Optics for Soft X-ray Seeding of LCLS-II
- Grating and Mirrors

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J. Krzywinski, J. Hastings, et al.
Outline

- Motivations
- Requirements
  - Input FEL parameters
  - Transform-limited pulses
  - Seeding power
- X-ray optics
  - Grazing-incidence Grating Monochromator
    - Fixed-focal point operation
    - Resolving power
    - Efficiency
  - Mirrors
    - Pre-mirror
    - Vertically focusing mirror
    - Horizontal focusing mirror
- Ray-tracing results
- Summary
Motivations

- SASE FEL temporal characteristics
  - Coherence time $\ll$ pulse duration

6 Å SASE FEL spectrum at 26 m in the first undulator

$\tau_c \sim 12$ fs

Goal $\Rightarrow$ make temporally fully coherent pulses
**Requirements**

- **Input FEL parameters**
  - **Energy range**
    - 200 – 2000 eV
  - **Pulse length**
    - 200 eV: 34 fs rms*, peak current 1 kA
    - 2000 eV: 12 fs rms*, peak current 3 kA
  - **Pulse energy**
    - 200 eV: 1.2 µJ, peak power ~ 10 MW
    - 2000 eV: 40 µJ, peak power ~ 1 GW
  - **e-beam size**
    - 200 eV: 50 µm rms†
    - 2000 eV: 15 µm rms†

*Note: FWHM = √12 rms
†Note: FWHM = 2.354 rms
Requirements

- Input FEL parameters (cont’d)
  - X-ray beam size
    - Energy dependent
    - Loosely speaking
      \[ w_0 \sim w_e \sim \sqrt{\varepsilon} \]
    - Transversely fully coherent
      - Gaussian optics necessary
  - X-ray pulse length
    - “Design goal” pulse length
    - Maximum pulse length
      - Afforded by optics to be transform-limited

![Grating Performance for Fixed Focus](image1)

![Grating Performance for Fixed Focus](image2)
Requirements

- Rigorous definition for transform-limited pulses

\[ \sigma_t \cdot \sigma_\omega \geq \frac{1}{2} \quad \sigma_t, \sigma_\omega \text{ are rms values} \]

- For a (temporal) Gaussian beam

\[ \sigma_t \cdot \sigma_\omega = \frac{1}{2} \]
\[ \sigma_t \cdot \Delta \omega_{FWHM} = \sqrt{2 \ln 2} \]
\[ \Delta \omega_{FWHM} = \frac{\sqrt{2 \ln 2}}{\sigma_t} \]
\[ R = \frac{\lambda}{\Delta \lambda_{FWHM}} = \frac{\omega}{\Delta \omega_{FWHM}} = \frac{\pi}{2 \ln 2} \frac{\Delta T_{FWHM}}{T} = 2.266 \frac{\Delta T_{FWHM}}{T} \]

- For a (temporal) flat-top beam

\[ \sigma_t \cdot \Delta \omega_{FWHM} = 1.607 \]
\[ \Delta \omega_{FWHM} = \frac{1.607}{\Delta T_{FWHM} / \sqrt{12}} \]
\[ R = \frac{\lambda}{\Delta \lambda_{FWHM}} = \frac{\omega}{\Delta \omega_{FWHM}} = \frac{2\pi}{1.607 \sqrt{12}} \frac{\Delta T_{FWHM}}{T} = 1.129 \frac{\Delta T_{FWHM}}{T} \]
Requirements

Performance requirements

- Resolving power to make pulse fully transform-limited, assuming flat-top profile
  - 200 eV
    - $\Delta T_{\text{FWHM}} = 117.78 \text{ fs}$
    - $R = 6428$
  - 2000 eV
    - $\Delta T_{\text{FWHM}} = 41.57 \text{ fs}$
    - $R = 22689$

- Seeding power after all optics
  - 200 eV: $> 10 \text{ kW}$
  - 2000 eV: $> 20 \text{ kW}$

- Seeding beam collinear w/ original beam
  - Transverse profile preserved if possible

- Time delay
  - $\sim 10 \text{ ps}$
  - Variable delay in tuning range is acceptable if within 10%
Operational requirements

