Thermal analysis of LN$_2$-cooled silicon crystals for Energy Recovery Linac monochromators

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Abstract. We discuss major features of the predicted power distribution in undulator beams at the proposed Cornell Energy Recovery Linac, and the anticipated consequences for monochromator performance. Finite element analysis of thermal deformation of LN$_2$-cooled Si crystal monochromators for the ERL is summarized. A new metric, the modified linear power density, is found to provide a clear description of crystal thermal deformation.

1. Introduction
Energy Recovery Linac (ERL) sources are expected to produce round, ultra-low emittance and low energy-spread electron beams, which when coupled with long undulators will produce x-ray beams with spectral brightness and spatial coherence, superior to existing sources with quasi-continuous time structure [1]. An adverse side effect of the decreased divergence of the harmonic radiation will be an increase of the radiation power density on the upstream beamline optics, in many cases the first crystal of the monochromator, potentially causing significant thermal deformation of the optics.

Both liquid nitrogen (LN$_2$) cooled silicon and water-cooled diamond crystals have been successfully used to mitigate the high heat loads at 3rd generation sources, with LN$_2$-cooled Si more widely used because of the availability of large perfect single crystals. For an ERL monochromator, a perfect crystal structure is needed to propagate the highly coherent beam without inducing wavefront distortions. Given the difference between the radiation power density of 3rd generation sources and that expected from the ERL, there is a need for evaluating the performance of such monochromators at the ERL.

In this paper, we will briefly discuss the radiation features expected from the Cornell ERL undulators and then present finite element analysis (FEA) results for ERL LN$_2$-cooled Si monochromators. We introduce the concept of modified linear power density, which provides a nearly scale-invariant metric to evaluate Si crystal deformation.

2. Power radiation from ERL undulators
Major parameters of the proposed 5.0 GeV Cornell ERL machine have been defined [1]; those parameters relevant to undulator radiation are summarized in table 1. Because of the very small source emittance, power radiated from the undulator has negligible difference compared to an ideal “zero-emittance” source (fig.1), as estimated by SPECTRA 8.1.3. [2]. The heat load in the central cone can be simply estimated by multiplying the on-axis power density for “zero-emittance” with the central cone size. Near-field effect can be expected even on axis for the 25m long undulator (fig.1).
Table 1. Cornell ERL source and undulator parameters

| Mode     | \(\Delta E/E (%)\) | Current (mA) | \(\epsilon_x/\epsilon_y\) (nm rad) | \(\sigma_x\) (\(\mu\)m) (S/L) | \(\sigma_y\) (\(\mu\)m) (S/L) | \(\sigma_x^{',}(\mu\text{rad})(\text{S/L})^a\) | \(\sigma_y^{',}(\mu\text{rad})(\text{S/L})^a\) |
|----------|---------------------|--------------|----------------------------------|-----------------|-----------------|----------------------------------|----------------------------------|
| 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) | \(B_{\text{max}}^a\) (T) (P/H) | \(K_{\text{max}}^a\) (P/H) |
|------|------------|-------------|---------------|----------|-------------------------------|----------------------------|
| 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                |

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

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**Fig.1** Due to the small emittance of ERL source, the power density given by zero-emittance formulas (solid lines) match the numerical results (circles and crosses) very well under far-field approximation for CHESS 25m long undulators. However, near field effects are expected even 45m from the source, on-axis (dash lines). The thick lines and circles are horizontal profiles, thin line and crosses are vertical profiles for a 25m planar undulator. Spectra [2] is used for numerical calculations.

**Fig.2** X-ray profiles calculated with SRW [4] at highest K (1st harmonic at 3.6keV) 70m from source, for ERL 5m undulator, high flux mode, using slits at 35m. Using 1mm \(\times\) 1mm slits, fringes will appear ((a): horizontal (b): vertical). With 1.5mm \(\times\) 1.5mm slits fringes will mostly disappear ((c): horizontal; (d): vertical)

These long undulators with short period will produce much higher flux and power density than normally seen at 3\(\text{rd}\) generation sources. For a 3\(\text{rd}\) generation undulator, especially in the horizontal direction, the larger beam central cone means that a higher percentage of radiated power is “mixed” into the central cone. In the end, although the ERL undulator radiates much high power density, the total power within the “central cone” of a 5GeV ERL undulator is not much different than that of 3\(\text{rd}\) generation sources, not more than a few hundred watts. The very small source emittance in both directions allows operation of a unique “Delta” undulator design with flexible polarization modes [3]. When operating in helical mode to produce elliptical polarization, the higher harmonics are pushed off-axis, reducing power in the central cone. For Cornell ERL undulators, longer undulators produce...
beams with smaller angular size, so the power density increases, but total power in the central cone is similar for different length undulators. With minimum slit size to accept the central cones, the intercepted power is around 400W for both 25m and 5m long planar undulators at maximal K, and around 100W for both helical ones with K=0.707.

At a 3rd generation source, power on the first optic can be reduced by using slits to accept only part of the central cone. For an ERL source, however, because of the higher degree of coherence, such an aperture may produce interference fringes downstream, even for the so-called “high flux” mode of operation at the Cornell ERL, as shown in fig 2. For that reason, we assume the heat-limiting aperture just upstream of the monochromator accepts the entire central cone, verified with SRW [4], for the thermal analysis in this paper.

