5. Session 3
Limiting Radiation/Matter Interactions in Focused LCLS Beams

Seb Doniach
Stanford University
Limits on focused beam intensity
for molecular structure measurements
using an XFEL*

S. Doniach

* J. Synchrotron Radiation (1996) 3 260-267
how many photons to make a hologram of a small bio molecule?

For a small protein of ~ 1000 atoms need ≥ 300 photons/atom coherently scattered

$\rightarrow 3 \times 10^9$ photons/atom incident in 50 Fs

$\Rightarrow E_{x-ray} \sim 6 \times 10^5$ volt/Å (10'' watt)

Rate & absorption of EM energy by outer electrons:

electrons ionize in ~ 1 Bohr orbit

$\rightarrow \approx 100$ attoseconds

plasma temperature ~ 10^6 C (10 orbit velocities)

Conclusion: plasma forms too fast to see hologram
Plasma Formation by Focused photon beam

Classical motion of electron in $E^2$ field:

$$m \ddot{x} = -\frac{eV}{\dot{x}^3} + eE(t)$$

$x$ oscillates by $eE/m$ per cycle (attains $10^{-18}$)

escape velocity reached for Bohr orbits for which

$$E_B = \left(\frac{eEa_0}{\hbar}\right)^2 E_{\text{Ryd}}$$

quantum mechanically: inverse bremsstrahlung
atom in xray field $E=13$
Ion temperature heating rate

\[
\frac{dT_i}{dt} \sim \frac{8n_e e^4 z^2}{3M} \frac{[\ln \left( \frac{mv_e^2}{w} \right)]^2}{v_e}
\]

\[
\approx \frac{z^2 E_{\text{Ryd}}}{E_{\text{C}}} \left( \frac{E_{\text{Ryd}}}{E_{\text{C}}} \right) \left( \frac{m}{M} \right) \left( \frac{v_e}{a_e} \right) \frac{m}{M} \left\{ \ln A \right\}^2
\]

\[
\sim \frac{z^2 m}{M} \left\{ \ln A \right\}^2 \cdot 30 \text{eV/fs} \quad (\text{for } E_{\text{C}} \approx 100 \text{eV})
\]

ie ions reach around 1eV \sim 10^4 \text{eV} in 1 femtosecond

C rough estimate: need to include field induced wiggle velocities.

* Polishchuk, Meyer-Ter-Vehn

Smallest sample to make diffraction pattern before it ionizes?

$1 (\mu m)^3 \sim 4 \times 10^4$ protein molecules:

$5 \times 10^{12}$ photons / pulse $\sim 10^7$ coh. diffracted photons

$\sim 7 \times 10^3$ photoionization events per molecule

$\sim > 1$ photoionization/atom

$\rightarrow$ 1 shot/sample

$10 (\mu m)^3$ maybe $> 1$ shot/sample
DXS measurement

$I(\vec{q}, t)$

$I(\vec{q}, t+\tau)$

 photons incoherent in time
**DXS**

*(dynamic X-ray scattering)*

Measure $I_q(t)$ at different times

Perform *post-detection interferometry*

$$C(q,z) = \frac{1}{T} \int_0^T I_q(t) I_q(t+z) \, dt$$

$$= \langle S_q(0) S_q(0) S_q(z) S_q(z) \rangle - \langle S_q(0) S_q(0) \rangle^2$$

For liquids this becomes

$$C(q,z) \equiv \{ S_q(0)^2 + S_q(z)^2 \}$$

when $S_q(z) = \langle S_q(0) S_q(z) \rangle$

Complementary to slow neutrons
DxS event rates for FEL versus synchrotron source (intrinsic advantage) (i.e., storage ring)

time tagged photons

\[ e_1, e_2, \ldots, t \rightarrow \left\lfloor \frac{N}{T} \text{photons in time } T \right\rfloor \rightarrow \]

DxS events: \( N^2 \) events in \( M \) time bins

Synchrotron bunch trains vs. FEL bunch trains

\( R \) repetitions/\( \text{sec} \) vs. \( S \) repetitions/\( \text{sec} \)