- Energy tuning should be simple
- Use fewer gratings as possible
  - Use one or two gratings to cover entire energy range if possible
  - Design has just one grating
- Use fewer mirrors as possible
  - Reflection loss minimized
  - Easy alignment
  - Alignment easily maintained during energy tuning
- Use fewer and simpler mechanical motion as possible
  - Keep incident angle constant if possible especially for curved-mirrors
  - Use simple not convoluted motions if possible
- Optical components
  - Cylindrical horizontal focusing $M_1$
    - Focusing at re-entrant point
  - Planar pre-mirror $M_2$
    - Varying incident angle to grating $G$
  - Planar variable-line-spacing grating $G$
    - Focusing at exit slit
  - Exit slit S
  - Spherical vertical focusing mirror $M_3$
    - Re-collimate at re-entrant point
Grating Monochromator

**Grating Equation**

\[ \sigma ( \cos \theta - \cos \theta' ) = n \lambda \]

Since \( \theta \) and \( \theta' \) are both arbitrary, special conditions relating \( \theta \) and \( \theta' \) can be imposed for special modes of operation

- **Constant incidence angle mode**
  \[ \theta = \text{const.} \]

- **Constant included angle mode**
  \[ \alpha + \beta = \text{const.} \]

- **Constant focal-point mode**
  \[ \frac{\cos \beta}{\cos \alpha} = \frac{1}{\kappa} = \text{const.} \]

Grating \( \Rightarrow \) Angular dispersion

Focusing is needed for obtaining resolving power
Variable Line Spacing Grating

- **VLS focusing**
  - **Focusing condition**
    - **Linear coefficient**
      \[
      \frac{\Delta \sigma}{\Delta x} = \frac{\sigma^2}{\lambda} \left[ -\frac{\cos^2 \alpha}{r} - \frac{\cos^2 \beta}{r'} \right]
      \]
      - \(r, r'\) are positive
  - **If operate in fixed focal-point mode**
    - \(\Delta \sigma / \Delta x\) weakly energy dependent
    - Can only have a fixed linear coeff.
      - Defocusing effect (to be discussed)
        - No impact on resolving power
        - Big impact on transverse profile

**Grating Performance for Fixed Focus**

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>(-1.560E-07)</th>
<th>(-1.558E-07)</th>
<th>(-1.556E-07)</th>
<th>(-1.554E-07)</th>
<th>(-1.552E-07)</th>
<th>(-1.550E-07)</th>
<th>(-1.548E-07)</th>
<th>(-1.546E-07)</th>
</tr>
</thead>
</table>

- Small angle (high energy) limit
- Required for exact fixed focal-point

\[ \Delta \sigma / \Delta x = \frac{\sigma^2}{\lambda} \left[ -\frac{\cos^2 \alpha}{r} - \frac{\cos^2 \beta}{r'} \right] \]
Fixed focal-point mode

\[ \sigma (\sin \alpha - \sin \beta) = n \lambda \]

\[ \frac{\cos \beta}{\cos \alpha} = \frac{1}{\kappa} = 5.939 > 1 \]

- \( \sigma = 0.45 \, \mu m \, (2222 \, l/mm) \)
- \( n = 1 \)

“Fixed” focal-point
- “Fixed” exit slit
- Included angle \( \alpha + \beta \) variable
  - Rotation of pre-mirror
  - Rotation of grating

Use outside order
- Smaller \( \theta \) for larger footprint

![Diagram showing incident angle \( \theta \), exit angle \( \theta' \), and critical angles for Si, B\(_4\)C, and Be.]
Resolving Power

- Contributions
  - Quadrature addition of all terms
    - # of grating grooves
    - Size of incident beam
    - Footprint
  - Entrance slit
    - Slit-less, defined by incident beam
  - Exit slit
    - Image size
    - Slit settings
  - Slope error of optics

![Graph showing effective resolving power vs. energy](image-url)
Coherent Beam Propagation

- Use Gaussian beam propagation as 1\textsuperscript{st} order approx.
- Formulated based on ABCD matrix for ray-optics

\[
\begin{bmatrix}
A_{\text{total}} & B_{\text{total}} \\
C_{\text{total}} & D_{\text{total}}
\end{bmatrix} =
\begin{bmatrix}
1 & r & A & 0 \\
0 & 1 & C & 1/A
\end{bmatrix}
\begin{bmatrix}
1 & r' \\
0 & 1
\end{bmatrix}
\]

\[
A + Cr' \quad Ar + Crr' + r'/A
\]

\[
C \quad 1/A + Cr
\]

\[
\begin{bmatrix}
-M & 0 \\
-1/f_t & -1/M
\end{bmatrix}
\]

\[
A = \frac{\cos \beta}{\cos \alpha} = \frac{1}{\kappa}
\]

