MBN Research Center

TECHNO-CLS

Funded by the European Union

# *Work Package 2*
# *Theory and modelling*


**Andrey V. Solov'yov**

*MBN Research Center, Frankfurt am Main, Germany*

www.mbnresearch.com



**2nd Year Progress Review Meeting,**

**EIC-PATHFINDER TECHNO-CLS project 101046458**

***"Emerging technologies for Crystal-based gamma-ray Light Sources (CLS)"***

**26 June 2024, on-line**

# TECHNO-CLS consortium

# Outline

MBN Research Center

- Introduction to EIC-PATHFINDER TECHNO-CLS project
  - Gamma-ray Crystal-based Light Sources (CLS): basic ideas
  - Overview of the main tasks of the Working Package 2 (WP2)
- WP2 Theory and modelling
  - Task 2.1
  - Task 2.2
  - Tasks 2.3 and 2.4
- Conclusions and outlook

# Oriented crystal based light sources

MBN Research Center

Selected examples of the novel gamma-ray Crystal based Light Sources (CLSs). Black circles and lines mark atoms of crystallographic planes, wavy curves show trajectories of the channeling particles, shadowed areas refer to radiation.

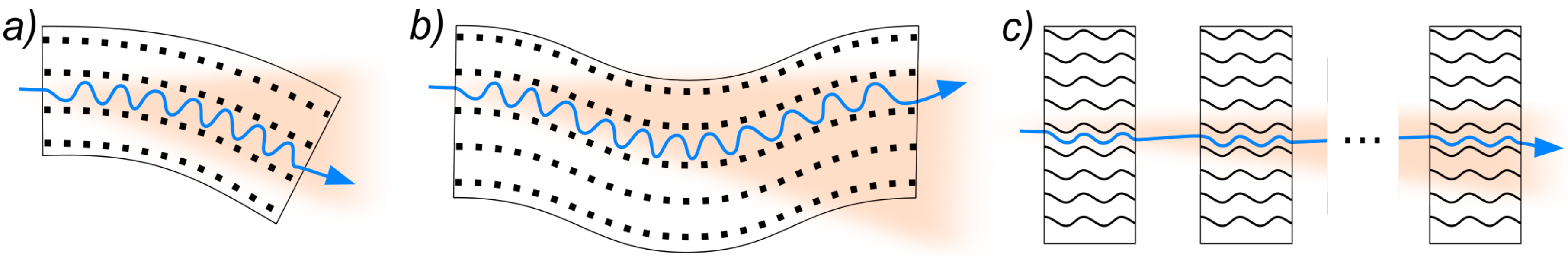
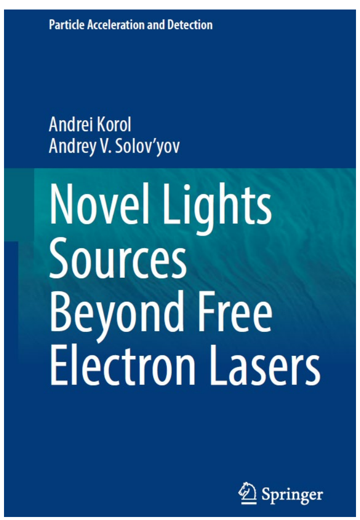
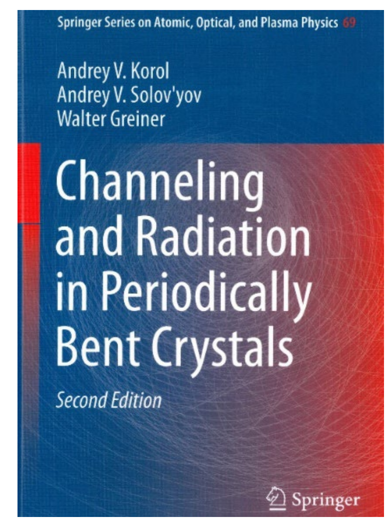



Figure from A.V. Korol, and A.V. Solov'yov, Eur. Phys. J. D (2020) 74: 201





- A.V. Korol, A.V.Solov'yov, *Novel Lights Sources Beyond Free Electron Lasers*, Particle Acceleration and Detection series, Springer Nature Switzerland, Cham (2022)
- A.V. Korol and A.V. Solov'yov, *Crystal-based intensive gamma-ray light sources* (Topical Review), Eur. Phys. J. D, vol. 74, 201 (2020)
- A.V. Korol, G.B. Sushko, and A.V. Solov'yov, *All-atom relativistic molecular dynamics simulations of channeling and radiation processes in oriented crystals* (Topical Review), Eur. Phys. J. D, vol. 75, 107 (2021)
- A.V. Korol, A.V. Solov'yov, Greiner, *Channeling and Radiation in Periodically Bent Crystals*, Second Edition, Springer–Verlag, Berlin, Heidelberg (2014)

# Crystalline vs magnetic undulator

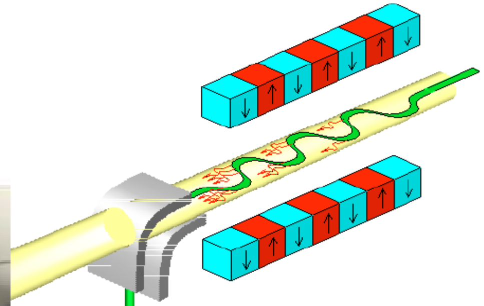


Magnetic undulator:

$\lambda_u$~1 cm, ħω~10 keV

Crystalline undulator:

$\lambda_u$~10 μm, ħω~0.1 …10 MeV



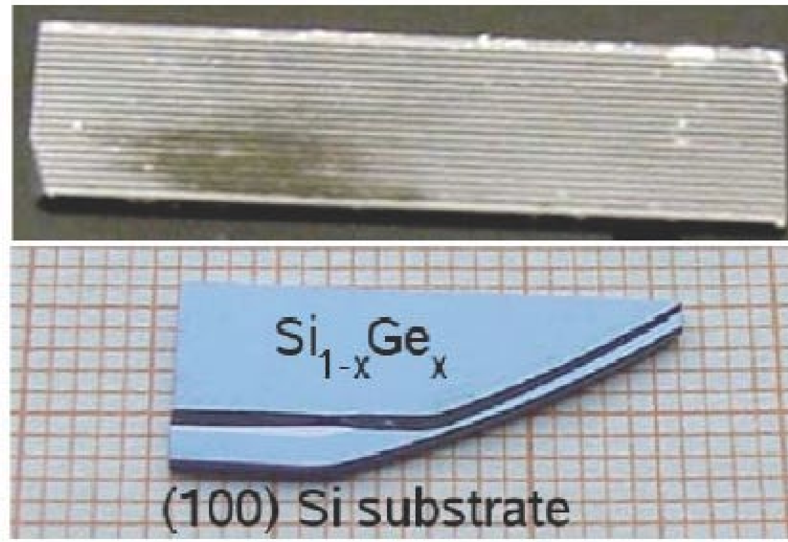



**Fig. 1.3** *Left:* Magnetic undulator for the X-ray laser XFEL [179]. The picture is taken from [180]. *Right top:* laser-ablated diamond crystal. The crystal size is $4 \times 2 \times 0.3$ mm$^3$. The undulator period is $\lambda_u = 50\,\mu$m. The picture is taken from [74]. *Right bottom:* a $Si_{1-x}Ge_x$ superlattice crystalline undulator with four periods. Periodically varied Ge content (from $x = 0$ to $x_{max} = 0.5\%$) gives rise to the undulator period $\lambda_u = 50\,\mu$m. The picture is courtesy of J.L. Hansen, A. Nylandsted and U. Uggerhøj (University of Aarhus).

# CU-LSs versus FEL and SR

MBN Research Center

Brilliance of a photon source relates the number of photons of a given energy emitted per unit time interval, unit source area, unit solid angle and per bandwidth:

$$B_n = \frac{\Delta N_{\omega_n}}{10^3\,(\Delta\omega_n/\omega_n)\,(2\pi)^2\,\varepsilon_x\varepsilon_y}\,\frac{I}{e}$$

- $n$ – harmonic number
- $\omega_n, \Delta\omega_n$ – energy and width of the $n$th harmonic
- $\Delta\omega_n/\omega_n$ – bandwidth (=BW)
- $\Delta N_{\omega_n}$ – number of photons with $\omega \in \left[\omega_n - \Delta\omega_n/2, \omega_n + \Delta\omega_n/2\right]$
- $I$ – electric current of the beam
- $\varepsilon_{x,y}$ – emittance of the photon source along

A.V Korol, A.V Solov'yov, Eur. Phys. J. D (2020) 74: 201

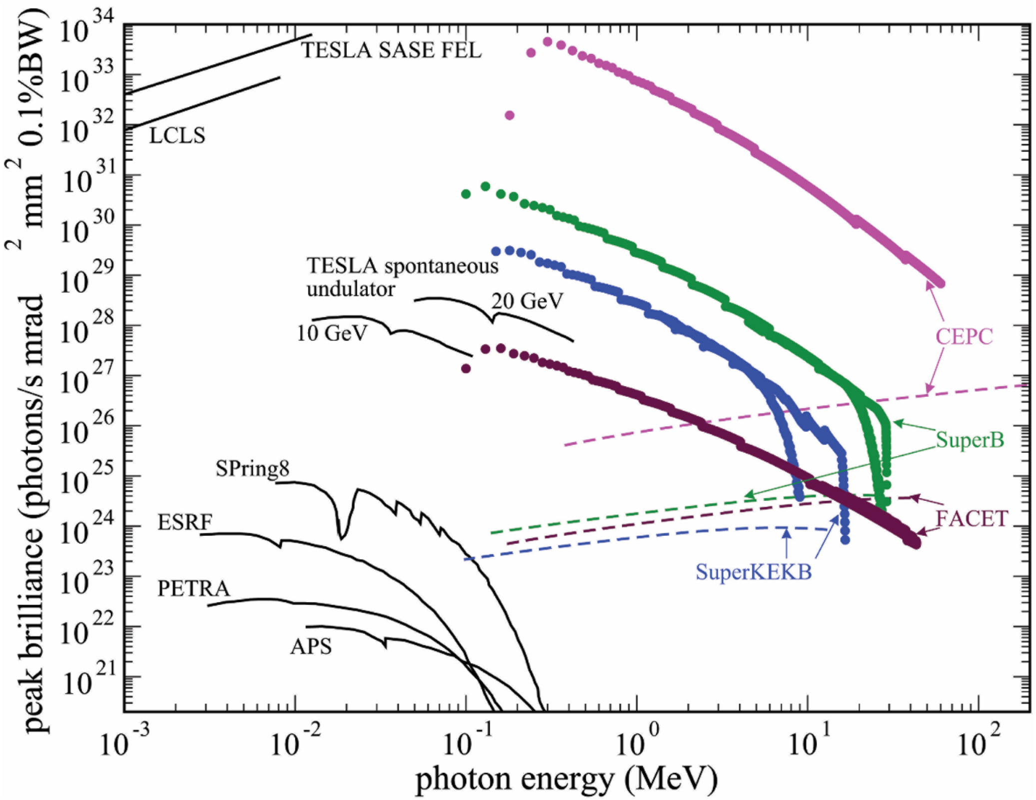
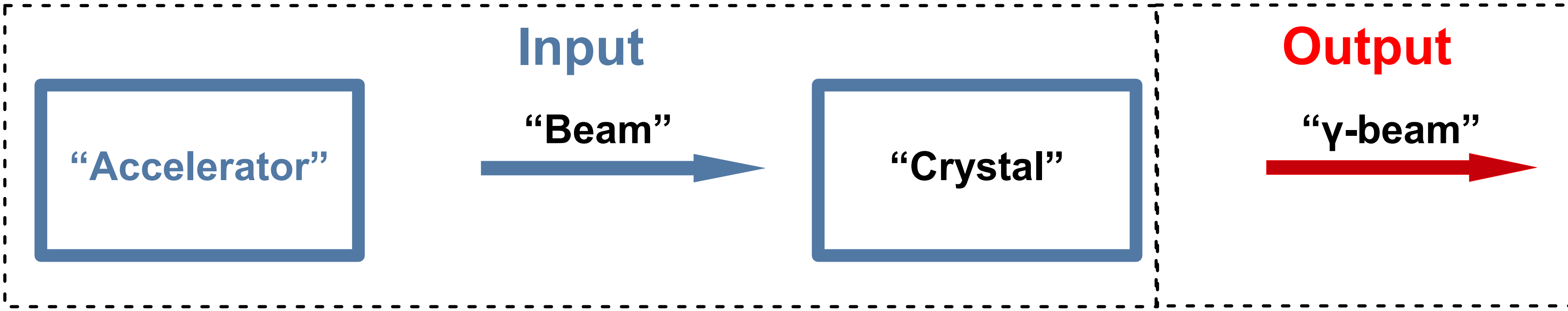



