from 2m long ERL undulator with perfect microbeam optics

Introduction The purpose of this calculation is to estimate the flux from an ERL 2m long undulator source when focused down to a 1 nm focal spot size by ideal optics.

ERL Undulator source

The source parameters of the ERL undulator for microbeam experiment was assumed as:

Machine parameters: G = 5.3GeV, I = 10mA, $\sigma_E/E = 0.0001$

Electron beam emittance: 0.01 nm-rad (horizontal or vertical), Beta function (H or V) = 1 m

RMS source size: $\sigma_x = \sigma_y = 0.0032$ mm;

RMS source divergence: $\sigma_x' = \sigma_y' = 0.0032$ mrad;

Undulator period length: $\lambda_u = 2$ cm

Undulator period number: 100

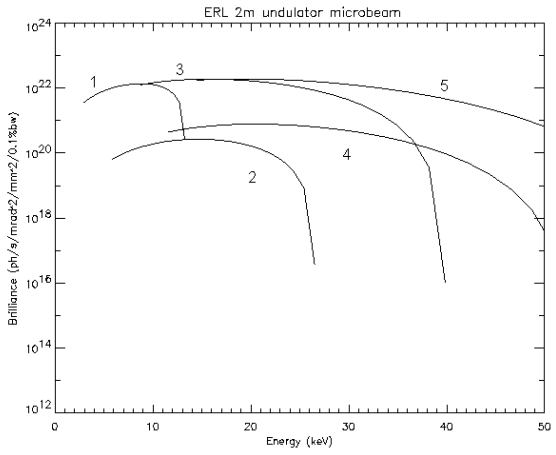
Undulator total length: 2.0 meters

Source to station hutch distance: 25 meters

ERL Microbeam Undulator radiation

(1) To use 10 keV, from the tuning curve (calculated with XOP v2.0) it can be seen that the strong-

Fig.1



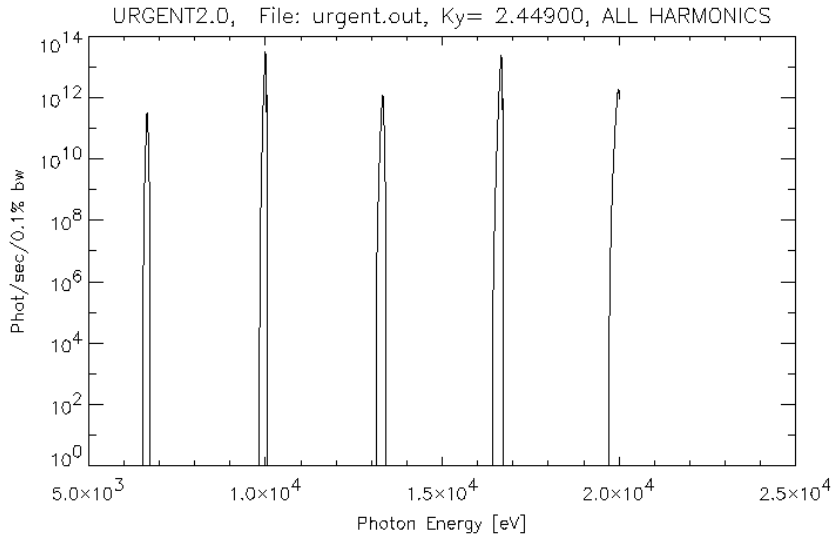
est radiation is the third harmonic.

Fig.1 the tuning curve of ERL 2m undulator source, calculated with first order harmonic energy range from 2.9keV to 13.3keV.

(2) From the equation[1]:

$$E_i[keV] = 0.94963 \frac{iE^2[GeV]}{\lambda_u[cm](1+0.5k^2)},$$

for the third harmonic (i=3) and E_i=10keV, λ_u=2cm, it was calculated that the deflection parameter k=2.450007



(3) The undulator flux at 25m away

Fig.2 Flux on an aperture. Calculated with k_y=2.449, observation distance of 25 meters, at position of V = H = 0, and aperture size of 0.3 mm x 0.3 mm. Calculation mode = 4 (means flux on aperture), ICAL = 1 (means non-zero emittance and finite N). Undulator type: plane, number of calculation points = 100.