\[
C = \frac{\Delta \sigma(\lambda)}{\sigma^2 \cos \alpha \cos \beta} = \left( \frac{\kappa + 1}{r \kappa r'} \right) = -\frac{1}{f_t}
\]

\[
M = \frac{\cos \alpha r'}{\cos \beta r}
\]
Coherent Beam Propagation

- (Total) ABCD matrix for Gaussian beam
  - Waist location \( \delta r \)
  - Rayleigh length \( z_R \)

\[
\delta r' - i z_R' = \left[ \frac{A(\delta r - i z_R) + B}{C(\delta r - i z_R) + D} \right]_{\delta r = 0}
\]

\[
z_R = \frac{\pi w_0^2}{\lambda}
\]

\[
\delta r'(\lambda) = \left[ \frac{(A \delta r + B)(C \delta r + D) + AC z_R^2}{(C \delta r + D)^2 + (C z_R)^2} \right]_{\delta r = 0}
\]

\[
z_R' = \left[ \frac{- (A \delta r + B)C z_R + (C \delta r + D)A z_R}{(C \delta r + D)^2 + (C z_R)^2} \right]_{\delta r = 0}
\]

\[
z_R' = \frac{\pi w_0'^2}{\lambda}
\]

\[
M_{\text{Gaussian}}(\lambda) = \sqrt{\frac{z_R'}{z_R}} = \left[ \frac{- (A \delta r + B)C + (C \delta r + D)A}{(C \delta r + D)^2 + (C z_R)^2} \right]_{\delta r = 0}
\]
Coherent Beam Propagation

ABCD matrix for Gaussian beam w/ const. $\Delta \sigma / \Delta x$

\[
\delta r' = i z_R' = \frac{A(\lambda)(-i z_R) + B(\lambda)}{C(\lambda)(-i z_R) + D(\lambda)}
\]

\[
\delta r'(\lambda) = \frac{B(\lambda)D(\lambda) + A(\lambda)C(\lambda)z_R^2}{[D(\lambda)]^2 + [C(\lambda)z_R]^2}
\]

\[
z_R' = \frac{-B(\lambda)C(\lambda)z_R + D(\lambda)A(\lambda)z_R}{[D(\lambda)]^2 + [C(\lambda)z_R]^2}
\]

\[
M_{\text{Gaussian}}(\lambda) = \sqrt{\frac{-B(\lambda)C(\lambda) + D(\lambda)A(\lambda)}{[D(\lambda)]^2 + [C(\lambda)z_R]^2}}
\]
Dispersion Plane

- Optical components
  - Deflecting mirror
  - Pre-mirror
  - VLS Grating
  - Collimation mirror

![Dispersion Plane Diagram]

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>$L_1$</th>
<th>$L_{M1M2}$</th>
<th>$r_{M2G}$</th>
<th>$r_G'$</th>
<th>$r_{M3}$</th>
<th>$r_{M3}'$</th>
<th>$\Delta L_{Re-entrant}$</th>
<th>$r_{total}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>200 eV</td>
<td>13.761030</td>
<td>4.204372</td>
<td>0.036709</td>
<td>5.981053</td>
<td>0.351780</td>
<td>1.993796</td>
<td>1.656204</td>
<td>27.984945</td>
</tr>
<tr>
<td>2000 eV</td>
<td>13.761030</td>
<td>3.901582</td>
<td>0.339127</td>
<td>6.021674</td>
<td>0.311159</td>
<td>3.400840</td>
<td>0.249160</td>
<td>27.984572</td>
</tr>
</tbody>
</table>
Beam Size in Dispersion Plane

- Beam size evolution
  - Grating
    - \( w_0 \) object
    - \( w_0' \) image
    - \( z_R \)
    - \( r'(\lambda) \)
    - \( \delta r'(\lambda) \)
    - \( r'_{\text{non-coherent}} \)
  - Collimation mirror
    - \( w_0 \) object
    - \( w_0' \) image
    - \( z_R' \)
    - \( r'_{\text{non-coherent}} \)

Grating Performance for Fixed Focus

- Source
- Ray-optics
- Re-entrant point

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Time Delay

Optical delay
- Variable when tuning energy
  - ~ 10 ps +/- 10%
  - Variation Minimized by optimize $\Pi$

![Grating Performance for Fixed Focus](image)

- $\delta T$ (ps)
- Energy (eV)

