Thermal, mechanical deformation and stability of Monochromator Crystals under high heat load
Outline

- Cooling strategy
  - Water or LN2, direct or indirect, crystal size and cooling scheme
- Crystal material, properties
  - Crystals, Silicon, doping, anisotropic elasticity, pure isotope
- Thermal deformation
  - Finite element analysis (FEA)
  - Measurement techniques
  - Comparison between measurements and simulations
  - Some extended FEA results
    - Power and power density, beam size, grazing angle, cooling coefficient,…
    - Focusing effects
- Initial deformation of the crystal
  - Manufacturing, mounting, and cooling down to LN2 temperature
- Stability and vibration
  - Some measurement results
Cooling strategy: mirror and monochromator

Thermal deformation - comparison of mirror and monochromator

➢ For an incident beam at 30 m
  ● Power density $P_{a0}=200 \text{ W/mm}^2$
  ● Beam size $H \times V=2 \times 1 \text{ mm}^2$

White beam mirror

- typical grazing angle: 2 mrad
- footprint: 500 ~ 1000 mm
- Power density $P_a \sim 1 \text{ W/mm}^2$
- Topside cooling by water

- typical length: 1000 mm

Monochromator crystal

- typical Bragg angle: 12° (209 mrad)
- footprint ~ 1% as long as for mirror
- Power density $P_a \sim 50 \text{ W/mm}^2$
- Cooling scheme?
Cooling strategy: white beam mirror

Solution to minimize thermal deformation for white beam mirror (smart shape + full illumination):

- Mirror size: 800x80x80
- Grazing angle 3.1 mrad
- 2~3 coatings
- Heat load: **834 W**
  Gaussian distribution
  \( \sigma = 3.86 \text{ mm} \)

**ESRF UPBL06 (ID16)**

- Heat load: \( 834 \text{ W} \)
- Gaussian distribution
- \( \sigma = 3.86 \text{ mm} \)

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**Cooling strategy: mirror and monochromator**

Can monochromator crystal be cooled as mirror (full illumination) ?

**White beam mirror**

- \( P_a = 1 \text{ W/mm}^2 \)
- \( W_{bm} = 2 \text{ mm}, \ H_{cool} = 10 \text{ mm} \)
- \( h_{cv-eq} = 5000 \text{ W/m}^2/\text{°C} \)

\[
\Delta T_{\text{min}} = T_{\text{min}} - T_f = \frac{P_a}{h_{cv-eq}} \frac{W_{bm}}{2H_{cool}}
\]

\[
\Delta T_{\text{min}} = 20^\circ\text{C}
\]

For **Monochromator crystal**

- \( P_a \sim 50 \text{ W/mm}^2 \)

\[
\Delta T_{\text{min}} = 1000^\circ\text{C} \quad !!!
\]

Impossible to cool the Monochromator as the mirror
Cooling strategy for monochromator crystal

Full side cooling (to increase cooling surface area)

- $P_a \sim 50 \text{ W/mm}^2$
- $W_{bm}=2 \text{ mm}, L_{bm}=5 \text{ mm}$,
- $H_{cool}=t_{\text{mono}}=50 \text{ mm}$
- $L_{cool}=L_{\text{mono}}=100 \text{ mm} \gg L_{bm}$
- $h_{cv-eq} = 5000 \text{ W/m}^2/\text{oC}$

\[
\Delta T_{\text{min}} = \frac{P_a * W_{bm} * L_{bm}}{h_{cv-eq} * 2 * H_{cool} * L_{cool}}
\]

\[
\Delta T_{\text{min}} = 10^\circ \text{C}
\]

Cooling of monochromator needs crystal significantly longer than beam footprint

Bottom cooling

- Cooling surface area reduced

Direct cooling

- No thermal contact resistant
- Sealing difficulty
- Sealing induced stress and deformation
Crystal material, Properties of Si

Materials for Monochromator crystal

- **Silicon:**
  - Perfect crystal
  - Large size Φ100x500
  - Very reasonable price
    (900€/kg, 9000€ for Φ100x500)
  - Interesting properties at low temperature

