Expected performance of cryogenic silicon monochromator for high power density and high coherence ERL beamlines

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Abstract. With small emittance and a high degree of X-ray coherence, the Energy Recovery Linac beamlines, proposed at Cornell, need excellent optics to preserve the high quality of X-ray beam. In this paper, thermal deformation of cryogenic silicon monochromators and its effect on wavefront deformation are studied. For crystal thermal deformation analysis, we introduce the so-called modified linear power density as a universal parameter of heat load. For the wavefront simulation, using synchrotron radiation workshop, we study the focusing of source under one-to-one demagnification ratio, for the full central cone of undulator radiations. The studies conclude that cryogenic Si monochromators, in general, are suitable for Cornell energy recovery linac beamlines.

1. Introduction

Future Energy Recovery Linac (ERL) beamlines, with smaller source emittance and higher degree of X-ray coherence than available at existing 3rd generation sources [1], need excellent optics to preserve the high quality of the X-ray beam. For Cornell ERL, 5m and 25m long undulators with 19 mm periods will produce extremely low-divergent central cones with very high power density; therefore, the potential thermal deformation of monochromator crystals has to be carefully studied. LN₂-cooled Si crystal monochromators have been widely used at 3rd generation sources with success [2,3], and the perfect atomic structure of Si crystals is good for preserving X-ray wavefront. Since crystal thermal deformation is sensitively related to many factors, including power density, total power, and the dimensions of heating footprint, we introduce the so-called modified linear power density (MLPD), with which the Si thermal deformation can be better understood with given heat load.

With crystal deformation profiles calculated with ANSYS, the wavefront distortion can be evaluated with the simulation tool, Synchrotron Radiation Workshop (SRW) [4]. In this paper, the wavefront distortion by monochromator is evaluated by simulating a one-to-one focusing of the X-ray source through an ideal thin lens set right after monochromator.

2. Modified linear power density and the thermal deformation of cryogenic Si monochromator

Cornell ERL is proposed to run with current of either 25mA (high coherence mode) or 100mA (high flux mode). ERL round source allows a unique Delta undulator design with its polarization changeable between planar mode and helical mode [1]. For clarity, major source and undulator parameters are summarized in table 1

The on-axis radiation power density of CHESS ERL undulators can be as high as 1.1×10⁶ W/mrad² for 25m undulator at planar mode and 3.4×10⁵ W/mrad² at helical mode. As a comparison, APS...
undulator A maximal on-axis power density is about $1.6 \times 10^5 \text{W/mrad}^2$. On the other hand, because of the small ERL emittance in both transverse directions which creates small radiation cone, the maximal total power in central cone is about 400 W and 95 W for ERL planar and helical undulators respectively, comparable to the heat load on third generation sources. There will be 8 different kinds of beamlines for Cornell ERL out of the different combinations of machine currents, undulator lengths and undulator polarization modes. Before we start to use ANSYS to simulate all the 8 kinds of beamlines, we use a simplified model to understand what we can expect for cryogenic monochromators. With the assumption that the surface heating area is much smaller than crystal dimensions, the maximum temperature at the center of thermal footprint can be estimated as [5]:

$$T = T_a + (T_0 - T_a) \exp(0.0183P_M),$$  \(1\)

with

$$P_M = [1 + \ln(L/W)/2.571]Q/L,$$  \(2\)

which we call modified linear power density (MLPD). Q is the heating power; L and W are the length and width ($L \geq W$) of X-ray footprint, and $T_0$ is the temperature at the “far-away” crystal boundary and $T_a$ is a constant of 47.4K. The coefficient in eq.(1) is calculated with $P_M$ in the unit of W/mm. Eq.(1) tells us that it is the linear power density that determines crystal temperature increase.