Events/\( \text{sec/} \)bin

\[
\frac{N^2R}{M} \quad \text{vs} \quad \left[ N\left(\frac{R}{S}\right) \right]^2 \frac{S}{M}
\]

\[
\therefore \quad \frac{\text{FEL events}}{\text{synchrotron events}} = \frac{R}{S} \approx 10^4
\]
Fastest events in protein Folding

helix ↔ random coil (Schwarcz 1965)

helix nucleation
(Zimm-Brass model)

ccc ⇄ che

\[ T_{\text{ccc}} \sim T_{H-bond} e^{-\frac{U}{kT}} \]

\[ \tau_{\text{ccc}} \approx 10^4 \text{ picosec} \]

\[ \Rightarrow <10^{-8} \text{ sec} \]

(Schwarcz estimate \( 2 \times 10^{-8} \text{ sec} \))

Recent T-jump data: 10's of nanosec for small peptide (Woodrut et al)
Crystal Optics for the LCLS

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CRystal Optics
For the LCLS
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LCLS Workshop, Stanford, January 23 and 24, 1997

Outline

1. Optics for Third Generation Sources:
   - Examples of optics used at the ESRF
     - Source properties
     - Cryogenic cooling
     - Diamond crystals

2. Crystal Optics for the LCLS:
   - Source properties
   - Crystal geometries
### Basic Optical Elements for Hard Synchrotron X-Rays

<table>
<thead>
<tr>
<th>Mirrors</th>
<th>Multilayers</th>
<th>Single Crystals</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total external reflection</td>
<td>Bragg diffraction</td>
<td></td>
</tr>
<tr>
<td>Fresnel equations</td>
<td>Bragg equation: (2d \sin(\theta_B + \delta) = n \lambda)</td>
<td></td>
</tr>
<tr>
<td>Reflection</td>
<td>Reflection</td>
<td>Reflection and transmission</td>
</tr>
<tr>
<td>Rayleigh-Rice theory</td>
<td>Scalar theory</td>
<td>Dynamic theory, perfect mosaic model, imperfect</td>
</tr>
<tr>
<td>Other theories</td>
<td>Vector theory</td>
<td></td>
</tr>
<tr>
<td>Surface roughness = 2 A</td>
<td>4 ≤ (\theta_B) ≤ 90 degrees</td>
<td></td>
</tr>
<tr>
<td>Source size (vertical, low-(\beta) undulator) is 90 pm (FWHM)</td>
<td>4 ≤ (\theta_B) ≤ 90 degrees</td>
<td></td>
</tr>
<tr>
<td>Beam divergence (vertical, high-(\beta) undulator) is (FWHM)</td>
<td>4 ≤ (\theta_B) ≤ 90 degrees</td>
<td></td>
</tr>
</tbody>
</table>

### Functions

- **High energy cut-off**
- **Focusing - Collimating**
- **Power filter**
- **Energy resolution**: \(\Delta E/E = \frac{2\epsilon}{\Delta\theta \cdot \cot \theta_B}\)

### Conservation of Emittance: Optics Quality

#### Beam Quality

(FPR, 1987: \(\epsilon_v = 0.7\) nm; 1995: \(\epsilon_v = 0.04\) nm, diffraction limit effects appear)
- Source size (vertical, low-\(\beta\) undulator) is 90 pm (FWHM), ±9 pm stability.
- Beam divergence (vertical, high-\(\beta\) undulator) is 20 \(\mu\)rad (FWHM), ±2 \(\mu\)rad stability.

#### Mirror Requirements

- Surface: microroughness ≈ 3 A; slope error = 2 \(\mu\)rad (rms) for blur = source size.
- Ultra-precise shaping and superpolishing are required.
- Very accurate and stable mechanical mounting, UHV environment.

#### Multilayer Properties

- Surfaces and interfaces must be very smooth and flat, of the order 3 A and 1 \(\mu\)rad (rms).
- Nanometric tailored structures of various materials are required.
- Uniformity of the d-spacing of about 1% over 300 x 50 mm\(^2\) is required.
- Well controlled deposition process is necessary.
- Very accurate and stable mechanical mounting in UHV environment is required.

