Applications of a pnCCD Detector Coupled to Columnar Structure CsI(Tl) Scintillator System in Ultra High X-Ray Energy

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Outline

• pnCCD: 4-D detector
• Efficiency limitation
• Configuration of pnCCD+CsI(Tl) and detection process
• Determination of Energy Resolution
• Application: structure factor determination
• Summary
pnCCD: 4D detector

• Every event is recorded with it’s position (x,y), Energy and intensity

• Typical energy resolution of 2% at 10keV and 0.7% at 100 keV

• Spatial resolution less than one pixel (pixel size = 75 x 75µm)

• Fast readout frequency: 300Hz in normal mode and 1000Hz in burst mode

Laue pattern recorded by pnCCD


Norbert Meidinger, Robert Andritschke, Robert Hartmann, Sven Herrmann, Peter Holl, Gerhard Lutz, Lothar Strüde; pnCCD for photon detection from near-infrared to X-rays.
Limitation!

- Quantum Efficiency of silicon based detectors drops to less than 1% at photon energy 100keV
- Causes limitation for experiments using hard X-ray energies.
- Alternative approaches: replace Si by Ge/GaAs, but crystal quality cannot compete with that of Silicon
Columnar structure CsI(Tl) + pnCCD

Configuration

700µm

Columnar CsI(Tl)

Al substrate

Optical coupler

450µm

pnCCD

128 x 128 pixels

Pixel size = 75 x 75µm

X-ray

Quantum efficiency of pnCCD, CsI(Tl) and pnCCD+CsI(Tl).

D. Schlosser, M. Huth, R. Hartmann, A. Abboud, T. Conka Nurdan, M. Shokr, U. Pietsch, L. Strüder; Direct and indirect signal detection of 122 keV photons with a novel detector combining a pnCCD and a CsI(Tl) scintillator, 2015

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Detection Process

- **Direct detection**: Photon creates e-h pairs. e⁻ clouds directly drifted into the pixels creating the “direct signal” proportion to photon’s energy.

- **Indirect detection**: photon creates optical photons (550nm) in CsI(Tl). Generated photons isotropically radiated toward pnCCD with efficiency of 85%. Each optical photon is then generates 1 e-h pair. Generated e⁻ cloud is drifted to the pixels creating the “indirect signal”.

**Example**: 80keV Laue spot:

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Characterization

EDDI beamline

Laue pattern

Direct image

Indirect image

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Using spots detected directly and indirectly at the same time, we obtain a linear relation between direct and indirect energy

\[ E_d \text{ (keV)} = 5.4 \times E_{\text{indir}} \text{ (keV)} + 5.8 \]

Using the obtained relation, the indirect ppot energies can be determined

<table>
<thead>
<tr>
<th>Spot ( X_i )</th>
<th>Energy (keV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( X_1 )</td>
<td>99.78</td>
</tr>
<tr>
<td>( X_2 )</td>
<td>126.54</td>
</tr>
<tr>
<td>( X_3 )</td>
<td>111.7</td>
</tr>
<tr>
<td>( X_4 )</td>
<td>107.53</td>
</tr>
<tr>
<td>( X_5 )</td>
<td>95.56</td>
</tr>
<tr>
<td>( X_6 )</td>
<td>117.39</td>
</tr>
<tr>
<td>( X_7 )</td>
<td>112.46</td>
</tr>
<tr>
<td>( X_8 )</td>
<td>107.6</td>
</tr>
</tbody>
</table>

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Determination of Energy Resolution

For direct peak (pnCCD):

\[
R = \frac{FWHM}{E} = \frac{2.35\sqrt{(ENC^2 + FE/w)}}{E}
\]

\[w = 3.67\text{ eV}\]

\[ENC = 5.5\text{ equivalent noise charge}\]

\[F = 0.115, \text{ Fano factor in Si}\]

For indirect peak (pnCCD+CsI(Tl)):

\[
R = \frac{FWHM}{E} = 2.35 \sqrt{\frac{F_{CsI}}{N_{e}}} + \frac{\nu(T) + \nu(\eta) + \frac{1-\eta}{N_e} - \frac{ENC^2}{N_e^2}}{E}
\]

\[N: \text{ number of generated electrons}\]

\[\nu: \text{ the variance}\]

\[F_{CsI} = 0.28, \text{ Fano factor in CsI}\]

\[T = L * w_{CsI} = 60 \text{ photons/keV x 14eV = 0.84}\]

\[\eta: \text{ quantum efficiency}\]

16.5% < R < 18.5%

0.7% < R < 0.9%

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Application: X-Ray Structure Factor determination

- X-ray structure factor ($F_{hkl}$) is a mathematical function describing the amplitude and phase of a wave diffracted from crystal lattice planes characterised by Miller indices $h,k,l$.