$\xi$

$\gamma$

$\Pi$

$H'$

$H$

$\eta$

$\xi$

$\gamma$

$\Pi$

$H'$

$H$

$\eta$
**Sagittal Plane**

- **Optical components**
  - (Sagittally) Focusing mirror
  - Deflecting pre-mirror
  - Deflecting VLS Grating
  - Deflecting collimation mirror

---

**Table**

<table>
<thead>
<tr>
<th></th>
<th>$L_1$</th>
<th>$r^\prime_{M1}$</th>
<th>$\Delta r_{\text{Re-entrant}}$</th>
<th>$r_{\text{total}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>200 eV</td>
<td>13.761030</td>
<td>13.731681</td>
<td>0.492233</td>
<td>27.984945</td>
</tr>
<tr>
<td>2000 eV</td>
<td>13.761030</td>
<td>14.247250</td>
<td>-0.023708</td>
<td>27.984572</td>
</tr>
</tbody>
</table>
Beam Size in Sagittal Plane

- Beam size evolution
  - Focusing mirror

![Diagram showing beam size evolution and focusing mirror](image)

**Grating Performance for Fixed Focus**

- at designed location (ray-optics)
- re-entrant point
- source

**Graph showing energy (eV) vs. beam size (µm)**
Optimization of groove depth

For square wave lamella

\[
\eta_\lambda = \left( \frac{2}{m\pi} \right)^2 \sin^2 \left( \frac{\delta}{2} \right)
\]

\[
R_\lambda \approx R_\lambda \left( \frac{2\theta}{2} \right)
\]

\[
\delta = \frac{2\pi}{\lambda} (\cos \alpha + \cos \beta) \cdot h
\]

\[
\delta_{\text{peak}} = Q = m\pi, \text{ where } m = \pm 1, \pm 3, \ldots
\]

\[
\eta_{\text{peak}} = \left( \frac{2}{m\pi} \right)^2 \sin^2 \left( \frac{Q}{2} \right)
\]

\[h_{\text{peak}} \text{ only good for one energy}\]

\[
\delta(\lambda) = \frac{2\pi}{\lambda} (\cos \alpha + \cos \beta) \cdot h_{\text{peak}}
\]

\[
\frac{\eta(\lambda)}{R_\lambda(\alpha, \beta)} = \left( \frac{2}{m\pi} \right)^2 \sin^2 \left( \frac{\delta(\lambda)}{2} \right)
\]
Grating Efficiency

- Overall throughput
  - $M_1 \sim 100\%$
  - $M_2 \sim 100\%$
  - $G \sim R_\lambda \cdot \eta_\lambda \cdot b \sim 0.2\% - 0.005\%$
    - Reflectivity $R_\lambda$
    - Estimated grating efficiency $\eta_\lambda$
    - Bandwidth factor $b$
    - Beam size mismatch (very small)
  - $M_3 \sim 100\%$
- More rigorous calculations
  - Done by J. Krzywinski*
    - $\eta_\lambda$ agrees with estimate at 2000 eV
    - $\eta_\lambda$ 1/3 of estimate at 200 eV
    - Feature at 450 eV is evident

*Derived by solving Helmholtz equation in *inhomogeneous media*, in paraxial approximation

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Seeding Power

- Output power
  - \( p_{\text{output}} \sim p_{\text{input}} \cdot R_{\lambda} \cdot \eta_{\lambda} \cdot b \)
  - Estimates indicate goal is met
    - Simple amplitude grating estimate
    - J.K. rigorous calculation

![Graph showing grating performance for fixed focus](image)
## Optics Specs

### Grating specifications

<table>
<thead>
<tr>
<th>Parameter</th>
<th>symbol</th>
<th>value</th>
<th>unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Line spacing</td>
<td>$\sigma$</td>
<td>0.45</td>
<td>$\mu$m</td>
</tr>
<tr>
<td>Linear coeff</td>
<td>$\Delta\sigma/\Delta x$</td>
<td>-1.5527x10^{-7}</td>
<td></td>
</tr>
<tr>
<td>Groove height</td>
<td>$h$</td>
<td>4.984</td>
<td>nm</td>
</tr>
<tr>
<td>Grating profile</td>
<td></td>
<td>Lamella/Steps</td>
<td></td>
</tr>
<tr>
<td>Incident angle</td>
<td>$\theta$</td>
<td>8.963 – 28.26</td>
<td>mrad</td>
</tr>
<tr>
<td>Exit angle</td>
<td>$\theta'$</td>
<td>53.3 – 168.6</td>
<td>mrad</td>
</tr>
<tr>
<td>Included angle</td>
<td>$2\theta$</td>
<td>176.4 – 168.7</td>
<td>degree</td>
</tr>
<tr>
<td>Object distance</td>
<td>$L_{\text{obj}}$</td>
<td>~ 18</td>
<td>m</td>
</tr>
<tr>
<td>Image distance</td>
<td>$L_{\text{img}}$</td>
<td>~ 6</td>
<td>m</td>
</tr>
<tr>
<td>Exit slit</td>
<td>$s$</td>
<td>4 – 13</td>
<td>$\mu$m</td>
</tr>
</tbody>
</table>

