Spectroscopy & Coherent Scattering (SCS) Scientific Instrument

Andreas Scherz for WP86 European XFEL

Study of electronic, spin, and atomic structures on the nanoscale using soft X-rays explore excited-state dynamics on ultrafast time scales and unravel the function of complex materials in applied and quantum material science, basic energy science as well as bioscience
Electron energy working points and SASE3 Photon energies
Hutch planning with PSPO, WTM and DERU
WP-74, DESY - K. Tiedtke

- Pulse-resolved monochromatic beam intensity (abs. err. <10%, rel. err. <1%)
- Sensitivity to work in low-charge mode (<5fs monochromatic pulses)
- Absolute beam position monitor

- Production
- Delivery to WP74

2015-Mid

K. Tiedtke et al. (DESY)
**Technical Specifications**
- $1 \times 10^{-4} \rightarrow 1 \times 10^{-9}$ mbar
- 18mm apertures / tubes
- $N_2$, and Kr as well as Xe

- Components ordered. Device tests end of 2015-Q1 at Hera-South
**KB best refocusing:**
- Minimum beam size: 1.5x1.5 µm²

**Near-focus conditions soft x-rays:**
- 1.5 - 10µm  
  0 - 1.6 x Rayleigh range

**Out-of-focus by bent mechanism:**
- Maximum beam size: 1 x 1 mm²
SCS BEAMLINE: KB mirror system

- Invitation to tender
- Award of contract

Substrate length: ~500mm (vert.) and ~700mm (horz.)
KB bender mechanics: maximum tangential slope error 150nrad

Users' Meeting 2015

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**Flexible Design**
- 4 mirrors for wide wavelength range
- Large mirrors for high energy pulses
- External x, y and z translation on stable translator
- Internal $\theta$, $\Phi$ (piezo motor)
- On-axis and off-axis geometry
SCS BEAMLINE: LASER IN-COUPING

Permanent Beamline Components

Interchangeable Endstations / Detectors

Alignment Laser

Development by CIE for the instruments

Instrument Beam Dump

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**SCS Interchangeable Endstations and Detectors**

**Endstations:**
- **SCS**
- FFT (Forward scattering Fixed Target)
- XRD (X-ray resonant diffraction)
  - *hRIXS User consortium*
  - hRIXS.RIXS for solid samples and liquid jet
  - *PES User group*
  - PES Photoemission spectroscopy endstation

**Detectors:**
- DSSC
- FastCCD
  - *hRIXS User consortium*
  - RIXS Spectrometer
  - *PES User group*
  - ARTOF
Probing Spin dynamics on the smallest space-time dimensions
Non-local transfer of angular momentum.

Graves et al., Nature materials 12, 293 (2013)
SCS BEAMLINE: Forward-scattering fixed target endstation and DSSC detector integration

Permanent Beamline Components

Interchangeable Endstations / Detectors

Photon energy | \( \xi_{\text{min}} \) [nm] | \( \xi_{\text{max}} \) [nm]
---|---|---
0.5 keV | 3.6 | 2.0
0.95 keV | 1.9 | 1.0
1.2 keV | 1.5 | 0.8
2.0 keV | 0.9 | 0.5
3.0 keV | 0.6 | 0.3

Shortest Sample-Detector Distance:
270mm with gate valve
150mm without gate valve
Single-shot Coherent Diffraction Imaging using holographic and Phase retrieval approaches

SCS BEAMLINE: Detector Geometries

<table>
<thead>
<tr>
<th>Permanent Beamline Components</th>
<th>Interchangeable Endstations / Detectors</th>
</tr>
</thead>
</table>

### Sample size $\phi_{obj}$ [µm]

<table>
<thead>
<tr>
<th></th>
<th>1</th>
<th>3</th>
<th>5</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>FEL diameter [µm]</td>
<td>3</td>
<td>9</td>
<td>15</td>
<td>30</td>
</tr>
</tbody>
</table>