- It is the Fourier transform of the atomic positions within the crystal unit cell.

- Using measured $F_{hkl}$ one can determine the electron density distribution within a unit cell.

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Application: X-Ray Structure Factor determination

Example GaAs

Experimentally

Using kinematic theory: \( |F_{\text{exp}}|^2 = \frac{I_{\text{hkl}}}{C\varepsilon I_0 LPA} \)

- \( I_{\text{hkl}} \) is the measured intensity
- \( I_0 \) is the primary intensity hits the sample at the given energy
- \( C\varepsilon \) takes into account the absorption factor of the sample
- \( \varepsilon \) is the quantum efficiency of the detector
- \( L \) is a scale factor

Theoretically

\[
|F_{hkl}|^2 = \begin{cases} 
16 \left( f_{Ga} T_{Ga} + f_{As} T_{As} \right)^2 & \text{for } h+k+l=4n \\
16 \left( f_{Ga} T_{Ga} - f_{As} T_{As} \right)^2 & \text{for } h+k+l=4n+2 \\
16 \left( f_{Ga}^2 T_{Ga}^2 + f_{As}^2 T_{As}^2 \right) & \text{for } h+k+l=4n+1 \text{ or } 4n+3 
\end{cases}
\]

\( i \)s the Lorentz Factor

A takes into account the absorption factor of the sample
\( \varepsilon \) is the quantum efficiency of the detector
\( C \) is a scale factor
\( P = \frac{1}{2} \left( 1 + \cos^2 2\theta \right) - \frac{1}{2} \cos^2 2\rho \sin^2 2\theta \) is the polarized Factor
\( L = \frac{\lambda^2}{\sin^2 \theta} \) is the Lorentz Factor

\( f \) is the form factor,
\( T_i = e^{-B_i \sin^2 \theta / \lambda^2} \) is the temperature factor And \( B_i \) is the Debye Waller factor

\( F_{\text{exp}} \) is the experimentally determined structure factor

Strong reflection
Weak reflection
Moderate

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Laue Diffraction experiment

- **FCC structure**: $hkl$ should be **all even** or **all odd**
- $\sqrt{h^2 + k^2 + l^2} = \frac{a}{d_{hkl}}$ with $d_{hkl} = \lambda / \sin \Theta$ and $a = 5.653\,\text{Å}$
- $\cos \phi = \frac{h_1 h_2 + k_1 k_2 + l_1 l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2} \sqrt{h_2^2 + k_2^2 + l_2^2}}$

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Experimental X-Ray Structure factor

Using kinematic theory:

\[ |F_{\text{exp}}|^2 = \frac{I_{hkl}}{C \varepsilon I_0 \text{LPA}} \]

- \( I_{hkl} \) is the measured intensity
- \( I_0 \) is the primary intensity hits the sample at the given energy
- \( A \) takes into account the absorption factor of the sample
- \( \varepsilon \) is the quantum efficiency of the detector
- \( C \) is a scale factor

\[ P = \frac{1}{2} (1 + \cos^2 \theta) - \frac{1}{2} \tau \cos^2 2\rho \sin^2 \theta \] is the polarized Factor

\[ L = \frac{\lambda^2}{\sin^2 \theta} \] is the Lorentz Factor

\[ I_{hkl} = \frac{I_0}{QE_{ph}} \]

Error propagation in intensity calculation =

\[ \sigma_{sys} = \frac{I_{hkl}}{QE_{ph}^2} \times \sigmaQE_{ph} \quad \text{and} \quad \sigma_{stat} = \frac{\sqrt{I_{hkl}}}{QE_{ph}} \]

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X-ray Structure factor: Experimental (direct & indirect) vs. Theoretical

\[ |\Delta F/F| = \left( F_{\text{theo}} - F_{\text{exp}} \right) / F_{\text{theo}} = \]

- strong reflections: 18% for direct, 3% for indirect
- weak reflections: 35% for direct, 15% for indirect

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summary

• By combination of CsI(Tl) scintillator with silicon based pnCCD detector, hard X-Ray radiation (50-100keV) photons can be measured indirectly with an efficiency equivalent to the pnCCD efficiency at low energy (1-10keV) without scintillator

• Measured Energy resolution is between 0.7 and 0.9% for direct Bragg peaks and between 16.5 and 18.5% for indirect peaks in the energy range [50, 100] keV

• When intensity determination is required, the errors in the experimental values in the hard X-ray applications were reduced by an average of 15% w.r.t the old system

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