**Fig. 7.** Peak brilliance of superradiant CUR (thick solid curves) and spontaneous CUR (dashed lines) from diamond(110) CUs calculated for the SuperKEKB, SuperB, FACET-II and CEPC positron beams versus modern synchrotrons, undulators and XFELs. The data on the latter are taken from reference [8].

# Prototypes of gamma-ray CLSs




**Principal elements**:
- Type of accelerator
- Apparatus
- Beam line
- Infrastructure

**Characterisation of the beam:**
- Type of projectile
- Energy and energy spread
- Size
- Emittance
- Current

**Relevant issues:**
- Crystal manufacture;
- Structure characterisation
- Crystal manipulation
- Channeling experiments
- Advanced simulations

**Experimental and theoretical characteri-sation of the radiation**:
- Spectral-angular distribution
- Number of photons
- Brilliance
- Power

# WP2 objectives



- O2.1 Computer modelling of BC & PBC structures fabricated by means of different technologies.
- O2.2 Multiscale simulations of particle propagation in LC, BC & PBC.
- O2.3 Atomistic level characterisation of related phenomena (multiple scattering, channeling, dechanneling, rechanneling, volume reflection and capture, energy losses).
- O2.4 Characterisation of radiation emitted in CLS under conditions matching existing experimental setups and those beyond.
- O2.5 Comparison of the results of simulations with experiment.
- O2.6 Characterisation of CLSs

# WP2: Theory & modelling (Lead team: MBN-RC)

MBN Research Center

**T2.1: (HMU, MBN-RC)**

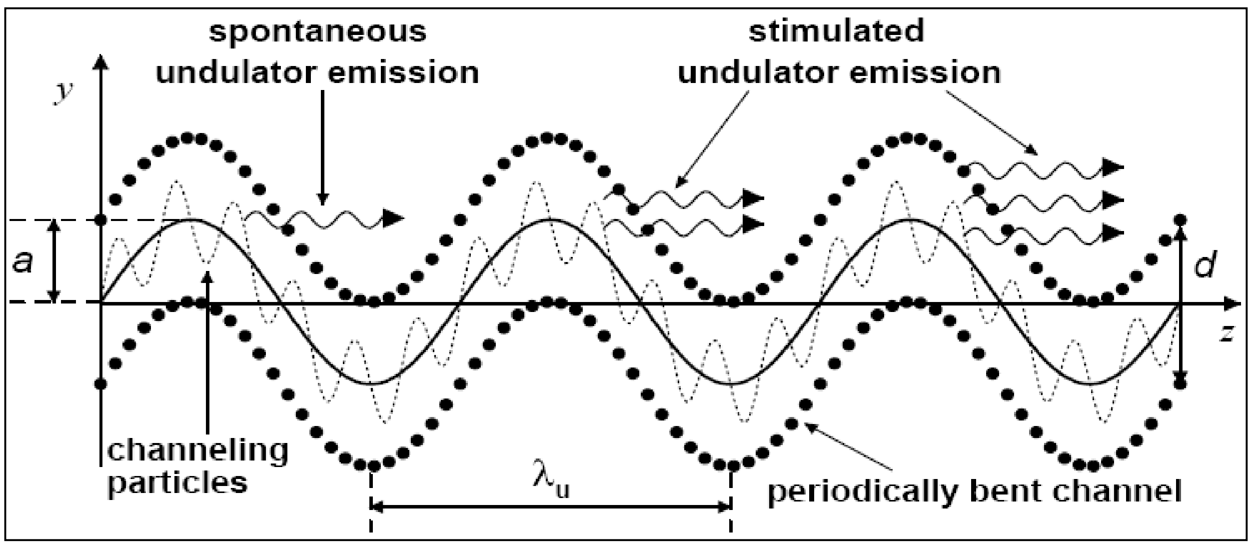
- **Modelling of *crystal structure modification due to AW excitation* by means of (i) a piezoelectric transducer**, (ii) a laser pulse.
- Verification of the results against the experiment.
- **Determination of the optimal parameters of the piezoelectric element**/laser **pulse to achieve highest photon yield.**

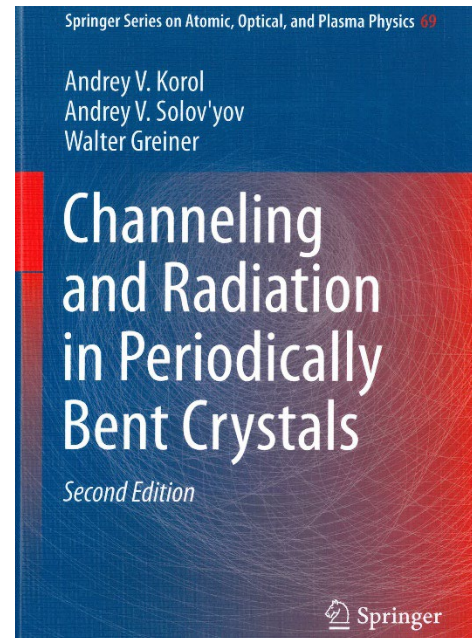
# Radiation from a crystalline undulator