---

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## Mirror specifications

<table>
<thead>
<tr>
<th>Parameter</th>
<th>symbol</th>
<th>value</th>
<th>unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylindrical mirror</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Radius $R_1$</td>
<td>$R_1$</td>
<td>0.2106</td>
<td>m</td>
</tr>
<tr>
<td>focal length $f_1$</td>
<td>$f_1$</td>
<td>7.800</td>
<td>m</td>
</tr>
<tr>
<td>Incident angle $\xi/2$</td>
<td>$\xi/2$</td>
<td>13.50</td>
<td>mrad</td>
</tr>
<tr>
<td>Planar mirror</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Incident angle $\gamma/2$</td>
<td>$\gamma/2$</td>
<td>8.14 – 75.4</td>
<td>mrad</td>
</tr>
<tr>
<td>Spherical Mirror</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Radius $R_3$</td>
<td>$R_3$</td>
<td>63.780</td>
<td>m</td>
</tr>
<tr>
<td>focal length $f_3$</td>
<td>$f_3$</td>
<td>0.30215</td>
<td>m</td>
</tr>
<tr>
<td>Incident angle $\eta/2$</td>
<td>$\eta/2$</td>
<td>9.475</td>
<td>mrad</td>
</tr>
<tr>
<td>Offset-1</td>
<td>$H$</td>
<td>0.1200</td>
<td>m</td>
</tr>
<tr>
<td>Offset-2</td>
<td>$H'$</td>
<td>0.1145</td>
<td>m</td>
</tr>
<tr>
<td>Offset-3</td>
<td>$II$</td>
<td>5.518</td>
<td>mm</td>
</tr>
</tbody>
</table>
# Optics Specs

## Performance

<table>
<thead>
<tr>
<th>Parameter</th>
<th>symbol</th>
<th>value</th>
<th>unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy range</td>
<td>$\varepsilon$</td>
<td>200 – 2000</td>
<td>eV</td>
</tr>
<tr>
<td>Pulse length (rms)</td>
<td>$\tau$</td>
<td>34 – 12</td>
<td>fs</td>
</tr>
<tr>
<td>Pulse energy</td>
<td>$E$</td>
<td>1.2 - 40</td>
<td>$\mu$J</td>
</tr>
<tr>
<td>Peak Power</td>
<td>$P_{\text{input}}$</td>
<td>10 - 1000</td>
<td>MW</td>
</tr>
<tr>
<td>E-beam size (rms)</td>
<td>$s$</td>
<td>50 -15</td>
<td>$\mu$m</td>
</tr>
<tr>
<td>Resolving power</td>
<td>$R$</td>
<td>&gt; 23000</td>
<td></td>
</tr>
<tr>
<td>Throughput</td>
<td>$\eta_{\text{total}}$</td>
<td>0.2 – 0.005</td>
<td>%</td>
</tr>
<tr>
<td>Output peak Power</td>
<td>$P_{\text{output}}$</td>
<td>26 - 49</td>
<td>kW</td>
</tr>
<tr>
<td>Time delay</td>
<td>$\Delta T$</td>
<td>10.837 – 9.595</td>
<td>ps</td>
</tr>
</tbody>
</table>
Ray-Tracing Calculations

- **Input parameters**
  - **Source**
    - **Spatial**
      - Gaussian
    - **Angular**
      - Gaussian
  - **Grating parameters**
    - **Object/image distances**
      - \( L_{\text{object}} = 18.000 \, \text{m}, \, L_{\text{image}} = 6.000 \, \text{m} \)
    - **Input/exit angles**
      - \( \alpha = \beta = 2\theta/2 = 88.2175^\circ \)
    - **Polynomial (variable-line-spacing)**
      - Groove density = 22222.22 l/cm
      - Linear coefficient = 76.89 l/cm²
      - Mount = TGM/Seya
      - Auto-tuning
      - Signed

- Best focus
  \[ g_1 = 76.89 \]