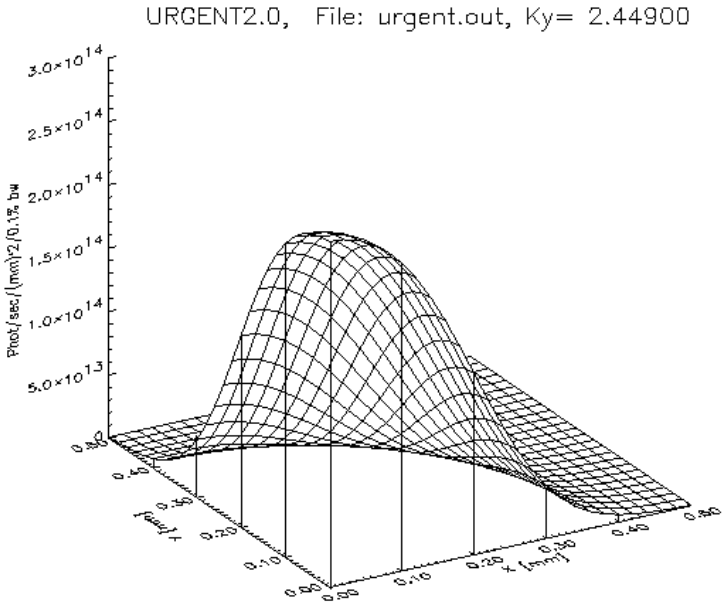


Fig.3 Spatial profile at 25 meters away from source, calculated at energy of 10 keV (E_{min}=10000eV), all harmonic included, and at position of H = V = 0. Other input parameters: 5.3GeV and 10mA beam, $\sigma_x = \sigma_y = 0.0032$mm, $\sigma_x' = \sigma_y' = 0.0032$mrad, D=25m, mash grid number of points: 25 x 25, non-zero emittance, finite N, mode=1 (means angular/spatial flux at E_{min}), acceptance (i.e. the calculation spatial range): 1mm x 1mm.

With assumption that x-ray station is about 25 meters away from the source and deflection parameter k_y=2.449, the flux through a 0.3mm x 0.3mm slit, 5--20 keV was calculated as in fig.2. The spectrum has very sharp peaks of harmonics.

The spatial profile of the radiation at 10 keV, 25 meters away from source is shown in fig.3, where the spot size (FWHM) looks about 0.3 or 0.4 mm. With a 0.3 mm aperture we should be able to collect most of the photon flux from the source without much waste.

In order to calculate the x-ray flux after a monochromator, we calculated the x-rays flux through a 0.3 mm x 0.3 mm area, on axis, with a narrow energy range around 10 keV. As shown in fig.4, the flux intensity is about $2x10^{13}$ ph/sec/0.1%bw within the calculated +/-10eV range.