MBN Research Center

Basic idea (Korol, Solov'yov, Greiner, J.Phys.G, v.24, L45 (1998); reviews: *International Journal of Modern Physics E*, v.8, p.49-100 (1999); v.13, p.867-916 (2004) ); PRL, 98, 164801, (2007); Monograph, Second Edition, Springer–Verlag, Berlin, Heidelberg (2014)

The radiation is generated by a bunch of ultra-relativistic positrons (ε=0.5…10 GeV) channeling in a crystal along periodically bent crystallographic planes. The periodicity of trajectories results in the undulator-type radiation due to the constructive interference of the photons emitted from similar parts of the trajectory.




***d*=1…2 *Å*** **- the interplanar spacing**
***a*=(10…50)*d*** **– the amplitude of bending**
**$\lambda_u$=(10$^4$…10$^5$)*a*** **– the period of bending**

→ $d \ll a \ll \lambda$

# Spectral and angular distribution of spontaneous radiation in CU

MBN Research Center

$$\frac{\mathrm{d}E_N}{\mathrm{d}\omega\,\mathrm{d}\Omega_{\mathbf{n}}} = D_N(\eta)\,F(\omega;\gamma,p;\theta,\varphi)$$

Here, $F(\omega;\gamma,p;\theta,\varphi)$ is a smooth function of the arguments

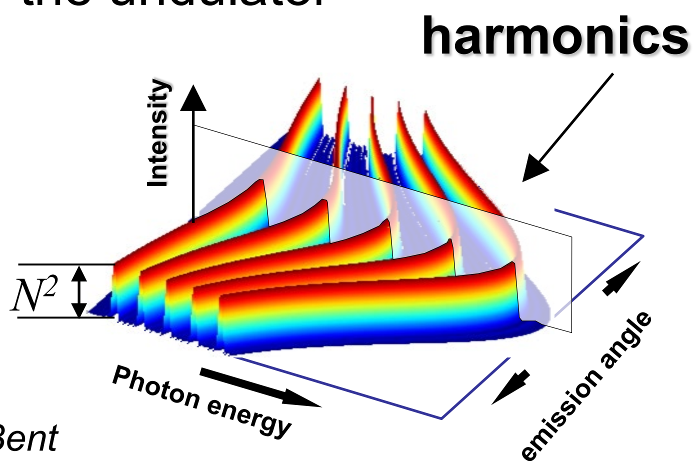
$$D_N(\eta) = \left(\frac{\sin N\pi\eta}{\sin\pi\eta}\right)^2 \qquad \omega^{(K)} = \frac{4\gamma^2\Omega_u\,K}{2+2\theta^2\gamma^2+p^2}, \quad K=1,2,\dots$$

$$\eta = \frac{\omega}{\Omega_u}\left(\frac{1}{2\gamma^2}+\frac{\vartheta^2}{2}+\frac{p^2}{4\gamma^2}\right)$$

The characteristic frequencies (harmonics) of the undulator radiation

$$p^2 = 2\gamma^2\,\frac{\overline{\dot{y}^2}}{c^2}$$

p is undulator parameter
dipole regime: p << 1
non-dipole regime: p >> 1




A.Korol, A.V. Solov‘yov, W.Greiner, *Chan. and Rad. In Periodically Bent Crystals*, Second Edition, Springer–Verlag, Berlin, Heidelberg (2014)

# Feasibility of a crystalline undulator

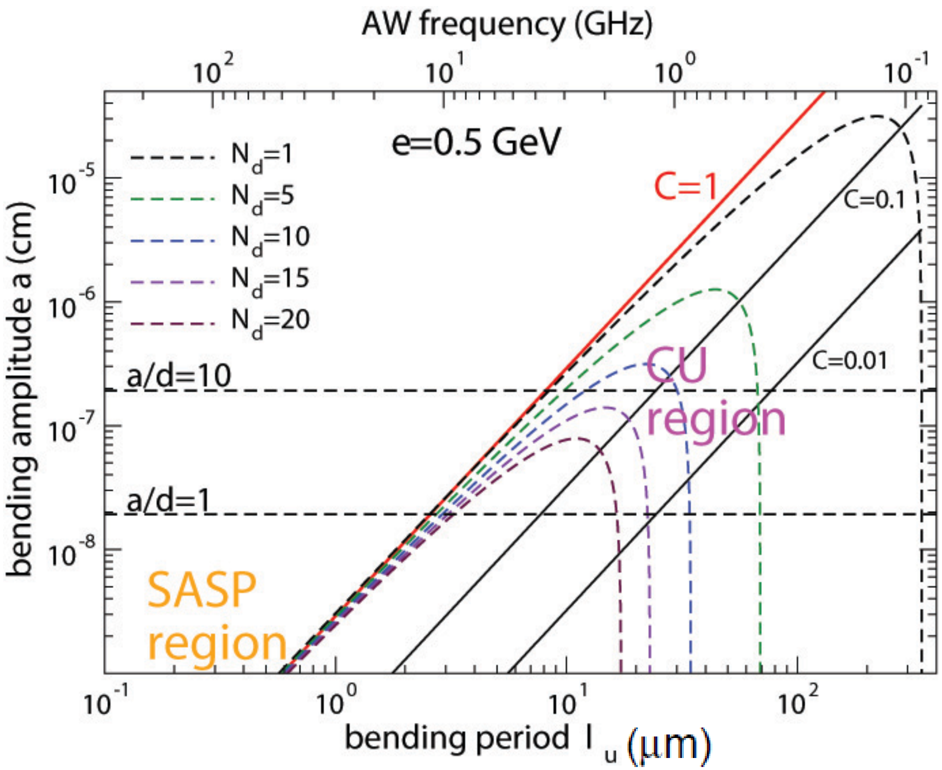
The summary of all essential conditions (Korol, Solov'yov, Greiner 1998, 2004):