- **Germanium**
  - Less perfect
  - Medium size Φ100x75
  - 4 ~ 40 times more expensive than Si

- **HPHT Synthetic Diamond**
  - Imperfect
  - Small size 10x10x1
  - Expensive
Anisotropic elasticity of Si

- Silicon: cubic diamond crystal structure
- Stiffness coefficient matrix
  - 3 three independent elastic coefficients for Si (100)
  - Can be calculated for any crystallographic orientation
    - Analytically
    - By codes (MatLab, Python)

\[
\begin{bmatrix}
  c_{11} & c_{12} & c_{12} \\
  c_{12} & c_{11} & c_{12} \\
  c_{12} & c_{12} & c_{11}
\end{bmatrix}
\]

- Important for bent silicon crystal
- For thermal deformation?

\[C_{100} = \begin{bmatrix}
    c_{11} & c_{12} & c_{12} \\
    c_{12} & c_{11} & c_{12} \\
    c_{12} & c_{12} & c_{11}
\end{bmatrix}\]

Figure 6
(a) Elastic modulus in the directions $e_1'$ and $e_3'$. (b) Shear modulus and (c) Poisson’s ratio in the directions 12 and 23 for silicon (3 1 1). The vector $e_1'$ is fixed in the normal direction [3 1 1], and the vectors $e_2'$ and $e_3'$ are in the crystal plane (3 1 1). The angle $\alpha$ is between the vectors $e_1'$ and [1 -1]21/2 in the crystal plane: $e_2'(\alpha=0^\circ) = [0 1 -1]2^{1/2}$, $e_3'(\alpha=90^\circ) = [2 -3 -3]/(2)^{1/2}$.

Anisotropic elasticity of Si

- **Thermal deformation**
  - Depends on the Poisson’s ratio:
    \[ \Delta \theta \propto \frac{(1 + \nu) \alpha}{k} \]
  - Poisson’s ratio depends on the crystal orientation
  - Thermal slope error
    \[ \Delta \theta = \frac{\partial u_1}{\partial x_2} \propto \left( \nu_{12} + \nu_{13} \right)/2 \]
  - But the average \( \nu_{av} = (\nu_{12} + \nu_{13})/2 \) is constant

- **Thermal deformation with anisotropic elasticity of silicon \( \rightarrow \) Simulation with isotropic and constant elasticity \( (\nu_{av}) \)

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Si related Crystal material: Germanium doped silicon

- **Germanium doped silicon** $\text{Si}_{100-x}\text{-Ge}_x (x \leq 2\%)$
  - Ge doping decreases dislocation mobility, and modifies dislocation nodes in Si crystalline lattice
  - Increasing semi-conducting device efficiency: material strength, current carrier mobility
  - Application to DCM: $\text{Si}_{100-x}\text{-Ge}_x$ for $1^{st}$ crystal (LN$_2$), Si for $2^{nd}$ crystal (water)

  - Vegard’s law: 
    $$ \Delta d/d_{\text{Si}} = \mu x $$
    ($\mu = 4.18 \times 10^{-4}$)
  - Concentration $x \sim 0.7\%$

- Ge doping reduces dramatically the thermal conductivity of Si especially at LN2 temperature
  - Therefore the application of Si-Ge crystals to cryogenic cooling cannot be recommended


Si related Crystal material: pure isotope silicon

- Three stable isotopes in natural silicon:
  - Silicon-28 : 92%
  - Silicon-29 : 4.7%
  - Silicon-30 : 3.3%

**Single-isotope** silicon-28 crystal (99.9%)

- Very high thermal conductivity \( k = 30000 \text{ W m}^{-1} \text{ K}^{-1} \) at 20 K, 6 times higher than natural Si
- Available, used in semiconductor industry
- Small size, very expensive
- Technology challenge for effective cooling
  - Huge size and high cost of cooling system for 500 W cooling power

natSi, $^{28}$Si and Diamond for very high heat-load monochromator

Macro-pulse train effects ($f=10$Hz)

