Automatic Optimization of X-ray Free-Electron Laser at SACLA

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3rd ICFA Beam Dynamics Mini-Workshop on Machine Learning Applications for Particle Accelerators

Hosted by Brookhaven National Laboratory

November 1–4, 2022

Introduction

- The brightness of an X-ray free-electron laser (XFEL) should be maximized for each experimental user by fine-tuning of accelerator components.
- An optimizer based on Gaussian process regression (GPR) has been successfully applied to XFEL facilities [1].
- We have developed a GPR-based optimizer for the XFEL facility, SACLA.

SACLA

Main Linac [2]

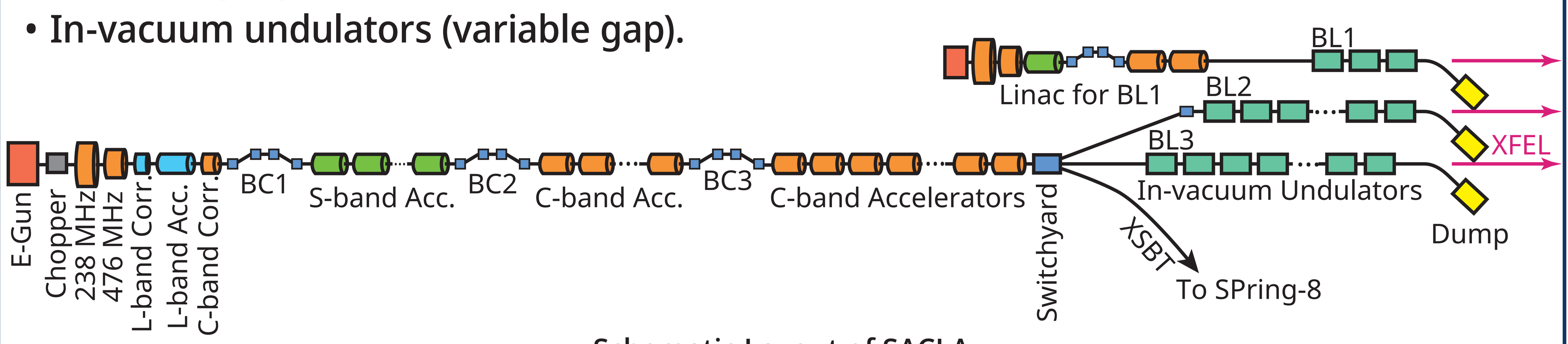
- Beam energy: 8 GeV maximum
- XFEL photon energy: 4 – 15 keV (BL2, BL3)

Second Linac

- Beam energy: 0.8 GeV maximum
- XFEL Photon Energy: 20 – 150 eV (BL1)

Key Technologies

- Low-emittance CeB6 thermionic electron gun.
- C-band high-gradient linear accelerator.
- In-vacuum undulators (variable gap).



Schematic Layout of SACLA

Optimizer Design

- We implemented the GPR based on scikit-learn [3], GPyTorch [4], and BoTorch [5].
- The GP kernel is the convolution of a radial basis function (RBF), constant kernel, and white noise kernel.

$$K(\mathbf{x}_i, \mathbf{x}_j) = k \times \mathrm{RBF}(\mathbf{x}_i, \mathbf{x}_j) + \sigma\delta(\mathbf{x}_i - \mathbf{x}_j)$$

- The hyperparameters are the factor, k, noise factor, σ, and the length scale of RBF.
- We can set upper and lower limits for each parameter.
- The optimizer can handle up to 32 parameters at a time.
- The optimizer uses the maximum point of the expected improvement, α_{EI}, to determine the parameters for the next trial.

$$\alpha_{\mathrm{EI}}(\mathbf{x}^*) = \int_{y_{\max}}^{\infty} (y^* - y_{\max}) p(y^* | \mathbf{x}^*, \mathbf{y}, X, \boldsymbol{\theta}) dy^*$$