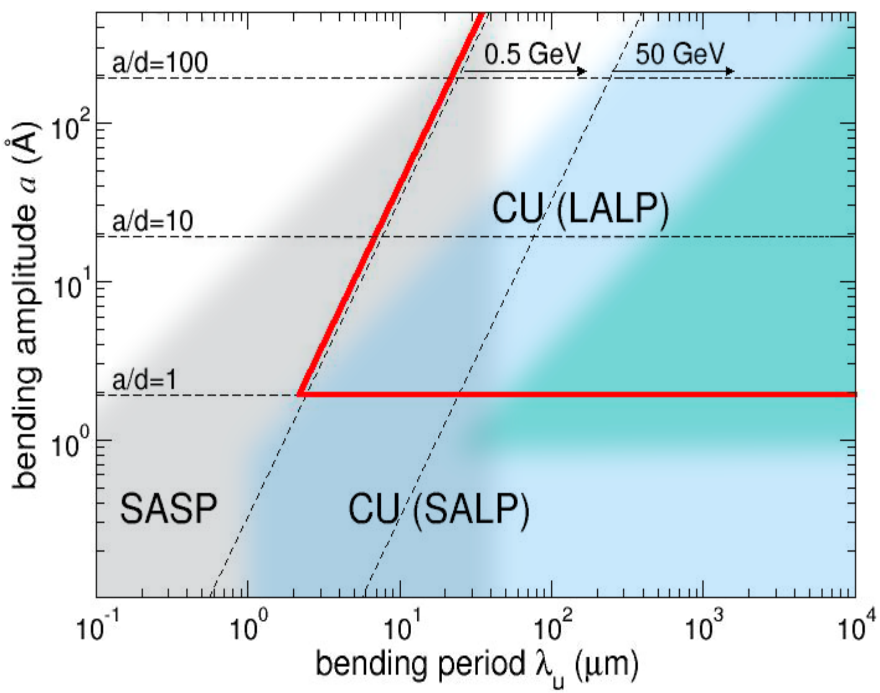
$$
\begin{cases}
C = (2\pi)^2 \dfrac{\varepsilon}{qU'_{\max}} \dfrac{a}{\lambda^2} \ll 1 & \text{stable channeling} \\
d \ll a \ll \lambda & \text{large-amplitude regime} \\
N = \dfrac{L}{\lambda} \gg 1 & \text{large number of undulator periods} \\
L \leq \min\left[L_{\rm d}(C), L_a(\omega)\right] & \text{account for the dechanneling and photon attenuation} \\
\dfrac{\Delta\varepsilon}{\varepsilon} \ll 1 & \text{low radiative losses}
\end{cases}
$$

**If these are met then:**

- within the length *L* the particle experiences stable planar channeling
- characteristic energies of the undulator and channeling radiation are well separated
- intensity of the undulator radiation is higher than that of the channeling radiation.
- emission spectrum is stable towards the radiative losses.

# CU parameter ranges




**Left figure.** Bending amplitude, $a$, vs bending period, $\lambda$, consistent with the condition C<1 and calculated for various numbers of undulator periods $N_d$ as indicated for e=0.5 Gev ($\gamma = 10^3$) positron channeling in *Si* along (110) crystallographic plane. Bending profile $y=a\sin(2\pi z/\lambda)$.

A.Korol, W.Krause, A.Solov'yov, W.Greiner, J.Phys.G: Nucl.Part.Phys., v.26, L87-L95 (2000);

***From A.Korol, A.Solov'yov, W.Greiner, Chan. and Rad. In Periodically Bent Crystals, Second Edition, Springer–Verlag, Berlin, Heidelberg (2014)***;

**Right figure.** Shadowing indicates the ranges accessible by means of modern technologies: superlattices (grey), surface deformations (green), AWs (blue); ***From A.V. Korol and A.V. Solov'yov, Eur. Phys. J. D, vol. 74, 201 (2020)***

# Acousto-Optic Modulation (AOM)

MBN Research Center

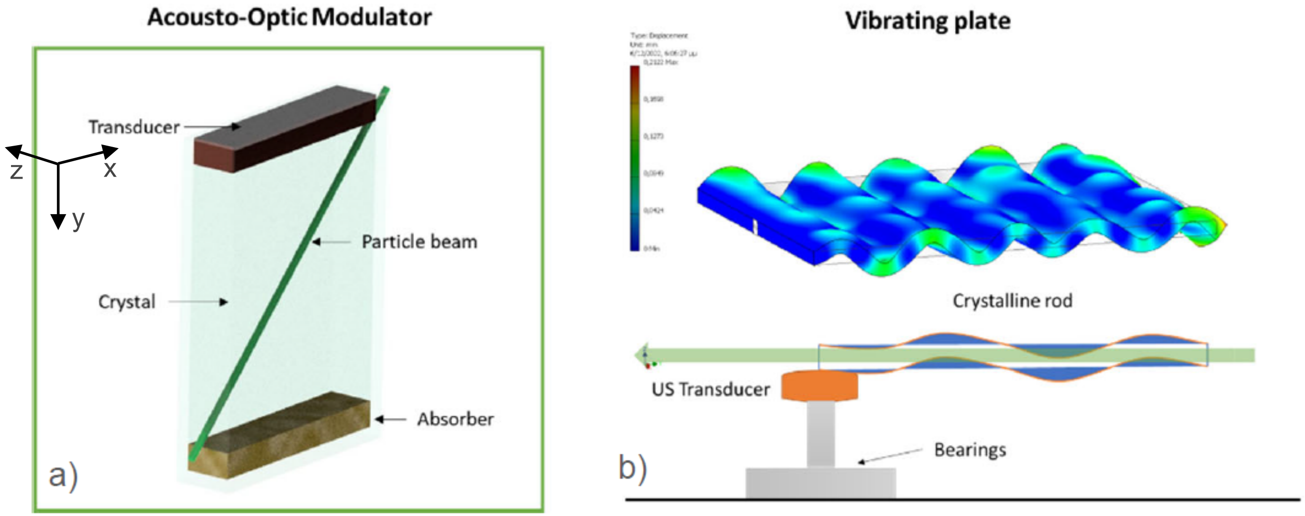



**Figure 2.1.1:** Schematic diagrams of novel acoustically excited crystalline undulator layouts, a) Acousto-Optic Modulator–type (AOM) AW CU and b) Vibrating Plate–type (VP) AW CU.