- LN2 cooled diamond crystal ($20\text{mm} \times 20\text{mm} \times 20\text{mm}$)
- LHe cooled single-isotope silicon-$28$ crystal ($20\text{mm} \times 20\text{mm} \times 20\text{mm}$)
- LHe cooled natural silicon crystal ($120\text{mm} \times 60\text{mm} \times 60\text{mm}$)

Time-structure proposal of TESLA X-FEL (repetition rate 10 Hz)

$L.\text{ Zhang et al., AIP Conference Proceedings, 705, pp.639-642 (2003)}$
Thermal deformation of the monochromator crystal

For monochromator crystal

- 3D temperature and deformation
- Non-linear material properties \((k, \alpha)\)
- Finite Element Analysis (FEA) for the modeling

Example of water cooling
Thermal deformation: side cooling versus bottom cooling

- Similar temperature distribution
  but low temperature with side cooling
- Very comparable thermal deformation:
  0.7% lower thermal deformation with side cooling
  → Thermal bump deformation predominant!

How to reduce this huge thermal slope error $\theta_{th} = 1085 \, \mu{rad}$?
Thermal deformation: water cooling versus LN2 cooling

Water cooling vs LN2 (Liquid Nitrogen) cooling

For LN2 cooling
\[ \theta_{th} = 18 \, \mu \text{rad} \]
\[ \theta_{RMS} = 3 \, \mu \text{rad} \]
Reduced by a factor of 61 for \( \theta_{th} \)
(96 for \( \theta_{RMS} \))
Thermal deformation: indirect measurement technique

- Thermal deformation → Rocking-curve broadening
- Rocking-curve width:

\[
FWM_{c} = \sqrt{(\theta_{th} + \theta_{0})^2 + FWM_{\text{intr}}^2}
\]

- Comparison of test and FEA results for ID09 LN2 cooled Si crystal (Channel-Cut Monochromator)

\[\text{FWHM}_{\text{exp}} = 9.3 \ \mu\text{rad} \quad \text{FWHM}_{\text{theory}} = 7.7 \ \mu\text{rad}\]

Zhang L. et al., JSR (2003). 10, 313-319
Thermal deformation: direct measurement technique

Applied to ID06, ID18 and ID26 LN2 cooled Si crystal

- Multiple angular scans across the Bragg peak (rocking curve) at various vertical positions of a narrow-gap slit downstream from the monochromator

\[ \Delta \theta_{th} = \theta^*_{\text{peak}} - \theta_B \]

Thermal deformation: direct measurement technique

ID06 LN2 cooled Si crystal (DCM)

- **FEA** (Gaussian distribution and volume power absorption, $h_{cv}$ determined by fitting temperature in only one case)

- For various other cases (I, HxV)

- Excellent agreement in Temperature

Thermal deformation: direct measurement technique

ID06 LN2 cooled Si crystal (DCM)

(1st) Direct comparison of test results and FEA results

Thermals slope versus Power and Bragg angle

For UPBL06 LN2 cooled monochromator crystal

- Si 111, 5~20 keV
- LxWxT = 100x60x80 mm³
- White beam mirror used to reduce the heat load
- Beam size HxV=2x1 mm²
- Indirect cooling \( h_{cv} = 4000 \text{ W/m}^2/\text{K} \)

- Bragg angle: 5.6 ~ 23.1°
For UPBL06 LN2 cooled monochromator crystal

- Bragg angle: 10.4,

**Effective cooling coefficients:**
- $h_{cv}$ (W/m²/K)
- 2000 poor contact
- 4000 correct contact
- 8000 excellent contact
- 12000 direct cooling
- 20000 enhanced direct cooling

**Indirect cooling vs direct cooling**
- $P_{\text{limit}}$ (Indirect cooling) = 345 W
- $P_{\text{limit}}$ (direct cooling) = 375 W
- Direct cooling is interesting for the heat load in a small range (345, 375) W