### Table 1. Cornell ERL source and undulator parameters

| Electron source parameters | Mode | $\Delta E/E$ (%) | Current (mA) | $\epsilon_x/\epsilon_y$ (nm rad) | $\sigma_x (\mu\text{m}(\text{S/L})^2$ | $\sigma_y (\mu\text{m}(\text{S/L})^2$ | $\sigma_x' (\text{mmrad}(\text{S/L})^2$ | $\sigma_y' (\text{mmrad}(\text{S/L})^2$ |
|---------------------------|------|-----------------|--------------|------------------------------|-----------------|-----------------|-----------------|-----------------|
| High flux                 | 0.0186 | 100             | 0.031/0.025  | 4.95/11.1                    | 4.45/9.95       | 6.22/2.78       | 5.59/2.50       |
| High coh.                | 0.0088 | 25              | 0.013/0.011  | 3.217/7.19                  | 2.904/6.49      | 4.042/1.81      | 3.649/1.63      |

| Undulator parameters | Type | Length (m) | Period (mm) | Period number | Gap (mm) | $B_{\text{max}}(T) (\text{P/H})^b$ | $K_{\text{max}} (\text{P/H})^b$ |
|---------------------|------|------------|-------------|--------------|---------|--------------------------------|-----------------|
| Short               | 5    | 19         | 263         | 5            | 1.2524/0.8856 | 2.222/1.571|
| Long                | 25   | 19         | 1315        | 5            | 1.2524/0.8856 | 2.222/1.571|

*aSource dimensions are calculated with $\beta$ functions set as undulator length over $2\pi$, and “S/L” stands for short/long undulators; b$^b$/P/H stands for planar/helical undulators.

Even eq.(1) is only accurate within a limited range of heat load [5], we found out that the MLPD, $P_M$, can be used to parameterize crystal thermal deformation when the assumption of surface heating is reasonable. The power load for ERL helical undulators, and for planar undulators not working at high value of deflection parameter $K$, can be approximated as surface heat. With MLPD, the severity of crystal thermal deformation can be evaluated independent of facilities and beamlines. It is believed that cryogenic Si crystal thermal deformation can be divided into three regions [6]. When heat load is small, the slope errors caused by thermal deformation increase linearly with heating power. As power increases to a level called transition region, the slope errors may not increase and could even decrease as heating power increases. Further increase the power to the so-called non-linear region, or run-away region, the slope errors increase dramatically as heating power increase. In terms of MLPD, we find out that the crystal deformation is in the linear region when MLPD is around 50 W/mm or less, and in the transition region when MLPD is around 50 – 100 W/mm and in the nonlinear region when MLPD is around 100 w/mm or higher [5].

The results of ANSYS simulations for CHESS ERL beamlines are summarized in table 2, with the I-weighted slope errors defined as $\alpha_{\text{rms}} = \sqrt{\int I(x)[E(x) - \text{mean}(E(x))]^2 dx} / \int I(x) dx$, where $I(x)$ is the monochromatic X-ray intensity, and $E(x)$ is surface slope, along position x on a crystal surface.

It can be seen from table 2 that the MLPD will be larger than 100 W/mm only when ERL machine runs at 100 mA, and meanwhile the planar undulators work at maximum $K$. Under that circumstance, the cryogenic mono will work in the nonlinear region with large deformation. If any future ERL beamlines need to have cryogenic Si monochromator work at this extreme condition, possible ways to
mitigate may include positioning monochromator further downstream of the beamline to reduce MLPD, using internal cooled Si crystal to increase cooling efficiency, and reducing the openings of power slit.

### Table 2. The summary of ERL monochromator slope errors simulated using ANSYS

| Undulator length (m) | Current (mA) | Mono to source (m) | Total power (W) | MLPD (W/mm) | I-weighted slope errors (μrad) | 1st harmonic energy (keV) |
|----------------------|--------------|--------------------|-----------------|-------------|-------------------------------|--------------------------|
| Helical undulator, K = 0.707, maximum on-axis power density condition | 25 | 25 | 45 | 24 | 12 | 0.52 | 8.33 |
| | 25 | 100 | 45 | 95 | 47 | 2.05 | |
| | 5 | 25 | 35 | 24 | 6.7 | 0.30 | |
| | 5 | 100 | 35 | 95 | 27 | 1.25 | |
| Planar undulator, K = 2.22, “closed-gap” condition | 25 | 25 | 45 | 98 | 78 | 1.35 | 3.6 |
| | 25 | 100 | 45 | 392 | 310 | 80 | |
| | 5 | 25 | 35 | 99 | 45 | 0.9 | |
| | 5 | 100 | 35 | 395 | 178 | 12.5 | |
| Planar undulator, K = 1.06. | 25 | 25 | 45 | 35 | 17 | 0.61 | 8.0 |
| | 25 | 100 | 45 | 141 | 70 | 1.94 | |
| | 5 | 25 | 35 | 35 | 10 | 0.35 | |
| | 5 | 100 | 35 | 140 | 40 | 1.47 | |