A 20 GeV positron beam (red arrow) of the size σ=150 μm (SLAC specification) enters the crystal. For these geometries, the **two FEM simulation sets** have been performed (HMU).

**SET1:** Harmonic pressure *P* ($P_{max}$=4 MPa; ν=10 and 40 MHz) is applied on the upper XZ plane. *Boundary conditions*: (i) free boundaries on the YZ and XY planes; (ii) non-reflective (absorber) boundaries on the lower XZ plane.

**SET2:** Harmonic pressure ($P_{max}$=4 MPa; ν=10 MHz) is applied on the upper XZ plane. *Boundary conditions:* (i) simply supported plate boundaries on the YZ and XY planes; (ii) non-reflective (absorber) boundary conditions at the bottom XZ plane.

Work in progress: MBN-RC & HMU.

# Simulated bending profiles

MBN Research Center

## SET 1: Excitation frequency 40 MHz

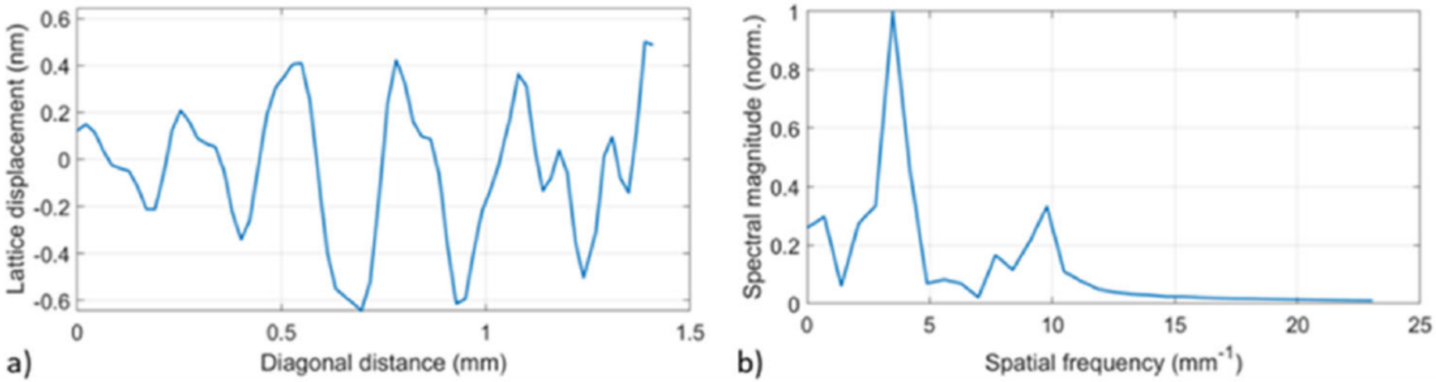
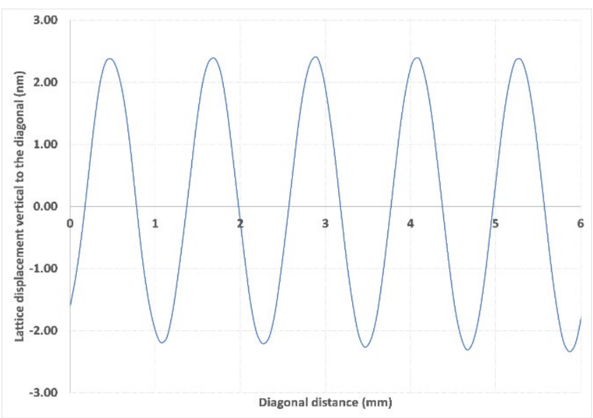



**Figure 2.1.3:** FEM simulations of the acoustically induced lattice modulation of the Si1 crystal excited with 42 MHz, 4 MPa harmonic pressure a) space domain, b) spatial frequency domain.

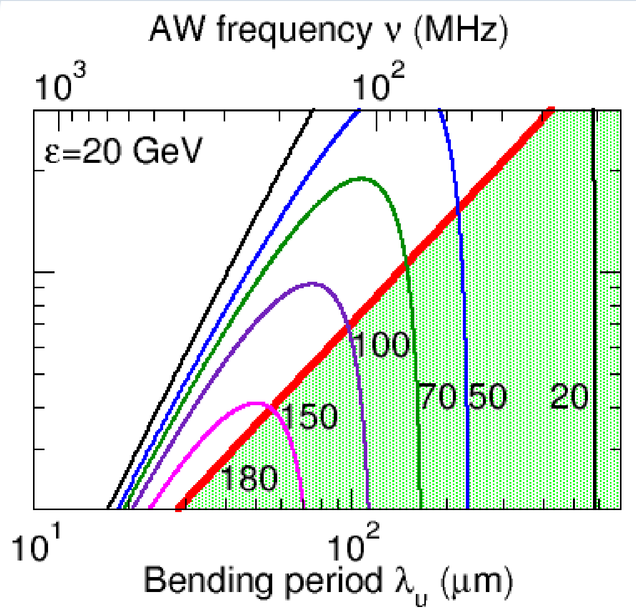
## SET 2: Excitation frequency 10 MHz

Bending profiles along the central path




Potential experimental realization of SET 2 can be difficult and require further feasibility investigation.

