Differentiable modeling of x-ray scattering

April 3, 2025

Abstract

We examine how the spectral properties of Self-Amplified Spontaneous Emission (SASE) pulses at X-ray Free-Electron Laser (XFEL) facilities affect measured scattering patterns, focusing on shot-to-shot variability and finite bandwidth. A hierarchy of models is presented, from a monochromatic approximation to approximate spectral modeling using differentiable 3D Gaussians and the reparameterization trick.

1 Introduction

In X-ray scattering experiments at XFEL facilities, the measured signal depends on the SASE pulse characteristics. These pulses exhibit shot-to-shot fluctuations in central energy, spectral width, and overall shape. Depending on resolution requirements and the relative size of broadening contributions from other factors, such as mosaicity, different approximations might be used.

2 Physical Framework

2.1 Scattering Model

Let $I(\mathbf{q})$ be the total scattering intensity as a function of the momentum transfer vector $\mathbf{q}$. It comprises Bragg (lattice) and diffuse components:

$$I(\mathbf{q}) = I_B(\mathbf{q}) + I_d(\mathbf{q}). \tag{1}$$

2.2 SASE Pulse Properties

SASE pulses feature a spectral intensity distribution $I_{\text{SASE}}(\omega)$, subject to:

- Shot-to-shot fluctuations in central energy ω_0 and spectral width σ_ω

2.3 Measurement Process

The intensity at pixel (x, y) is

$$I_{\text{det}}(x, y) = \int \left[I_B(\mathbf{q}(x, y, \omega)) \cdot G_B(x, y, \omega) + I_d(\mathbf{q}(x, y, \omega)) \cdot G_d(x, y, \omega) \right] I_{\text{SASE}}(\omega) \, d\omega, \tag{2}$$

where $\mathbf{q}(x, y, \omega)$ maps pixel position and photon energy to momentum transfer, while $G_B(x, y, \omega)$ and $G_d(x, y, \omega)$ represent the distinct geometric, partiality and polarization factors for Bragg and diffuse components, respectively.

3 Modeling Approaches by Complexity

3.1 Case 1: Stable Monochromatic Approximation

Assumptions:

- Negligible shot-to-shot jitter

- Negligible bandwidth

Model:

$$I_{\text{SASE}}(\omega) \approx \delta(\omega - \omega_0), \tag{3}$$

$$I_{\text{det}}(x,y) \approx I_B(\mathbf{q}(x,y,\omega_0)) \cdot G_B(x,y,\omega_0) + I_d(\mathbf{q}(x,y,\omega_0)) \cdot G_d(x,y,\omega_0). \tag{4}$$

3.2 Case 2: Shot-to-Shot Jitter, Monochromatic per Shot

Assumptions:

- Energy jitter included

- Each pulse treated as monochromatic

- Bandwidth still small compared to other effects

Model: For shot j,

$$I_{\text{SASE},j}(\omega) \approx \delta(\omega - \omega_j), \tag{5}$$

$$I_{\text{det},j}(x,y) \approx I_B(\mathbf{q}(x,y,\omega_j)) \cdot G_B(x,y,\omega_j) + I_d(\mathbf{q}(x,y,\omega_j)) \cdot G_d(x,y,\omega_j). \tag{6}$$

An approximate fractional change in intensity due to jitter:

$$\frac{\Delta I_{\text{det}}}{I_{\text{det}}} \approx \left| \nabla_{\mathbf{q}} \ln I \cdot \frac{\mathbf{q}}{|\mathbf{q}|} \right| \frac{\Delta\omega}{\omega} |\mathbf{q}|. \tag{7}$$

Question

How sharp are the features in the diffuse map? Is this fractional change negligible or not, for the diffuse scattering component?

3.3 Case 3: Shot-to-Shot Jitter with Gaussian Bandwidth

Assumptions:

- Energy jitter and bandwidth both matter

- SASE spectrum approximated as Gaussian

Model:

$$I_{\text{SASE},j}(\omega) \approx \exp\left[-\frac{(\omega - \omega_j)^2}{2\sigma_{\omega,j}^2}\right], \tag{8}$$

$$I_{\text{det},j}(x,y) \approx \int \left[I_B(\mathbf{q}(x,y,\omega)) \cdot G_B(x,y,\omega) + I_d(\mathbf{q}(x,y,\omega)) \cdot G_d(x,y,\omega)\right] \exp\left[-\frac{(\omega-\omega_j)^2}{2\sigma_{\omega,j}^2}\right] d\omega. \tag{9}$$

In reciprocal space, this corresponds to integrating over a "slab" of thickness proportional to $\Delta\omega/\omega \times |\mathbf{q}|$.

Differentiable Modeling (Monte Carlo)

Represent the SASE spectrum in $\mathbf{q}$-space as a 3D Gaussian, with covariance $\Sigma_j = L_j L_j^T$. The reparameterization trick samples

$$\mathbf{q} = \mathbf{q}_j + L_j \, \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \mathcal{N}(0, I),$$

yielding a Monte Carlo estimate of $I_{\text{det},j}(x, y)$. The distinct geometric factors must be applied to Bragg and diffuse components at each sampled point.

3.4 Case 4: Full SASE Spectral Shape

Assumptions:

- General shot-to-shot jitter

- No simple analytical form for the SASE spectrum

Model:

$$I_{\text{det},j}(x, y) = \int \left[I_B(\mathbf{q}(x, y, \omega)) \cdot G_B(x, y, \omega) + I_d(\mathbf{q}(x, y, \omega)) \cdot G_d(x, y, \omega) \right] I_{\text{SASE},j}(\omega) \, d\omega. \tag{10}$$

Implementation

Measure or reconstruct each pulse's spectral profile per shot. Discretize and integrate numerically.

Tradeoffs

Significantly more computationally expensive than case 4.

4 Practical Implications

5 PyTorch Example (Case 3)

```
def scattering_model(q_0, L, I_B_func, I_d_func, G_B_func, G_d_func, num_samples=100)
    # q_0: central q vector (or array) for a pixel
    # L: Cholesky factor of covariance matrix
    # I_B_func: function computing Bragg intensity at q
    # I_d_func: function computing diffuse intensity at q
    # G_B_func: function computing geometric/polarization factors for Bragg
    # G_d_func: function computing geometric/polarization factors for diffuse

    # Sample from standard normal
    epsilon = torch.randn(num_samples, 3)

    # Reparameterization
    q_samples = q_0.unsqueeze(0) + torch.matmul(epsilon, L.T)
```

```
# Compute Bragg + diffuse at each sampled q with appropriate geometric factors
I_samples = torch.stack([
    I_B_func(q) * G_B_func(q) + I_d_func(q) * G_d_func(q)
    for q in q_samples
])

# Monte Carlo average
return I_samples.mean()
```

6   Conclusion

A hierarchy of models provides a systematic way to incorporate SASE pulse effects in
X-ray scattering experiments. From the simplest monochromatic approximation to full
spectral modeling, one can balance computational effort against experimental fidelity.