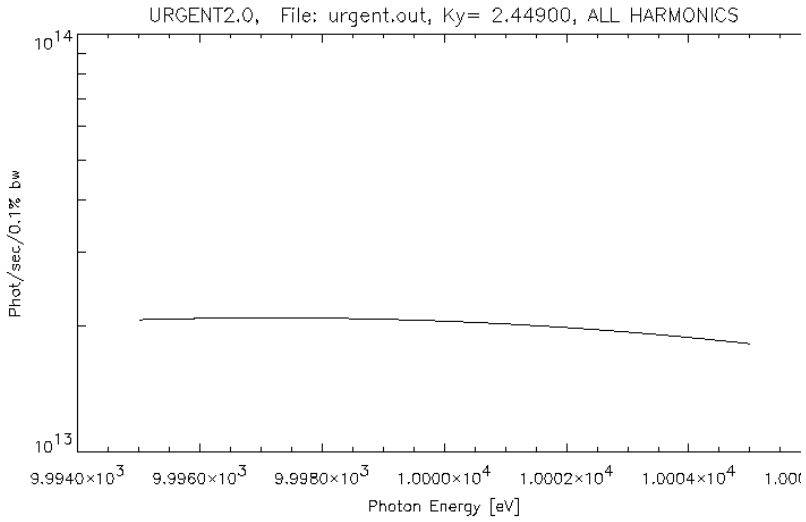


Fig.4 Flux on an aperture, similar input as used for fig.2, except the energy range is changed to 10keV +/- 5 eV. It can be seen from this plot that even though the undulator spectra are very narrow as shown in fig.2, the intensity is quite constant within 1.2eV range around 10keV that is accepted by a crystal monochromator.

(4) Bandwidth of double flat perfect Si(111).

Suppose a set of double (flat and perfect) Si(111) crystals will be used for the monochromator, the x-rays bandwidth of σ mode x-rays after the crystal is shown in fig.5, with integral width about 5 arc seconds. With other parameters output from the XOP code: d=3.1356Å, θ_B=11.4°, it can be calculated that $\Delta\lambda=1.5x10^{-4}$Å and ΔE=1.226 eV.

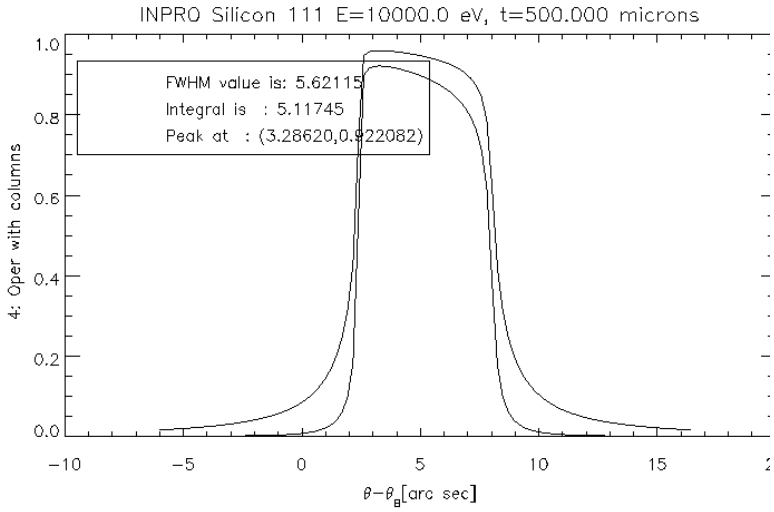


Fig.5 The reflectivity band width passing one and double flat perfect Si(111) crystals at 10 keV. Other input parameters are: asymmetry angle = 0, crystal temperature = 300 k, crystal thickness = 500 μm and the calculation mode = reflectivity in Bragg case.

(5) Undulator flux though both Si(111) monochromator and ellipsoidal mirror

From section (3) it has been known that the x-ray flux passing through 0.3 mm by 0.3 mm ($9x10^4$ μm^2) aperture is:

$F = 2x10^{13}$ ph/sec/0.1%bw ;

and from section (4) it has been known that the energy width of the flat perfect double Si(1111) is

$\Delta E = 0.001226$ keV; or: $BW = \Delta E/E = 1.2x10^{-4}$.

From "Possible 1 nm scale focusing on ERL" (another summary by R. Huang and D. Bilderback) it has been estimated that an ideal ellipsoidal mirror of making 5 nm focal size may have the acceptance of $6x10^4$ μm^2 (assuming ellipsoidal mirror maximum acceptance area is 1/4 of a whole ellipsoidal capillary). Therefore the total x-ray flux goes to the final 5 nm spot will be (also assume 100% reflectivity of the ellipsoidal mirror):

$2x10^{13}*(6x10^4/9x10^4)*(0.001226/10/0.1\%) = 1.63x10^{12}$ (ph/sec/5nmSpot)