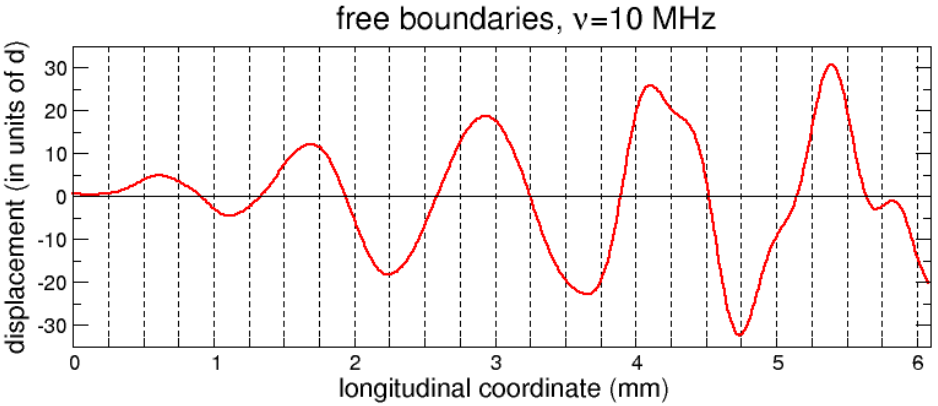
# CU via AW excitation for 20 GeV $e^+$

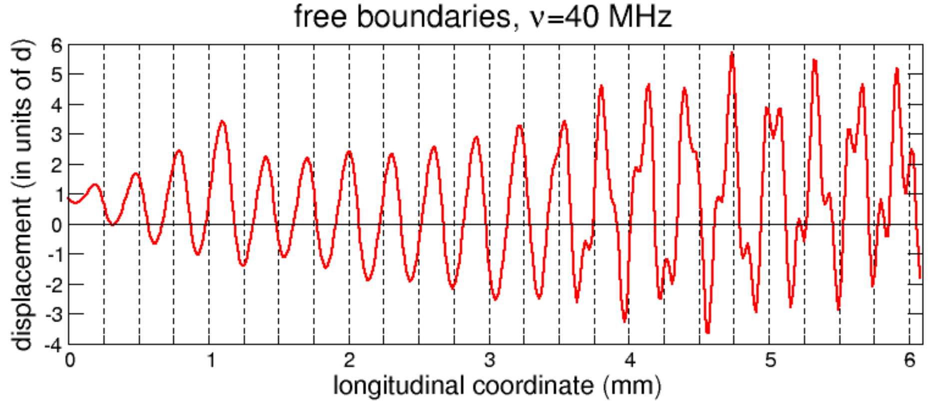



Work in progress: MBN-RC & HMU.

**Left figure:** Ranges of bending period $\lambda_u$ and amplitude $a > d = 1.92$ Å to be probed to construct a Si(110)-based CU for $\varepsilon = 20$ GeV positrons. The CU can be considered in the shadowed domain lying below the red line. Integers indicate the number of undulator periods within the dechanneling length.

The upper horizontal axis in shows the frequency of the AW transmitted along the <100> axial direction, that causes periodic bending of the (110) planes.