#### Single Crystal Monochromators

- Perfect Si and Ge crystals exist, but they must be transformed into monochromators by orientation, cutting, etching and polishing.
- Strain-free crystal preparation and accurate and stable mounting required.
- Other crystals must be developed for special purposes (Be, diamond, YB\(_{66}\) ...).
### SOME CRYSTAL PARAMETERS AT 8 KEV

<table>
<thead>
<tr>
<th>Material</th>
<th>(h k l)</th>
<th>$d_H = \frac{1}{2} \lambda_{\text{max}}$ (Å)</th>
<th>$\rho F H e^{2M/v_0}$ (10$^{-14}$ cm$^2$)</th>
<th>$\delta_{\text{FWHM}}$ (Å)</th>
<th>$\varepsilon_{\text{FWHM}}$ (10$^{-6}$)</th>
<th>$t_e$ (µm)</th>
<th>$t_a$ (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Be (002)</td>
<td></td>
<td>1.7916</td>
<td>5.59</td>
<td>10.7</td>
<td>22.8</td>
<td>5.0</td>
<td>1200</td>
</tr>
<tr>
<td>Be (110)</td>
<td></td>
<td>1.1428</td>
<td>4.27</td>
<td>6.49</td>
<td>7.1</td>
<td>10.3</td>
<td>1874</td>
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<tr>
<td>C$^*$ (111)</td>
<td></td>
<td>2.0593</td>
<td>11.1</td>
<td>24.1</td>
<td>59.7</td>
<td>2.20</td>
<td>250</td>
</tr>
<tr>
<td>C$^*$ (220)</td>
<td></td>
<td>1.2611</td>
<td>9.55</td>
<td>14.9</td>
<td>19.3</td>
<td>4.16</td>
<td>408</td>
</tr>
<tr>
<td>Si (111)</td>
<td></td>
<td>3.1354</td>
<td>10.82</td>
<td>34.3</td>
<td>135</td>
<td>1.48</td>
<td>8.7</td>
</tr>
<tr>
<td>Si (220)</td>
<td></td>
<td>1.9200</td>
<td>12.29</td>
<td>25.3</td>
<td>57.7</td>
<td>2.12</td>
<td>14.2</td>
</tr>
<tr>
<td>Ge (111)</td>
<td></td>
<td>3.2663</td>
<td>23.06</td>
<td>76.0</td>
<td>313</td>
<td>0.66</td>
<td>2.94</td>
</tr>
<tr>
<td>Ge (220)</td>
<td></td>
<td>2.0002</td>
<td>27.51</td>
<td>58.5</td>
<td>140</td>
<td>0.91</td>
<td>4.79</td>
</tr>
</tbody>
</table>

**Perfect (nearly perfect) single crystal**

**SILICON**

- Energy Difference (MeV)

  - 1.320 - 660 - 0 - 660 - 1.320

  - Back-scattering Si (13, 13, 13)

  - Rocking-curve, $T_{\text{free}}$ scan @ 26keV

  - $dE/E = 2 \cdot 10^{-8}$ (FWHM)

  - Best value ever achieved recently improved to $9 \cdot 10^{-9}$ !

  - F. Sot et al., ESRF Report (1993) 4

**GERMANIUM**

- Energy Difference (MeV)

  - 0 - 660 - 1.320

  - Ge double crystal in Laue case
diffraction pattern @ 1.4 MeV

  - Excess width: $2 \cdot 10^{-8}$ rad

  - Best value ever achieved

**BERYLLIUM**

- Diamond and Be

  - ESRF, ID10,

  - Undulator spectra

  - 0.5x0.5mm$^2$ @ 44m


  - Grobel et al., J. Phys. C. 4

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PERFECT CRYSTAL MONOCHROMATORS

The relative wavelength resolution of a perfect crystal put in a white incident beam of divergence \( \omega_0 \) ("white" means an energy bandwidth wider than that accepted by the crystal) can be obtained by differentiating Bragg's law and assuming Gaussian distribution functions when convoluting \( r(\Delta h) \) and \( I(\psi) \)

\[
\frac{\Delta E}{E} \left( = \frac{\Delta \lambda}{\lambda} \right) = (\omega_0^2 + \psi_0^2)^{1/2} \cot \theta_b
\]

We see that \( \psi_0 \) is the intrinsic crystal energy resolution that is to first order independent of energy (Bragg case only!) but varies with the square of the d-spacing and is proportional to the structure factor that in turn depends on \( (\sin \theta)/\lambda = 1/2d_h \).

The extinction thickness, i.e. the penetration depth \( t_e \) perpendicular to the lattice planes is given by

\[
t_e = v_o/(2d_h r_0 C | F_{hr} |)
\]

so that \( \psi_0 = t_e/d_h = 2\pi N_p \) where \( N_p \) is the number of lattice planes participating in the diffraction. Thus the crystal acts as a grating.