### DSSC distance [mm]

<table>
<thead>
<tr>
<th></th>
<th>0.5 keV</th>
<th>0.8 keV</th>
<th>1.2 keV</th>
<th>2.0 keV</th>
<th>3.0 keV</th>
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<tbody>
<tr>
<td></td>
<td>355</td>
<td>568</td>
<td>852</td>
<td>1420</td>
<td>2129</td>
</tr>
<tr>
<td></td>
<td>1065</td>
<td>1703</td>
<td>2555</td>
<td>4259</td>
<td>6388</td>
</tr>
<tr>
<td></td>
<td>1774</td>
<td>2839</td>
<td>4259</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>3549</td>
<td>5678</td>
<td>–</td>
<td>–</td>
<td>–</td>
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</tbody>
</table>

### Resolution [nm]

<table>
<thead>
<tr>
<th></th>
<th>4</th>
<th>12</th>
<th>20</th>
<th>39</th>
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Users’ Meeting 2015, The SCS instrument
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FFT endstation
Sample environment development by WP79

- THz delivery
- sample changer
- diagnostic stage
- FEL + OL
- camera port
- access port
- DSSC detector
- 1 T Magnet coils
- Piezo motor
Resonant Inelastic X-ray Scattering: Electronic structure, low-energy excitations and dispersion

\[ \omega - \omega' = \varepsilon_f - \varepsilon_i = \Delta \varepsilon \]


Sr\textsubscript{2}CuO\textsubscript{2}Cl\textsubscript{2}


Nature 485, 82 (2012)
hRIXS User Consortium

- Consists of over 40 international scientists (Spokesperson A. Föhlisch)
- Core team between Helmholtz Association, U Milano, DESY, XFEL guides the discussion for the instrument design and integration to the SCS instrument
- Technical design of the optical layout of the RIXS spectrometer is finished and will be reviewed in Feb. 2015

Lower resolution grating – TR-RIXS

High resolution grating – HR-RIXS

Yingying Peng, poster No. 37
Monochromator grating efficiency and resolving powers (WP73)

Baseline

HR hRIXS

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Monochromator grating pulse stretching

Instrumental pulse broadening
- G1: 50 l/mm
- G2: 150 l/mm

Pulse duration [fs] vs. Photon energy [eV]

SASE3 pulse duration (0.055 nC, 14 GeV)
Compensation of the pulse stretching

\[ \Delta \tau_{\text{rms}} = \sqrt{\int (\xi - \langle \xi \rangle)^2 t(\xi) d\xi} = \frac{1}{c} w_{\text{rms}} d_0 \lambda \]

\[ \frac{E}{\Delta E} = \frac{\lambda}{\Delta \lambda} = \frac{wd_0}{2c_B} = \frac{1}{2c_B} N \approx 1.13 \times N \]

Optimum grating illumination
Grating illumination tuning
SASE3 self-seeding

Soft x-ray energies [250-1200eV]
### SCS start-to-end simulation for the core operation modes

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</thead>
<tbody>
<tr>
<td>TR-spectroscopy,</td>
<td>14</td>
<td>1 (100 fs)</td>
<td>G1</td>
<td>50 / 20</td>
<td>100 x 100</td>
</tr>
<tr>
<td>TR-diffraction,</td>
<td>14</td>
<td>0.2 (20 fs)</td>
<td>G1</td>
<td>6 / 60</td>
<td>100 x 100</td>
</tr>
<tr>
<td>TR-PES (Fig. 2.2)</td>
<td>14</td>
<td>0.06 (5 fs)</td>
<td>G1</td>
<td>3 / 200</td>
<td>100 x 100</td>
</tr>
<tr>
<td>TR-RIXS (Fig. 2.3)</td>
<td>14</td>
<td>1 (100 fs)</td>
<td>G1</td>
<td>50 / 20</td>
<td>1000 x 10</td>
</tr>
<tr>
<td>HR-RIXS (Fig. 2.4)</td>
<td>14</td>
<td>0.2 (20 fs)</td>
<td>G2</td>
<td>6 / 20</td>
<td>1000 x 10</td>
</tr>
<tr>
<td>Mono CXDI on small targets,</td>
<td>14</td>
<td>0.2 (20 fs)</td>
<td>G1</td>
<td>50 / 20</td>
<td>&lt; 2 x 2</td>
</tr>
<tr>
<td>NLXS (Fig. 2.5)</td>
<td>14</td>
<td>0.06 (5 fs)</td>
<td>G1</td>
<td>3 / 200</td>
<td>&lt; 2 x 2</td>
</tr>
<tr>
<td>Mono CXDI on larger targets,</td>
<td>14</td>
<td>1 (100 fs)</td>
<td>G1</td>
<td>50 / 20</td>
<td>10 x 10</td>
</tr>
<tr>
<td>(Fig. 2.6)</td>
<td>14</td>
<td>0.2 (20 fs)</td>
<td>G1</td>
<td>6 / 60</td>
<td>10 x 10</td>
</tr>
<tr>
<td>Pink CXDI with intermediate focii (Fig. 2.7)</td>
<td>17.5</td>
<td>1 (100 fs)</td>
<td>Pink (M4)</td>
<td>Open</td>
<td>&lt; 2 x 2</td>
</tr>
<tr>
<td>Pink CXDI (Fig. 2.8)</td>
<td>17.5</td>
<td>0.2 (20 fs)</td>
<td>Pink (M4)</td>
<td>Open</td>
<td>&lt; 2 x 2</td>
</tr>
</tbody>
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SCS X-ray beam delivery using monochromator G1 for TR-Spectroscopy (100 x100 µm² spot) & hRIXS