3. The thermal deformation of monochromator crystal

Based on the success at 3rd generation sources [5], we consider an ERL Si monochromator with first crystal size 30 mm by 30 mm by 80 mm, contact cooled from two sides by LN$_2$ and assume a moderate effective cooling film coefficient of 5000 W/m$^2$/K [6]. Three regimes of crystal deformation have been identified previously [6]: the linear, transition and nonlinear (or runaway) regions, as shown in fig.3(a). However, it is not clear from previous studies how the crystal may deform for ERL beams, because the results vary not just with total power [5], but also with power density [6,7] and footprint (shape of the power distribution) [5,6].

![Fig.3. (a) Reproduction of FEA results for ESRF LN$_2$-cooled Si monochromator for different slit openings. (b) The ESRF results together with FEA results for Cornell ERL undulators, as a function of MLPD. Behaviour of Si deformation in “linear region” is scale-invariant with total power and beam footprint when evaluated with MLPD.](image)

When X-ray spot size is much smaller than its distance to LN$_2$ path, we introduce an empirical metric called the “modified linear power density” (MLPD) [8] as a measure of heat load on the crystal,  
\[
P_M = \left[1 + \ln(L/W)/2.571 \right]Q/L,  
\]

where $Q$ is the total accepted power, $L$ and $W$ are the length and width ($L \geq W$) of X-ray footprint and uniform power within the footprint is assumed. The MLPD yields a “empirical curve” of crystal deformation in the linear region (in terms of Peak-Valley slope error) that is scale-invariant in both total power and footprint, as shown in fig 3(b). The Cornell ERL data in fig.3(b) mostly assume worst case scenarios in terms of heat load. For Delta ID in planar mode, K=2.2218 (E=3.6 keV) is chosen for highest possible heat load. For helical mode ERL, K=0.707 (E=8.328 keV) is chosen. The distance from monochromator to source center is assumed to be 35 m for 5 m long undulator and 45 m for 25m undulator. The 1st (2nd) largest slope errors in fig.3(b) (the solid diamonds of 9000 µrad and 1300 µrad) corresponds to 25 m (5m) undulator, 100 mA, and K=2.2218. The calculated maximum temperature for these two data points are 2600 K and 770 K respectively, and are influenced by
systematic error associated with (1) black-body radiation that is not accounted for, (2) the material data tables we used only include thermal conductivity data up to 800 K and thermal expansion values up to 400 K. (for higher temperatures, ANSYS uses values for the closest available temperature beyond those tabulated). According to fig.3(b), crystal deformations are expected in the linear regime when the MLPD is no more than 50 W/mm, the transition regime when MLPD is around 50 – 100 W/mm, and in the nonlinear regime when the MLPD is higher than 100 W/mm. However, the MLPD for the onset of the nonlinear regime is dependent on details such as the effective cooling film coefficient, total power, and other factors.

To better compare FEA results with experiments measuring rocking curve broadening, we suggest the following definition of X-ray intensity weighted RMS slope errors for simulations,

$$\alpha_{RMS} = \sqrt{\frac{\int I(x)[E(x) - mean(E(x))]^2 dx}{\int I(x) dx}}$$

(2)

where $I(x)$ is the monochromatic X-ray intensity and $E(x)$ is the slope along X-ray footprint on crystal surface. This measure of RMS slope errors, for Cornell ERL monochromators, is mostly no more than 2-3 μrad as shown with squares in fig.3(b), which means nice rocking curve and good X-ray throughput. These results are close to the comprehensive measurement at ESRF with slope errors (FWHM) mostly in the range of 0.7 – 5 μrad [5].

It is important to note that for ERL sources, because of the small power footprint on crystal, the difference between surface heat load and volume heat load in FEA simulation is significant for planar undulators working at high K. The two largest slope errors in fig.3(b) and the corresponding high temperature are greatly reduced when FEA calculations are performed with a volume load, as seen in table 2 (for 25 m and 5 m planar undulators at 3.6keV). At lower K (for example, K=1.06), such difference becomes minor.

| Undulator type | Current (mA) | Slit size (mm²) | Distance to source (m) | Power (W) | MLPD (W/mm) | T max (K) | Weighted RMS slope (urad) | X-ray energy (eV) |
|----------------|--------------|-----------------|-----------------------|-----------|-------------|-----------|---------------------------|-----------------|
| Planar 25m     | 100          | 0.85x0.85       | 45                    | 390       | 310         | 311       | 80.0                      | 3600            |
| Planar 5m      | 100          | 1.5x1.5         | 35                    | 394       | 178         | 194       | 12.5                      | 3600            |
| Planar 25m     | 25           | 0.85x0.85       | 45                    | 97.5      | 77.6        | 101.5     | 1.35                      | 3600            |
| Helical 25m    | 100          | 0.75x0.75       | 45                    | 94.5      | 46.7        | 116.0     | 2.05                      | 8328*           |
| Planar 5m      | 100          | 0.75x0.75       | 45                    | 136       | 69          | 126       | 1.94                      | 8000*           |

*aCornell helical undulator has highest on-axis power at this energy; bA case of moderate K number

**Conclusion** FEA simulation shows trends in LN₂-cooled Si monochromator performance for the ERL will be similar to those at 3rd generation sources, but some improvements will be needed to support power loads from planar undulators operating with high K parameter.

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