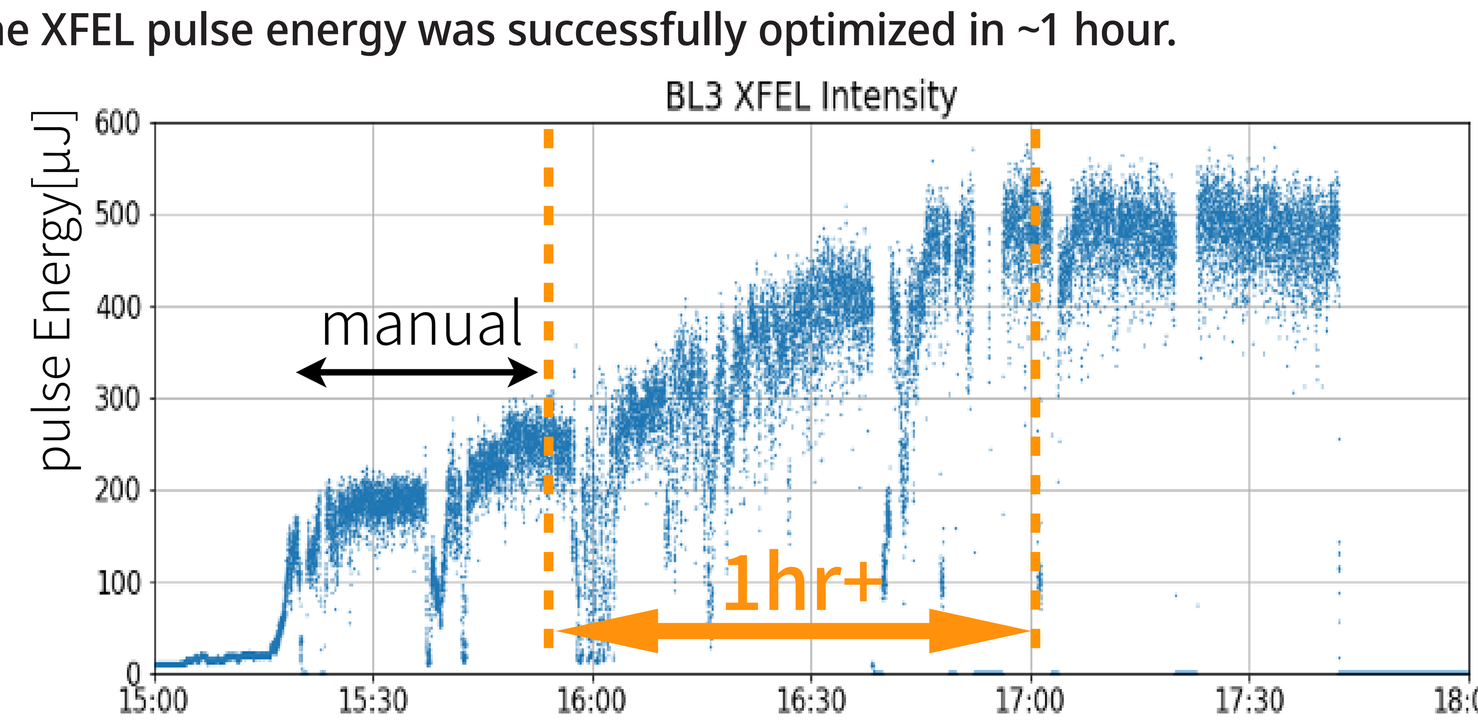
$\mathbf{x}^*$: the parameter vector to make an inference.
y^*: the value of objective function at $\mathbf{x}^*$.
X: the parameter vectors ever tried.
$\mathbf{y}$: the obtained data of objective function for X.
$y_{\max}$: the maximum value of $\mathbf{y}$.
$\boldsymbol{\theta}$: hyperparameter vector.

Tuning knobs

- RF phases of 238 MHz, 476 MHz, L-band (main and correction), S-band, and C-band (main and correction) accelerators. (7 parameters)
- Magnetic lens strengths in the low-energy region. (9 parameters)
- Quadrupole magnet strengths. (62 parameters)
- Steering magnet strenghts. (8 parameters)
- Taper of undulator K-values. (7 parameters)

Optimization of XFEL Pulse Energy

- The XFEL pulse energy was successfully optimized in ~1 hour.