(PINK BEAM: up to $10^{14}$ photons per pulse

up to $10^{18}-10^{20}$ W/cm²)

<table>
<thead>
<tr>
<th>Peak intensity [W/cm²]</th>
<th>Photon Energy [eV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 nC → 100 fs</td>
<td></td>
</tr>
<tr>
<td>0.2 nC → 20 fs</td>
<td></td>
</tr>
<tr>
<td>0.06 nC → 5 fs</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Fluence [mJ/cm²]</th>
<th>Photon Energy [eV]</th>
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<tbody>
<tr>
<td>Average</td>
<td></td>
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</table>
SCS High-quality floor for precision positioning / motion of large scale detectors

SCS high-quality Floor
- Contract signed.
- Installation in March 2015

[Diagram of experimental area with layers: pavement, filling material, marble, cement + sand mix, glue, hRIXS floor, and underground layers.]
The SCS team

Jan Torben Delitz
SCS Instrument Engineer

Robert Carley
SCS Instrument Scientist

Manuel Izquierdo
SCS Instrument Scientist

Alexander Yaroslavtsev
Visiting Scientist
Monochromatic Beam operations 250-3000 eV

Offset Mirrors
- < 1.5keV; 9mrad
- < 1.1keV; 12mrad
- < 850 eV; 15mrad
- < 700 eV; 20mrad

SCS Distribution
Mirror used for offset compensation

Monochromator
Premirror / VLS gratings

Intermediate focus / Vertical exit slits mono

KB mirror
Users' Meeting 2015

Pink Beam operations

Photon Energy: 3054 eV

Monochromator:
Premirror / flat mirror
Beam path in SCS Experiment Hutch

Horizontal beam size and position (x) [mm]

Vertical beam size and position (y) [mm]

Beam propagation direction z in SCS experiment hutch [m]
The race for RIXS at relevant energy scales

"Ideal" spectrum at Cu L₃

Energy loss (eV):
-0.3, -0.2, -0.1, 0.0

E/ΔE (combined):
7000, 10000, 20000, 30000, 40000, ∞

Instruments:
- SAXES@ADDRESS
- ESRF
- METRIXS
- Diamond
- NSLS II (Centurion)
hRIXS At XFEL: Get RIXS to the transform limit in time and energy

\[ \Delta t = \frac{h}{\Delta E} = \frac{E}{\Delta E} \times \frac{\lambda}{c} \]
Optical Laser delivery (Guido Palmer, Optical Laser Group, WP 78)

Optical table:
- Up and down frequency conversion setups
- Diagnostics
- Delay stages

THz setup near the endstation
Tilted pulse front THz generation (Hebling et al. Optics Express 21, 1161 (2002))

• Generates finite THz source
• Good beam properties i.e. focusable
• Scalable in pump pulse energy
• With 800 nm pump of LiNbO$_3$
  • 0.1 % energy conversion
• 1030 nm 100 mJ $\rightarrow$ 100 $\mu$J THz pulse
  • Electric fields of up to 5 GV/m