* In optics: "resolution power" (resolution = 1/resolving power)
The reflection pattern \( r(\Delta) \) of a crystal corresponds to the reflected intensity, normalized to the incident intensity of a monochromatic and parallel X-ray beam. Recorded as a function of the angle it is often called "rocking curve" and has the following shape

\[
r(\Delta) = L - (L^2 - 1)^{1/2}
\]

where \( L \) depends in a complicated way on the crystal structure factor, absorption, polarization and other parameters. The width of the rocking curve (Darwin width) for the symmetric case is given by

\[
\omega_s = 2(\lambda^2 r_o C |F_{hr}| e^{-M})/(\pi v_o \sin 2\theta_b)
\]

where \( r_o \) is the classical electron radius, \( C \) is the polarization factor (\(-1\) for \( \sigma \)-polarization and \( \cos 2\theta_b \) for \( \pi \)-polarization), \( F_{hr} \) is the real part of the structure factor, \( e^{-M} \) is the Debye-Waller factor and \( v_o \) is the volume of the crystallographic unit cell. This equation can be written as

\[
\omega_s = \varepsilon_s \tan \theta_b
\]

\[
\varepsilon_s = 4(d h^2 r_o C |F_{hr}| e^{-M})/\pi v_o
\]

see, e.g., Halszita & Hashizume, Handbook of Synchrotron Radiation, 1980.

(very good article on monochromators?)
CONSERVATION OF BRILLIANCE: THE HEAT LOAD

PRESENT-DAY X-RAY BEAM POWER AT THE ESRF
(at 100 mA, insertion device length = 1.6 m, 30 m from source point, F.P. Report, 1987)

- Undulators: total power: 100 W, central cone: 20 W, power density in central cone: 20 W/mm² normal to the beam.
- Wundulators: total power: 1.8 kW, power density: 40 W/mm² normal to the beam.
- Wigglers: total power: 5 kW, power density: 20 W/mm² normal to the beam.

FUTURE X-RAY BEAM POWER

- Will be 4 to 6 times higher, because:
  => Current increased to 200 mA.
  => Emittance 20 times smaller.
  => Longer and smaller-gap insertion devices will be installed.

CONSEQUENCES

- Materials must have small x-ray absorption ➞ low Z. (diamond, beryllium)
- Efficient cooling needed to prevent from melting.
- Thermal deformation to be minimised by cooling geometry. (thin elements, side-cooling)
- Small thermal expansion and big conductivity. (cryogenic)
- Materials must not degrade in intense x-ray beams.
- Cooling must not produce strains and vibrations.

SINGLE CRYSTAL MONOCHROMATORS

Perfect single crystals are generally used to select a more or less narrow monochromatic energy band out of wiggler or undulator radiation according to Bragg's law

\[ 2d_{\text{h}} \sin(\theta_{\text{h}} + \delta_{\text{h}}) = \lambda / n \]

where \( d_{\text{h}} \) is the lattice spacing of crystallographic planes belonging to the reflection, \( h \) stands for the Miller indices and \( \theta_{\text{h}} \) is the Bragg angle given by the angle between the incident (or the reflected) beam and the lattice planes.

- The integer \( n \) denotes the reflection order: \( d_{nh} = d_{h}/n \) and thus wavelengths \( \lambda_1, \lambda_{1/2}, \lambda_{1/3}, \ldots, \lambda_{1n} \) are reflected simultaneously as far as the reflections are not forbidden by the crystalline structure.

- Crystals can be used in reflection ("Bragg case") or in transmission geometry ("Laue case").
- The reflection can be symmetric or asymmetric.
- In all cases except the symmetric Laue case the reflection occurs at an angle different from the geometrical angle because of refraction. (refraction correction \( \delta_e \))
Fig. 3. Measured (a) and calculated (b) diffraction profiles of a parallel-sided silicon crystal in Laue geometry at the wavelength of 0.0731 nm. Solid lines for reflection and broken lines for transmission. Crystal thickness of 293 μm was assumed for calculation.