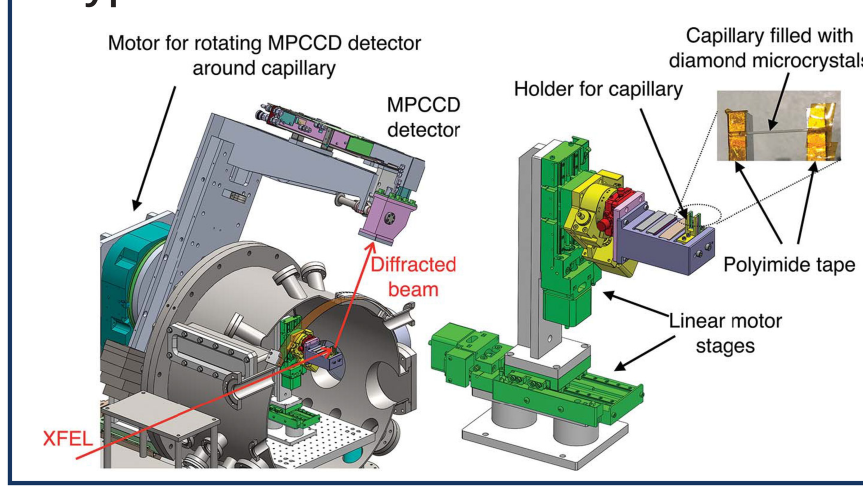
- The optimizer has been routinely utilized since 2020.
- However, XFEL spectral width, spatial profile, etc. are sometimes deteriorated after the optimization of XFEL pulse energy.
- Spectrum, spatial profile, etc. should be implemented to the objective function.

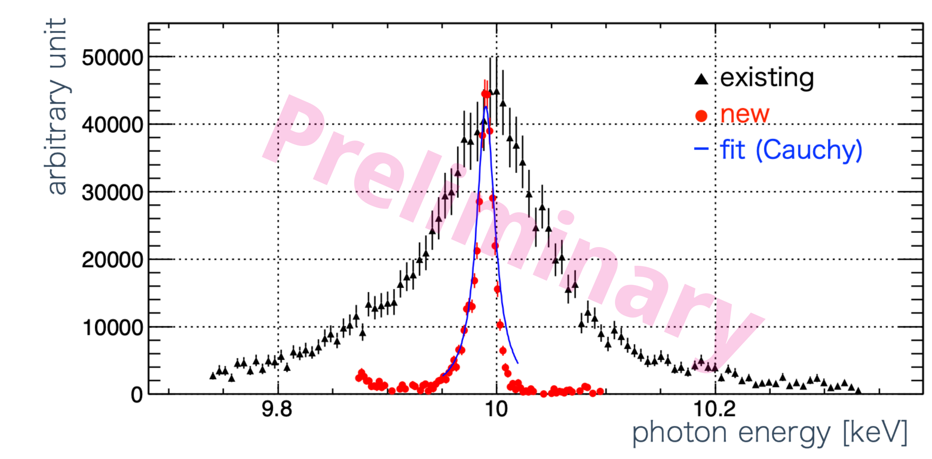
References

[1] J. Duris et al., Phys. Rev. Lett. **124**, 124801 (2020).
[2] T. Ishikawa et al., Nature Photonics **6**, 540 (2012).
[3] F. Pedregosa et al., Scikit-learn: Machine learning in Python, Journal of Machine Learning Research **12**, 2825 (2011).
[4] J. R. Gardner et al., Gpytorch: Blackbox Matrix-Matrix Gaussian Process Inference with GPU Acceleration, Advances in Neural Information Processing Systems **31** (2018).
[5] M. Balandat et al., BoTorch: A Framework for Efficient Monte-Carlo Bayesian Optimization, Advances in Neural Information Processing Systems **33** (2020).
[6] I. Inoue et al., J. Synchrotron Rad. **29**, 862 (2022).

New High-Resolution Inline Spectrometer

- To include spectral information to the objective function, a new high-resolution inline spectrometer (NIspec) was developed and installed [6].
- Halo part of XFEL is scattered by a diamond microcrystals filled in thin capillary and diffracted X-rays are detected by an X-ray image sensor (MPCCD).
- The resolution is a few eV for 10 keV XFEL, which is significantly narrower than the typical XFEL bandwidth of ~40 eV FWHM.