- Fixed linear coeff.
  \[ g_1 = 76.59 \]

- \[ g_1 = 76.39 \]

- \[ g_1 = 77.39 \]
End-to-end Results

- Source to re-entrant point simulation without exit slit

at source 
\((E, E+\Delta E, E-\Delta E)\)

at re-entrant point after M3 
(no slit)

at grating after M1

at exit slit location after grating 
(no slit)
End-to-end Results

- Source to re-entrant point simulation with exit slit

At source:
\[(E, E+\Delta E, E-\Delta E)\]

At re-entrant point after M3:

At grating after M1:

At exit slit after grating:
Summary

- **Design meets all requirements**
  - **High-resolution Grating Monochromator**
    - Fixed-focus operation excellent choice
      - Only single grating needed
      - Capable of tuning entire energy range
      - Defocusing effects understood
      - Few moving parts
    - Efficiency sufficient for seeding
      - Estimate and rigorous calculation indicate enough output power after mono
    - Delay is variable
      - but only weakly energy dependent
  
- **Mirrors**
  - Pre-mirror
    - Enables fixed-focus operation
  - Vertical collimation mirror
    - Re-collimates mono beam at entrance point
    - Has a short focal length, defocus effect is evident, but could be compensated
  - Horizontal focusing mirror
    - Focuses input beam at entrance point
Focusing requirements

- Image angular size < grating angular dispersion
  \[
  \frac{w_0'}{r'} \leq |\Delta \beta|
  \]
  - $r' \approx 6\, \text{m}$
  - Image angular size < 1.14 $\mu\text{rad}$
    - $w_0' < 6.84\, \mu\text{m}$

Possible solutions

- Focusing pre-mirror
- Spherical grating (fixed line spacing)
- Plane variable line spacing (VLS) grating
- Spherical +VLS grating
Angular Dispersion

Angular dispersion

\[ \Delta \beta = -\frac{\lambda}{R} \frac{1}{\sigma \cos \beta} \]

- At required resolving power \( R \)
- Much smaller than diffraction
  - Never be separated unless focused

\[
\begin{align*}
\lambda + \Delta \lambda &\quad \lambda \\
\alpha &\quad \beta \\
\Delta \beta &\quad \beta \\
\lambda &\quad \lambda
\end{align*}
\]

\[
\begin{align*}
\sqrt{2} w_0 &\quad w_0 \\
b &\quad w(z) \\
\Theta &\quad \Theta \\
z &\quad z
\end{align*}
\]

Diffraction-limited divergence
Grating dispersion \(|\Delta \beta|\)
VLSG focusing

Grating Performance for Fixed Focus

Energy (eV) vs. \(|\Delta \beta|\)
Grating Monochromator

- **Grating materials**
  - Si single crystal substrate
  - Proven fabrication technology
  - Superb roughness specs
  - But coating may be needed

- **Sustaining FEL full power**
  - At normal incidence
    - 200 eV: 1.2 µJ
    - 2000 eV: 40 µJ*
  - Peak energy deposition (per atom)
    \[ \varepsilon = \frac{2I_0}{\pi w_0^2(z) \alpha \frac{N_a \rho}{M}} \]
  - At \( z = 18 \) m
    - \( w_0(z = 18 \text{ m}) = 122 - 369 \) µm
    - Be is best, but coating unclear
    - \( \text{B}_4\text{C}, \text{C} \) coatings are safe but \( k \)-edge at \( \sim 283 \) eV
    - Si is also safe but \( k \)-edge at \( \sim 1824 \) eV

*Note: increased from original spec by 10x*
Grating Monochromator

- Use material void of absorption edges if possible
  - Be, Si are good for energy < 1800 eV
  - B₄C, C are good for energy > 300 eV
- Efficiency as high as possible
  - Must operate close to \( \theta_c \)
  - Critical angle \( \theta_c \)
    - Similar for almost all light material
    - Be, B₄C, C, and Si are fine
    - Almost linear in \( \lambda \)
Supporting Slides

- Alternative configurations
- ABCD formulations
  - Ray-optics
  - Gaussian beams
  - Arbitrary coherent beams
Alternative Configurations