T. Ishikawa (1992)

74 / SPIE Vol. 1740 Optics for High-Brightness Synchrotron Radiation Beamlines (1992)
HIGH ANGULAR AND ENERGY RESOLUTION

Resolutions achieved: \[ \frac{\Delta E}{E} = 3.5 \cdot 10^{-7} \] (5 meV at 14.4 keV)
\[ \psi = 2 \mu \text{rad} = 0.4 \text{ arcsec} \]
Heat Problem: Crystal case

- usually $P_s$ very high $\Rightarrow \Delta_{\text{bump}} > \Delta_{\text{bending}}$

\[ \Delta_{\text{bump}} \sim \frac{\alpha}{k} GPe^{-\mu x} \begin{cases} \mu x < 1 \Rightarrow x = t \\ \mu x > 1 \Rightarrow x = t_{\text{abs}} \end{cases} \]

- one reflection: increase of beam divergence and bandpass
- double reflection: loss of transmission

<table>
<thead>
<tr>
<th>Material</th>
<th>Re</th>
<th>C*</th>
<th>Si</th>
<th>Ge</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal</td>
<td>hcp</td>
<td>diamond</td>
<td>diamond</td>
<td>diamond</td>
</tr>
<tr>
<td>$\mu @8\text{keV [cm}^{-1}\text{]}$</td>
<td>1.8</td>
<td>7.5</td>
<td>141</td>
<td>402</td>
</tr>
<tr>
<td>$\kappa @297\text{K [Wcm}^{-1}\text{K}^{-1}]$</td>
<td>1.94</td>
<td>23</td>
<td>1.5</td>
<td>0.64</td>
</tr>
<tr>
<td>$\alpha @297\text{K [10}^{-6}\text{K}^{-1}]$</td>
<td>7.7</td>
<td>1.1</td>
<td>2.4</td>
<td>5.6</td>
</tr>
<tr>
<td>$\kappa/\mu\alpha @ 297\text{K [MK]}$</td>
<td>0.14</td>
<td>2.80</td>
<td>5 $\times 10^{-3}$</td>
<td>3 $\times 10^{-4}$</td>
</tr>
<tr>
<td>@ 77K [MK]</td>
<td>11</td>
<td>120</td>
<td>2 $\times 10^{-1}$</td>
<td>7 $\times 10^{-3}$</td>
</tr>
</tbody>
</table>
Cryogenic cooling for crystal (and multilayer substrates)

Thick crystal, side cooled
\[ P_s = 150 \text{W/mm}^2, P_t = 80 \text{W} \]
NSLS X2S


Thin crystal, direct cooled
\[ P_s = 415 \text{W/mm}^2, P_t = 167 \text{W} \]
ESRF BL3

peak power density is 2000 \text{W/mm}^2

DIAMOND SINGLE CRYSTALS - THE ULTIMATE

Recent heat load tests at the ESRF under extreme conditions:

Incident beam: 3.4 kW/mm² heat flux, 280 W total power.

Absorbed: 109 W/mm², 8.7 W. (3.1%)

Results: rocking curves (upper fig.)

"cold" beam (full circles)
"hot" beam (open circles)

FWHM: 3.2 arcsec, ΔT = 100 K.

Mounting strain/mosaic spread: 4 μrad

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Schematic of the experiments on Beamline 3 at the ESRF.


The wundulator beam is focused by a toroidal mirror onto an 4 x 8 x 0.1 mm³ synthetic diamond crystal (supplied by F. Sellschop, University of Johannesburg)

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MICROSCOPE PICTURE

X-RAY TOPOGRAPH

(provided by F. Sellschop)

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Beam width-

particle:

TROIKA

GUERRICA

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BEAM MULTIPLEXING

THE "TROIKA" CONCEPT (Alt-Hülsem, Freund, Grübel)

1 Undulator; 3 Experimental Stations!
THE PURSUIT OF BRILLIANCE

OPTICS FOR THE LCLS: GOALS

Two Main Objectives:

1. Provide the tools for source diagnostics:

=> source size, beam divergence, spectral properties, (time structure), peak brightness, flux, degree of coherence, polarization.

=> mostly known techniques, done with single crystal-based optical elements.

2. Provide the possibility to perform first and LCLS-specific experiments:

=> to be selected according to scientific applications (see later).

Guidelines:

following the ASAP-ASARA rule:

As Simple As Possible
As Sophisticated As Reasonably Achievable!