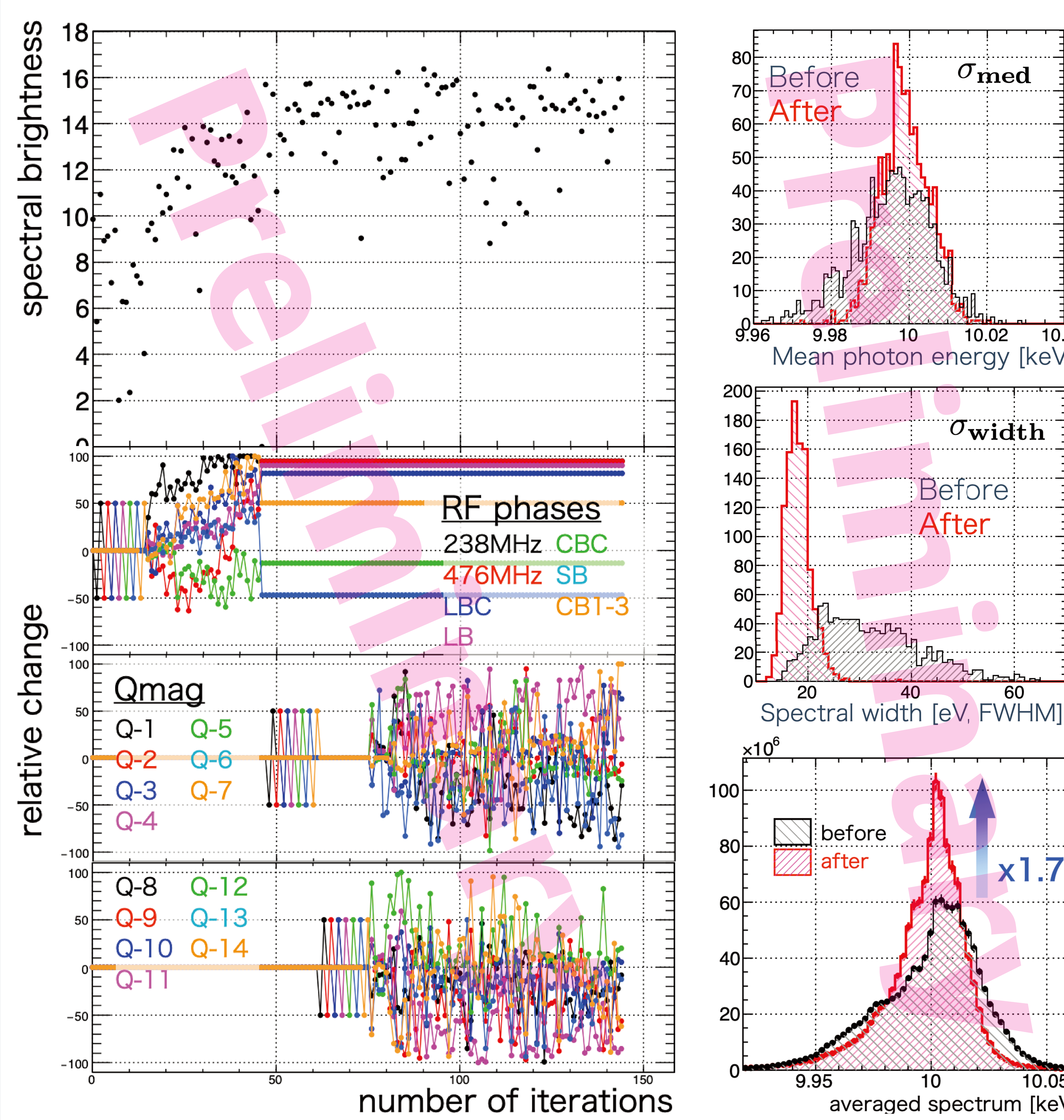
Optimization of Spectral Brightness

- The spectrum from the NIspec is fitted by Cauchy distribution.
- The spectral brightness, B_{avg}, is defined by:

$$B_{\mathrm{avg}} = \frac{P}{\sigma_{\mathrm{avg}}} \qquad \sigma_{\mathrm{avg}} = \sqrt{\sigma_{\mathrm{width}}^2 + \sigma_{\mathrm{med}}^2}$$

P: XFEL pulse energy.
σ_{width}: FWHM of the Cauchy distribution.
σ_{med}: FWHM of the median/peak photon energy of multiple (~90) shots.

- The spectral brightness was successfully optimized by our GP optimizer.
- The XFEL pulse energy was optimized first, then the spectral brightness was optimized in the case below.



- Both the photon energy jitter, σ_{med}, and the band width, σ_{width}, were improved.
- The width of the averaged spectrum was also made narrower and the spectral peak was increased by 1.7 times in this case.
- RF phases were more sensitive to the spectral brightness than the other tuning knobs.
- The spectrum was thought to be mainly affected by the longitudinal phase-space profile (bunch length, energy spread, etc.).
- Thus, the choice of the objective function is quite important for XFEL optimization.

Summary

- We developed a GPR-based optimizer for the XFEL facility, SACLA.
- Although we succeeded in the maximization of the XFEL pulse energy, the XFEL bandwidth sometimes became broader.
- Therefore, a new high-resolution inline spectrometer was developed and installed for optimization of the spectral brightness.
- The spectral brighteness was successfully improved by our optimizer.
- We plan to employ some other XFEL performance indices, such as XFEL spatial profile, to deliver better XFEL radiation.