Possible solutions

<table>
<thead>
<tr>
<th>Current configure</th>
<th>M₁</th>
<th>M₂</th>
<th>G</th>
<th>M₃</th>
<th>S</th>
<th>M₃</th>
<th>Note</th>
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<tr>
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<td>Planar-VLS</td>
<td>Fixed</td>
<td>Spherical</td>
<td>(small translation)</td>
<td>VLS needed</td>
<td></td>
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<tr>
<td>(sagittal plane)</td>
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<td>(tangential plane)</td>
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<tr>
<td>Configure - II</td>
<td>Cylindrical</td>
<td>Planar</td>
<td>Planar</td>
<td>Spherical</td>
<td>Fixed</td>
<td>Spherical</td>
<td>Extra mirror needed</td>
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<tr>
<td>(sagittal plane)</td>
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<td>(tangential plane)</td>
<td></td>
</tr>
<tr>
<td>Configure - III</td>
<td>Spherical</td>
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<td>Planar</td>
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<td>(tangential &amp; sagittal planes)</td>
<td></td>
<td>(tangential &amp; sagittal planes)</td>
<td></td>
</tr>
</tbody>
</table>

![Diagram showing the configurations with mirrors M₁, M₂, G, and M₃]
Example: design @ 2 keV

- **Optical pulse parameters**
  - $E = 2000$ eV
  - $\lambda = 6.200$ Å
  - $t = 2.068$ as
  - $\Delta T_{\text{FWHM}} = 41.57$ fs
    - $R = 22689$ to make it fully transform-limited

- **Transverse beam size**
  - Assuming predominantly TEM$_{00}$ mode
  - $\Delta x_{\text{FWHM}} = \Delta y_{\text{FWHM}} = 35.3$ µm
  - Beam waists $w_{0x} = w_{0y} = 30.0$ µm
  - Rayleigh length
    - $z_{Rx} = z_{Rx} = \frac{\pi w_{0x}^2}{\lambda} = 4.552$ m, if fully coherent
      - Diffraction-limited
    - $z_{Rx} < \frac{\pi w_{0x}^2}{\lambda} = 4.552$ m, if partially coherent
      - Not diffraction-limited
Variable Line Spacing Grating

- Fixed focal point operation
  \[
  \cos \beta = \frac{1}{\cos \alpha \kappa}
  \]

- Linear coefficient
  \[
  \frac{\Delta \sigma}{\Delta x} = -\sigma \frac{r' + r}{\sin \alpha - \sin \beta}
  \]
  \[
  = -\sigma \frac{\sin^2 \theta \left( \frac{1}{r} + \frac{1}{\kappa^2 r'} \right)}{\left( \sqrt{1 - \sin^2 \theta} - \sqrt{1 - \frac{1}{\kappa^2 \sin^2 \theta}} \right)}
  \]
  \[
  \approx -\sigma \frac{2 \left( \frac{1}{r} + \frac{1}{\kappa^2 r'} \right)}{\frac{1}{\kappa^2} - 1} \quad \text{if } \theta \ll 1
  \]
Variable Line Spacing Grating

If $\Delta \sigma / \Delta x = \text{constant at } \lambda_{\text{opt}}$

- Effective focus location

$$\frac{\lambda}{\sigma^2} \left[ \frac{\Delta \sigma}{\Delta x} \right]_{\lambda = \lambda_{\text{opt}}} = -\cos^2 \alpha - \cos^2 \beta$$

$$r'(\lambda) = \frac{\cos^2 \beta}{\cos^2 \alpha - \frac{\lambda}{r} \left[ \frac{\Delta \sigma}{\Delta x} \right]_{\lambda = \lambda_{\text{opt}}}}$$

- Effects of defocus
  - Larger image size at exit slit
  - Curved wavefront at exit slit

Grating Performance for Fixed Focus

- Larger image size at exit slit
- Curved wavefront at exit slit

Object $w_0$ to $\lambda$ to image $w_0'$

Energy (eV)

- $200$ to $2000$

Defocus (m)

- $-0.025$ to $0.035$
Operation of Pre-mirror

- Function of pre-mirror
  - Fixed focal point operation
    - Exit angle ($\beta$) variable
    - Rotation of grating
  - Incident ($\alpha$) & included ($2\theta$) variable
    - Motion of pre-mirror
      - Rotation and effective translation

![Graph showing grating performance for fixed focus](image)

- Included angle
- Incident angle
- Exit angle

Energy (eV) vs. $\alpha$, $\beta$, $2\theta$ (rad)

$M_1$, $M_2$, $M_3$
Operation of Pre-mirror

- Motion of pre-mirror
  - Rotation
    \[ \gamma' = \frac{1}{2}(\pi - 2\theta - \eta - \xi) \]
  - Translation
    - Variable
    ➔ Single rotation about a pivot point