(what is "reasonably achievable" ?? => budget, staff, timeframe...to be discussed)
ASYMMETRIC BRAGG REFLECTIONS

From: Kohra et al., in Matsushita & Hashimoto article.
PERFECT CRYSTAL MONOCHROMATORS

If the reflection is asymmetric meaning that the lattice planes make an angle $\alpha$ with the crystal surface the width is

$$\omega_o = \omega_s / b^{1/2}$$
$$\omega_h = \omega_s \cdot b^{1/2}$$

for the incident and exit beams, respectively, where

$$b = \frac{\sin(\theta_b - \alpha)}{\sin(\theta_b + \alpha)}$$

is the asymmetry factor. The energy resolution and the extinction depth have to be changed accordingly.

Associated with the angular beam transformation is the change in spatial cross section of the beam:

$$w_h = w_o / b \Rightarrow \omega_h w_h = \omega_o w_o$$

which expresses Liouville's theorem.

The angular shift of the Bragg peak is for the symmetric Bragg case

$$\delta_o = \omega_s F_{0r} / (2 \sqrt{C | F_{hr} | e^{-M}})$$

where $F_{0r}$ is the real part of the structure factor in forward direction. For the asymmetric case

$$\delta_o = (1 + 1/b) \delta_s / 2 \text{ and } \delta_h = (1 + b) \delta_s / 2$$
Schematic DuMond diagram for an asymmetrically cut crystal in the Bragg geometry. The horizontal dashed line represents divergent monochromatic radiation incident on the crystal. The enlarged insets show the Bragg-law curves (dot-dashed) and the reflectivity bands (between the solid lines) on the incidence and exit sides. The angular range emitted is |b| times the angular range accepted.


\[ \lambda/2d = \sin (\theta_i - \alpha - \Delta\theta_i) \]

\[ \lambda/2d = \sin (\theta_e + \alpha - \Delta\theta_e) \]

\[ (\lambda/d) \sin \alpha = \cos \theta_e - \cos \theta_i \]
RECI PROCAL SPACE AND MONOCHROMATIC BEAM

EWALD CONSTRUCTION

WHAT IS THE "DARWIN WIDTH"?

THE DARWIN WIDTH IS A SHEARING OF THE RECIPROCAL LATTICE VECTOR DUE TO FINITE PENETRATION DEPTH. IT IS NOT AN ANGULAR QUANTITY!

RECI PROCAL SPACE DIAGRAM

( MOMENTUM SPACE )

RADIATION

"DARWIN WIDTH"

"ANGULAR DARWIN WIDTH"

\[
\Delta k = \frac{\Delta t}{\pi} \cot \theta
\]

IN THE PRESENT CASE: \( k_0 \approx k_0' \) (FOR RELAXATION)
RECI PROCAL SPACE DIAGRAM

Asymmetric Bragg reflection
spherically expanding case

$\Delta k/k = 4\omega_0 c \cos \theta_0$

$\chi_0 \ll \omega_1$
**Reciprocal Space Diagram**

- Monochromatic beam

Asymmetric Bragg reflection
- Spatially expanding case

\[ \frac{\Delta \omega}{\omega} = \omega \cot \theta \]

**Liouville's theorem**

- Asymmetric Bragg reflection
- Spatially condensing case

\[ \theta = \theta_c \]
**Examples : Si and Diamond at 1.5A**

<table>
<thead>
<tr>
<th>Crystal</th>
<th>d(A)</th>
<th>qB</th>
<th>q</th>
<th>qE</th>
<th>b</th>
<th>foot (mm)</th>
<th>dE/E</th>
<th>t_ref (mm)</th>
<th>t_abs (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si (220)</td>
<td>1.9200</td>
<td>22.99°</td>
<td>0.1°</td>
<td>45.88°</td>
<td>411</td>
<td>85.9</td>
<td>1.2x10^-3</td>
<td>0.10</td>
<td>3-10^-9 0.124</td>
</tr>
<tr>
<td>C (III)</td>
<td>2.0593</td>
<td>21.36°</td>
<td>0.1°</td>
<td>42.62°</td>
<td>388</td>
<td>85.9</td>
<td>1.2x10^-3</td>
<td>0.11</td>
<td>0.65 2.33</td>
</tr>
</tbody>
</table>

*No refraction corrections of the Bragg angle included.*

**Isophases and Isochrones**

- Inclined optics
- Invariance effect
- Anomalous transmission
- Long beamlines

**Possibilities:**
- Time dispersion
- Time focusing
- Bunch lengthening
- Bunch compression

In connection with:
- Time-energy dependence of source
- Gradient crystals

**Isophasic and Isochronic**

Bunch lengthening due to penetration depth effect.
Power Considerations for the TESLA FEL: Photon Beam Transport and Monochromatization