**Good contact between cooling block and silicon crystal is needed**
Focusing effects of the monochromator crystal

For UPBL06 (ID20) LN2 cooled Si crystal

- Silicon crystal at $p=31$ m
- Beam size: $H \times V = (1.8\sim 2.8) \times 0.8$ mm² at 27m
- Bragg angle: $5.6 \sim 23.1°$
- Variable absorbed power
- Gaussian power distribution
- Thermal deformed crystal shape calculated by FEA: radius $R_{xtal}$
- Required radius $R_{req}$ for beam collimation ($q \to \infty$):

$$R_{req} = \frac{2p}{\sin(\theta_{Bragg})}$$

- Beam collimation is achievable by using only monochromator and by monitoring primary slits opening

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Diamond crystal monochromator

ID28 SS Diamond monochromator, U32g15

- **Parameters**
  - $e_{ph} > 12$ keV
  - At 28 m from the sources
  - Incident angle: 26 degrees
  - Beam size: $H \times V = 1.3 \times 0.5$ mm$^2$
  - Water cooling (indirect)
  - Diamond crystal size: $4 \times 8 \times 0.3$ mm$^3$
  - Darwin width at 311: $2 \mu$rad

- **Recommendations for $\Delta \theta < 0.4 \mu$rad, $T_{max} < T_{melt}(\text{In})$**
  - Beam size reduced to just cope with centre cone $H \times V = 1.3 \times 0.5$ mm$^2$
  - 0.8-mm (0.3+0.5) thick diamond attenuator in front
  - Maximize contact surface area
  - Thermal Contact Resistance (TCR) $> 7000$ W/m$^2$/°C (Indium foil to be used)
Initial deformation of the crystal

Heat load tests of the LN2 cooled monochromator → initial deformation of the crystal due to

- Monochromator components manufacturing, crystal cutting, mounting and assembling, cooling down from $T_{room}$ to $T_{LN2}$


### Parameters

<table>
<thead>
<tr>
<th></th>
<th>ID06 DCM</th>
<th>ID18 DCM</th>
<th>ID09 CCM</th>
</tr>
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<tbody>
<tr>
<td>$\theta_0$</td>
<td>0.45</td>
<td>1.0*</td>
<td>5.5</td>
</tr>
<tr>
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<td>2900</td>
<td>3500</td>
<td>$\mu\text{rad}$</td>
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<td></td>
<td></td>
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<td>1400</td>
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<td></td>
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<td>$W/m^2/K$</td>
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Stability and vibration of the monochromator

Example of ID06 Cinel mono

Correlation between X-ray intensity fluctuation and mechanical vibration
- $F=24.8, 66.2, 70.3, 78.7, 82.8$ Hz
- 1st peak due to vacuum pump 1, other 4 peaks due to pump 2

Remaining peaks probably due to mechanics \(\rightarrow\) room for improvement
Beam intensity fluctuation $\Delta I$ versus the cryo-cooler pump frequency

- For Oxford mono, high $\Delta I$ for $f_{\text{pump}} > 45$ Hz is due to the cooling scheme and mechanical structure of the mono
DCM vibration tests in ID22 (1997)

1997, ID22, 3D accelerometer
1st direct in-situ measurement on the LN2 cooled crystal

SET-UP

1997, ID22, LN2 cooled crystal
DCM vibration tests in BM25 (2004)

BM25 mono

Geophone L4C-H

Geophone L4C-V

Duo-beam Laser Vibrometer

FrF

PSD (μm/s²)/Hz

BM25 Mono - Frequency Responses w.r.t. Floor

BM25 - PSD relative to mono frame and on floor

Laser beam

Second crystal

First crystal

2014, L. Zhang
Summary

- Thermal deformation can be accurately modeled
- Crystal monochromator has focusing effects (R ~ 200 m)
- Thermal deformation depends on Poisson’s ratio $\nu$:
  $$\Delta \theta \sim (1 + \nu)$$
  but Anisotropic elasticity of the silicon can be taken into account by use of an average Poisson’s ratio in a simulation with isotropic and constant elasticity
- There are rooms for the improvement in terms of stability, and initial deformation of the crystal monochromator
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  - T. Weng*, M. Wulff

  (* Left ESRF)

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