![Graph showing the performance of a grating for fixed focus](image)
Rotation of Pre-mirror

- Rotation of pre-mirror
  - Center of rotation
  - ½ distance $\Pi$ above grating
  - Paraxial approximation

$$\lim_{\gamma' \to 0} \gamma' \cong \Gamma'$$

![Diagram showing pre-mirror rotation with center of rotation, half distance above grating, and paraxial approximation](image-url)
**Effective Source Location**

- Variation in source location
  - Optical path length difference
    - Extremely small (~ 0.40 mm)
  - Real concern
    - Jitter in FEL saturation point (~ 1 m)

---

![Grating Performance for Fixed Focus](chart)

**Virtual source point**

---

**Photon Division**

**X-ray Science Department**
Image at Exit Slit

- **Image formation**
  - Waist location shift about slit
  - Flat wavefront at waist
  - Curved wavefront at slit
    - Impact on collimation calculation

![Diagram of image formation with labels for waist, slit, and their respective locations](image)

![Graph showing Grating Performance for Fixed Focus with energy on the x-axis and s(µm) on the y-axis](graph)

- **Photon Division**
  - X-ray Science Department
Re-Collimation after exit slit

ABCD matrix

\[ A = \frac{\cos \beta}{\cos \alpha} = 1 \]

\[
\begin{bmatrix}
A_{\text{total}} & B_{\text{total}} \\
C_{\text{total}} & D_{\text{total}}
\end{bmatrix} = \begin{bmatrix}
1 & r & 1 & 0 & 1 & r' \\
0 & 1 & C & 1 & 0 & 1
\end{bmatrix}
\]

\[ = \begin{bmatrix}
1 + Cr' & r + Crr' + r' \\
C & 1 + Cr
\end{bmatrix}
\]

\[ = \begin{bmatrix}
M & 0 \\
-1/f_t & 1/M
\end{bmatrix}
\]

\[ M = -\frac{r'}{r} \]

\[ f_t = \frac{R \cos(\xi/2)}{2} \]
Coherent Beam Propagation

- ABCD matrix for Gaussian beam w/ const. $\zeta$

\[
\delta r' - i z_R' = \left[ \frac{M(\delta r - i z_R) + 0}{-(\delta r - i z_R)/f_t + 1/M} \right]_{\delta r = 0}
\]

\[
\delta r'(\lambda) = -M f_t z_R^2 \frac{f_t^2 + z_R^2}{(f_t/M)^2 + z_R^2}
\]

\[
z_R' = f_t^2 z_R \frac{z_R'}{z_R} = f_t \sqrt{\frac{z_R'}{z_R}} = \frac{f_t}{\sqrt{(f_t/M)^2 + z_R^2}}
\]

\[
M_{Gaussian}(\lambda) = \sqrt{\frac{z_R'}{z_R}} = \frac{f_t}{\sqrt{(f_t/M)^2 + z_R^2}}
\]

Grating Performance for Fixed Focus

- Designed Location of waist (ray-optics location)
- Designed location of re-entrant point
- Actual location of waist

Energy (eV) vs. Degree (m)

- $w_0$ to $w_0'$
- $z_R$ to $z_R'$
- $r$ to $r'$
- $\delta r'(\lambda)$
- $r'_{non-coherent}$

Photon Division
X-ray Science Department

SLAC
NATIONAL ACCELERATOR LABORATORY
Increase Input power?

6-Å FEL power along the **first undulator**

Saturation around 32 m with power ~10 GW

Present LCLS-II plan uses 40 meter long undulators
Coherent Beam Propagation

- ABCD matrix for Gaussian beam w/ const. $\zeta$

$$\delta r' - i z_R' = \left[ \frac{M(\delta r - i z_R) + 0}{-(\delta r - i z_R)/f_l + 1/M} \right]_{\delta r = 0}$$

$$\delta r'(\lambda) = -\frac{M f_l z_R^2}{(f_l/M)^2 + z_R^2}$$

$$z_R' = \frac{f_l^2 z_R}{(f_l/M)^2 + z_R^2}$$

$$M_{\text{Gaussian}}(\lambda) = \sqrt{\frac{z_R'}{z_R}} = \frac{f_l}{\sqrt{(f_l/M)^2 + z_R^2}}$$

Grating Performance for Fixed Focus

- Designed Location of waist
- Designed location of reentrant point
- Actual location of waist

Object $w_0$ to image $w_0'$ with reentrant point $z_R'$ and non-coherent $r'_{\text{non-coherent}}$.