Josef Feldhaus
HASYLAB at DESY
Power considerations for the TESLA FEL: Photon beam transport and monochromatization

J. Feldhaus, HASYLAB at DESY

1. TESLA FEL parameters
2. Beam transport: mirrors for deflection and focusing
3. Monochromatization
Average and Peak Power Density

\[ \sim 1 \text{ kW} \quad \text{average power} \]
\[ \sim 100 \text{ kW} \quad \text{peak} \]

\[ \text{minimise photon-matter interaction} \]
\[ \text{1. large distance} \quad \sim 1 \text{ km} \]
\[ \text{2. low-Z elements:} \]

<table>
<thead>
<tr>
<th>\text{Be}</th>
<th>\text{C}</th>
<th>(\text{Si})</th>
<th>\tilde{\text{X}}</th>
</tr>
</thead>
<tbody>
<tr>
<td>\sigma_{1\text{a}} \left(10^{-24} \text{ cm}^2\right)</td>
<td>3.2</td>
<td>20</td>
<td>790</td>
</tr>
</tbody>
</table>

Cu K-edge: \sim 4000 \text{ below}
30000 \text{ above}

increases with \(\lambda\)

\[ \sigma_{250\text{a}} \text{ (Mb)}: \quad 0.5 \quad 1.8 \quad 0.4 \quad 17 \]
<table>
<thead>
<tr>
<th>crystal</th>
<th>Be (002)</th>
<th>C (111)</th>
<th>Si (111)</th>
</tr>
</thead>
<tbody>
<tr>
<td>d-spacing (Å)</td>
<td>1.792</td>
<td>2.059</td>
<td>3.136</td>
</tr>
<tr>
<td>density (g/cm³)</td>
<td>1.85</td>
<td>3.52</td>
<td>2.33</td>
</tr>
<tr>
<td>thermal conductivity (W cm⁻¹ K⁻¹)</td>
<td>1.93</td>
<td>23</td>
<td>1.5</td>
</tr>
<tr>
<td>thermal expansion (10⁶ K⁻¹)</td>
<td>7.7</td>
<td>1.2</td>
<td>2.4</td>
</tr>
<tr>
<td>1/e absorption length at 1 Å (µm)</td>
<td>25100</td>
<td>2800</td>
<td>250</td>
</tr>
<tr>
<td>1/e absorption length at 2.4 Å (µm)</td>
<td>1420</td>
<td>165</td>
<td>20</td>
</tr>
<tr>
<td>1/e absorption length at 4 Å (µm)</td>
<td>280</td>
<td>35</td>
<td>4.8</td>
</tr>
<tr>
<td>1/e absorption length at 6.25 Å (µm)</td>
<td>70</td>
<td>9</td>
<td>1.5</td>
</tr>
<tr>
<td>1/e absorption length at 15 Å (µm)</td>
<td>5</td>
<td>0.8</td>
<td>1.6</td>
</tr>
</tbody>
</table>

Table 5.5.1. Properties of possible monochromator crystals.
Table 5.5.2. FEL photon beam parameters. The maximum tolerable average power density absorbed by a monochromator crystal is of the order of 20 kW/cm\(^2\) for diamond and 1 kW/cm\(^2\) for silicon.

\[
\frac{1}{P_{\text{tot}}} \approx 100 \text{W} ??
\]
Angular Power [kW/mrad$^2$]

FEL: $3 \times 10^{17}$ kW/mrad$^2$

Planar Undulator

Helical Undulator

$\theta = 500$ m: $5$ cm $\theta$

Angular Power [kW/mrad$^2$] vs Angle [\mu rad]

P. Gürtler, HASYLAB Dec 96
Power density

- everything evaporates near the undulator
  (except mirrors at grazing incidence)
  + well cooled low-Z material
- peak power o.k. at large distance
- " " probably o.k. for Be, C, (B, B, C...)
  near the undulator
- spontaneous emission:
  - penetrates thin low-Z crystals
  - larger divergence → pinhole
  
  no serious problem
Fig. 1. Photon energy dependence of the reflectivity of beryllium, diamond and silicon for a grazing angle of incidence of 2 mrad.
Fig. 2 Angular dependence of the reflectivity of beryllium (top) and diamond (bottom) for different x-ray wavelengths.
Table 5.5.4. Power density absorbed by beryllium, diamond and silicon mirrors at 2 mrad angle of incidence.