Assuming the further 1 nm x-ray squeezing channel will deliver 1/25 of the 5 nm diameter x-rays to 1 nm size spot, the final x-rays can be **focused into a 1 nm spot** with **ideal optics** will be: **$6.5x10^{10}$ ph/sec**

(6) Undulator flux at 1 nm spot by zone plate approach

From "Possible 1 nm scale focusing on ERL" it has been known that a $8.5x10^4 \mu m^2$ acceptance ideal zone plate (with diameter of 0.33 mm) may focus 0.1eV BW x-rays down to 1 nm in one step with efficiency of 0.406, therefore the total x-rays the zone plate delivered to this 1 nm spot will be:

$2x10^{13}*(8.5x10^4/9x10^4)*(0.1/10000/0.1\%)*0.406 =$ **$7.67x10^{10}$ ph/sec**

It seems that an ideal zone plate can deliver the same amount of photons to 1 nm spot as an ideal mirror can do even with a much narrow bandwidth because an ideal zone plate can focus x-ray into a larger divergence angle than any reflection optic can do. Meanwhile, using zone plate will have the advantage of make a 1 nm focal spot in one step.

(7) Using 1% multilayer to accept the whole 3rd harmonic and ellipsoidal mirror

The bandwidth of the 3rd harmonic of 2m ERL undulator is about $\Delta E/E = 1/iN = 1/300$, with ΔE about 33eV at 10keV, therefore a 1% bandwidth of multilayer will pass almost all of the photons of the 3rd harmonic. Fig.6 shows the spectrum of the flux through a 0.3mm x 0.3mm aperture 25 meters away from the source, with the integral of the flux from 9950eV to 10050eV of $9.5x10^{14}$ ph/sec/0.1%BW*eV = $9.5x10^{13}$ ph/sec.

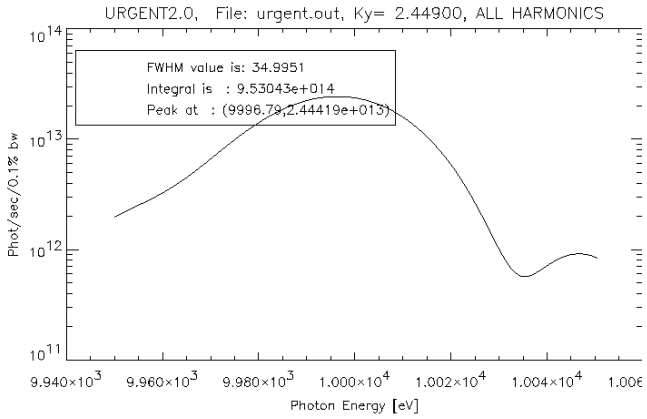


Fig.6 The spectrum of the flux through a 0.3mm by 0.3mm aperture 25 meters away from the undulator, from 9950eV to 10050eV. The integral intensity within this energy range is 9. $53x10^{14}$ ph/sec/0.1%BW*eV = $9.5x10^{13}$ ph/sec, assuming 0.1%BW = 10 eV at E=10keV.

The total x-rays collected by a $6x10^4 \mu m^2$ ellipsoidal mirror (see "possible 1 nm scale focusing on ERL") into 5 nm diameter spot will be:

$$9.5x10^{13} \text{ x } (6x10^4/9x10^4) = 6.3x10^{13} \text{ ph/sec}$$

If 1/25 of this photons can be collected by a micron channel to make a 1 nm spot, the x-rays flux into this 1 nm spot will be **$2.5x10^{12}$ ph/sec**, about 33 times higher than using double Si(111) crystal.

It can also be seen from this undulator tuning curve (fig.1) that at 10eV the radiation intensity of 1st order is only slightly smaller than 3rd order harmonic. Therefore if we use 1st harmonic at 10keV with broader energy width radiation, using multilayer may collect another factor of 2 to 3 times more photons.

Reference:

[1] A.W.Chao and M. Tigner, Handbook of Accelerator Physics and engineering, World Scientific Publishing Co.