3. **Wavefront propagation through cryogenic monochromator**

ERL ultra-low emittance is advantageous to the needs of high degree of transverse coherence and high-flux nano-focusing, which in turn requires high quality optics to maintain X-ray beam quality. In general, the Si crystal thermal deformation can be considered as a combination of a cylindrical curvature and a residual figure after cylindrical curvature subtraction. While the wavefront change by cylindrical curvature can be corrected with downstream focusing or defocusing optics, the changes arising from the residual figure may not be easily correctable, with a net effect of increase beam size in focusing. Using SRW [4] we simulate X-ray propagation starting from undulator, through monochromator crystal and a “perfect thin lens”, to make a 1:1 focusing of the source. We then evaluate the image changes caused by monochromator deformations.

Fig.2 shows the wavefront simulation results of 1:1 focusing for CHESS ERL 5 m long helical undulator source, working at the highest possible thermal load condition with K=0.707. For comparison, results with considering wavefront deformation from monochromator crystal and without considering the deformation are presented together in fig.2. It can be seen that when ERL machine runs at high coherence mode with current of 25 mA, there are almost no changes of focusing after considering wavefront deformation from monochromator crystal. For ERL machine running at 100 mA high flux mode, there are only minor changes after considering crystal deformation, with an increase of FWHMx from 15.4 μm to 15.6 μm, and FWHMy from 14.2 μm to 14.7 μm.

Similar wavefront simulations have been done for 25m long helical undulators and also for planar undulators with 1st harmonic X-ray energy at 8 keV. The results are summarized in table 3, from which it can be seen that when ERL machine runs at 25 mA, the crystal thermal deformation has negligible effect on wavefront deformation. Minor increase of focal size can be seen when ERL machine runs at 100 mA high flux mode.
Figure 1. Wavefront simulations of Cornell ERL 5m long helical undulators at 8.32 keV. (a) The comparison of the 1:1 focusing of the source with and without considering Si crystal thermal deformation, when ERL machine runs at 25 mA high coherent mode. (b) The same simulation for ERL machine working at 100 mA high flux mode.

Table 3. Summary of wavefront simulation with and without considering crystal deformations

| Undulator type | Current (mA) | 1st harmonic energy (keV) | Without crystal deformation | With crystal deformation |
|----------------|--------------|---------------------------|-----------------------------|-------------------------|
|                |              |                           | FWHM_x (μm) | FWHM_y (μm) | FWHM_x (μm) | FWHM_y (μm) |
| 5m helical     | 25           | 8.32                      | 13.1          | 12.9         | 13.2          | 12.9         |
|                | 100          |                           | 15.4          | 14.2         | 15.6          | 14.7         |
| 25m helical    | 25           |                            | 28.8          | 27.9         | 29.2          | 27.8         |
|                | 100          |                           | 34.7          | 32.1         | 34.8          | 33.2         |
| 5m planar      | 25           | 8.0                       | 12.9          | 12.6         | 12.9          | 12.7         |
|                | 100          |                           | 15.4          | 14.4         | 15.9          | 15.2         |
| 25m planar     | 25           |                            | 28.4          | 27.5         | 28.7          | 27.4         |
|                | 100          |                           | 35.0          | 32.4         | 35.1          | 34.0         |

4. Summary
Cryogenic Si monochromators in general will be suitable for CHESS ERL beamlines with small slope errors and negligible or minor wavefront distortions.

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