<table>
<thead>
<tr>
<th>λ (Å)</th>
<th>Be mirror at z = 0m (Wcm⁻²)</th>
<th>Be mirror at z = 600m (Wcm⁻²)</th>
<th>C mirror at z = 0m (Wcm⁻²)</th>
<th>C mirror at z = 600m (Wcm⁻²)</th>
<th>Si mirror at z = 0m (Wcm⁻²)</th>
<th>Si mirror at z = 600m (Wcm⁻²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6.25</td>
<td>96</td>
<td>0.02</td>
<td>291</td>
<td>0.05</td>
<td>3183</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>41</td>
<td>0.13</td>
<td>69</td>
<td>0.21</td>
<td>1023</td>
</tr>
<tr>
<td>3</td>
<td>15</td>
<td>225</td>
<td>0.01</td>
<td>589</td>
<td>0.04</td>
<td>471</td>
</tr>
<tr>
<td>4</td>
<td>2.4</td>
<td>37</td>
<td>0.04</td>
<td>122</td>
<td>0.14</td>
<td>1437</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>380</td>
<td>0.05</td>
<td>1212</td>
<td>0.15</td>
<td>12442</td>
</tr>
<tr>
<td>6</td>
<td>1</td>
<td>264</td>
<td>0.33</td>
<td>449</td>
<td>0.56</td>
<td>6638</td>
</tr>
</tbody>
</table>

deformation? : FEM simulations

problem: defocussing over large distance
Beam transfer and focusing

- highest reflectivity for lowest θ:
  \[ \Rightarrow \text{power density reduced by } \sim 10^5 \]
  (at θ = 2 mrad)

- mirrors at large distances o.k.
  \[ \Rightarrow \text{focusing "no problem"} \]

- many reflections possible

  \[ R = 0.995 \Rightarrow R \approx 2\% \text{ for U-turn} \]
  (at 2 mrad)

  - 5° - 10° deflection leaves \( \approx 90\% \) flux
    \[ \Rightarrow \text{reducing radiation background in the experimental hutch} \]
    \[ \text{combining radiation from different sources on one sample ("pump-and-probe")} \]

- focusing down to \( \approx 1:1000 \Rightarrow 50 \mu m \) ?
  \( (\leq 0.5 \text{ m } : 500 \text{ m}) \)

- general problem: surface accuracy

  1) \( \sigma' = 0.7 \mu \text{rad} \)
  2) 25 \( \mu \text{m in } 250 \text{m} \)
  \[ \text{or } 50 \text{nm in } 50 \text{cm} \]
  \[ 10^{-7} \text{ rad} ! \]
Figure 5.6: Spectrum of the radiation pulse near the saturation point for an 1 Å FEL with parameters presented in Table 5.3. Graph (a) is plotted over the full width of the radiation pulse spectrum and graph (b) presents enlarged fraction of graph (a). Calculations have been performed with linear simulation code.
Monochromatization

- \( \frac{\Delta E}{E} \) = 0.2% too large for most exper. FEL \[ \Rightarrow \text{use diamond}(Be), (Si). \]

- \( \lambda \leq 6.2 \text{Å} \) (for Si) \( \lambda \leq 4 \text{Å} \) for C(111)
- \( \lambda \geq 6.2 \text{Å} \):
  - single pulses on other (disposable) crystals (beryl, YBa, ...)
  - gratings?
  - under developed energy range?

- Si requires \( P \leq 1 \text{KW/cm}^2 \)
  \[ \Rightarrow \text{can only be used at reduced flux} \]

- diamond takes \( \approx 20 \text{KW/cm}^2 \) and 90\% is transmitted at 1 Å
  \[ \Rightarrow \text{OK at } 600 \text{mJ, but: total power?} \]

- Little experience with Be
  (no perfect crystals, small mosaic spread)

- Cooling needs R&D

* Two-stage FEL with monochromator between two undulators?
  \[ \text{OK for diamond at } 1 \text{KW and } 20 \text{KW/cm}^2, \]
**CONCLUSIONS**

- optimistic for $h\nu \geq 4\text{keV}$

  but

- all optical components will probably spoil the diffraction, limited collimation significantly.

- VUV-FEL will be exciting due to large cross-sections