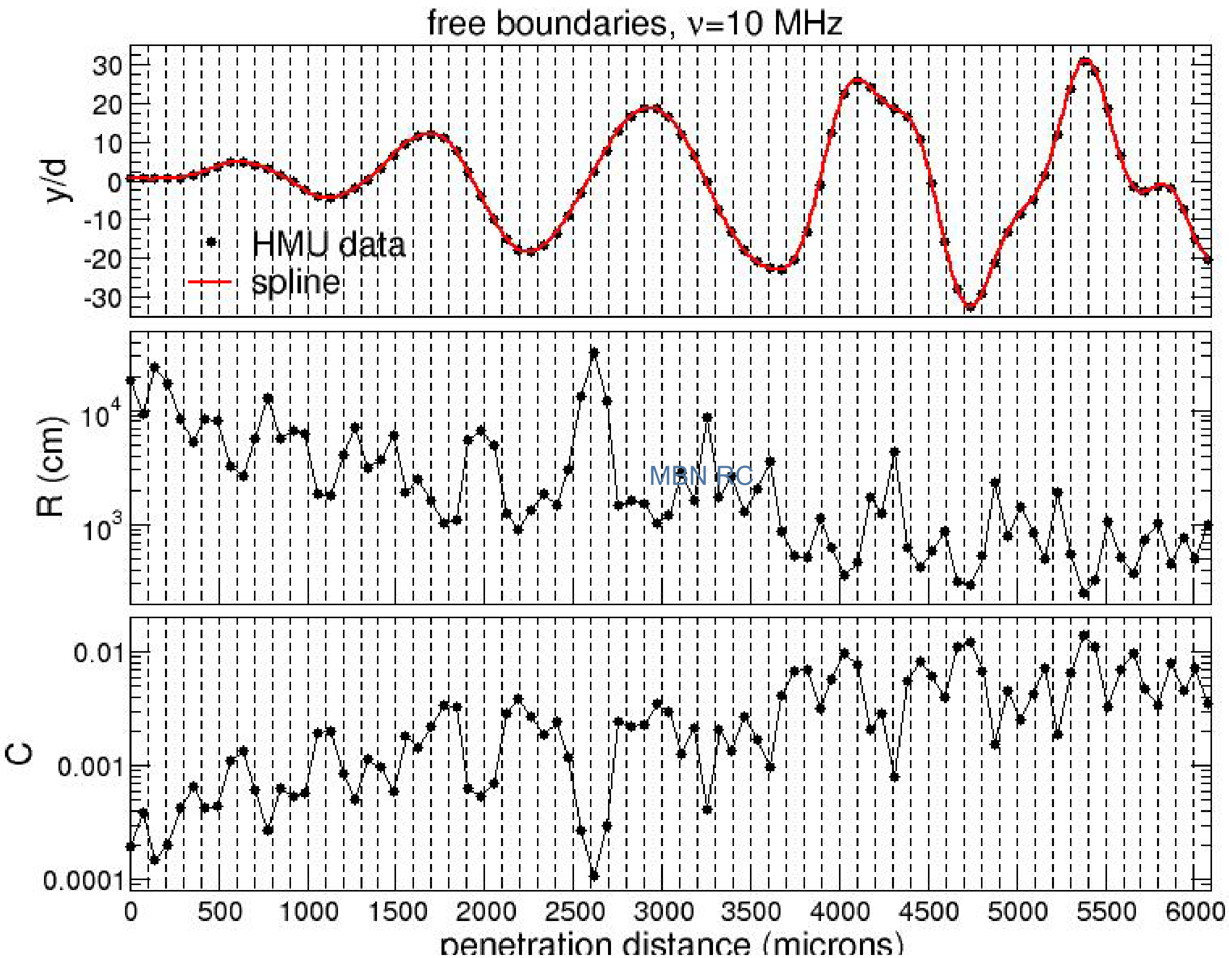




Bending profiles of (110) planes in Si due to AW with free boundary conditions. Left panel corresponds to the AW frequency 10 MHz, right panel – to 40 MHz.

# Initial analysis of channeling properties

MBN Research Center

## SET 1: Excitation frequency 10 MHz




Work in progress: MBN-RC & HMU.

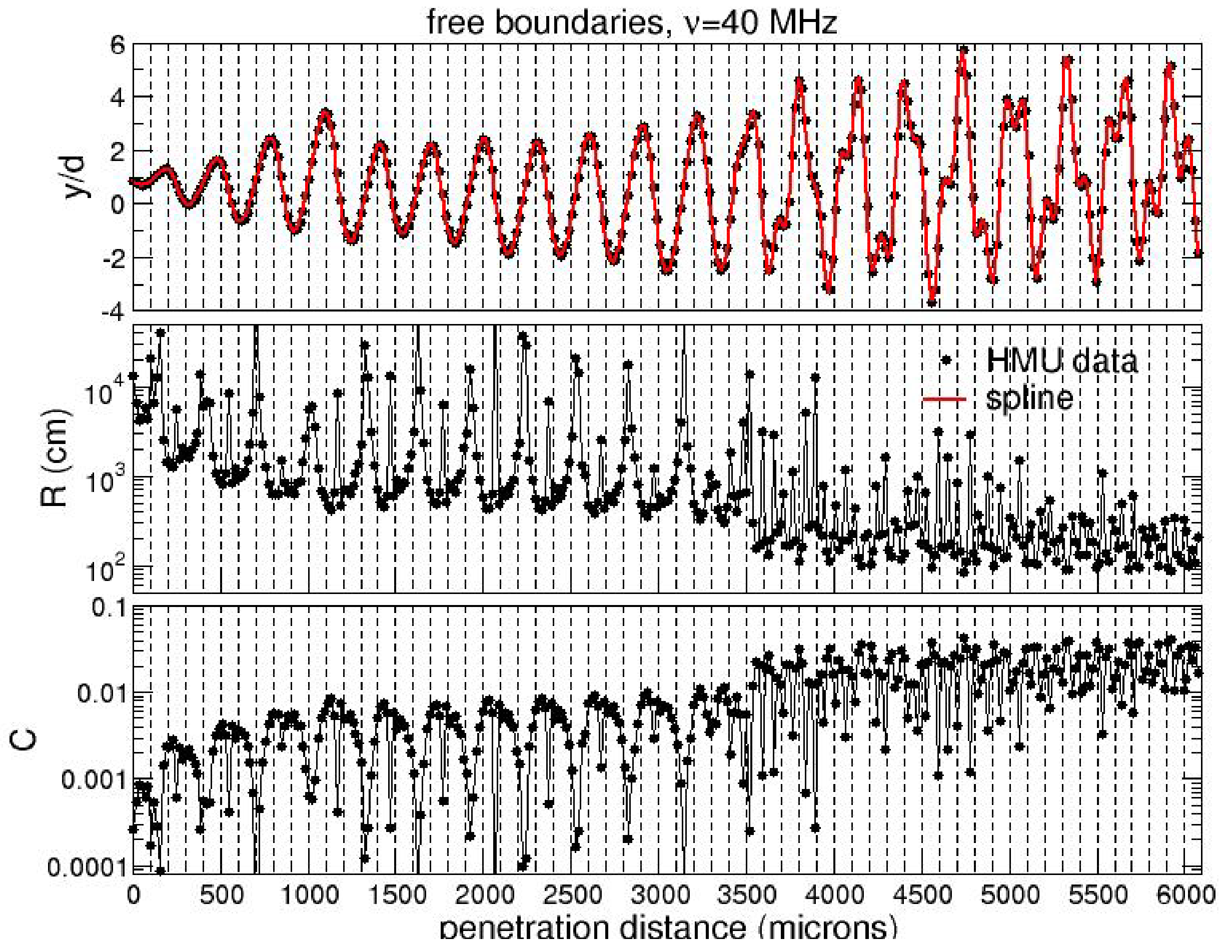
Top: Bending profiles of (110) planes in Si due to AW. Middle: Local curvature radius.

Bottom: Bending parameter C=centrifugal force / interplanar force.

# Initial analysis of channeling properties

MBN Research Center

## SET 1: Excitation frequency 40 MHz




Work in progress: MBN-RC & HMU.

Top: Bending profiles of (110) planes in Si due to AW. Middle: Local curvature radius. Bottom: Bending parameter C=centrifugal force / interplanar force.

# WP2: Theory & modelling (Lead team: MBN-RC)

MBN Research Center

**T2.2 (UoK, MBN-RC**, UNIFE, UNIPD, ESRF**)**

- ***Atomistic modelling* of Si- & diamond-based BC and PBC fabricated via different technologies.**
- **Studying the processes responsible for crystal imperfections**.
- Comparison with the data on experimental characterization.

# MBN Explorer: relativistic dynamics

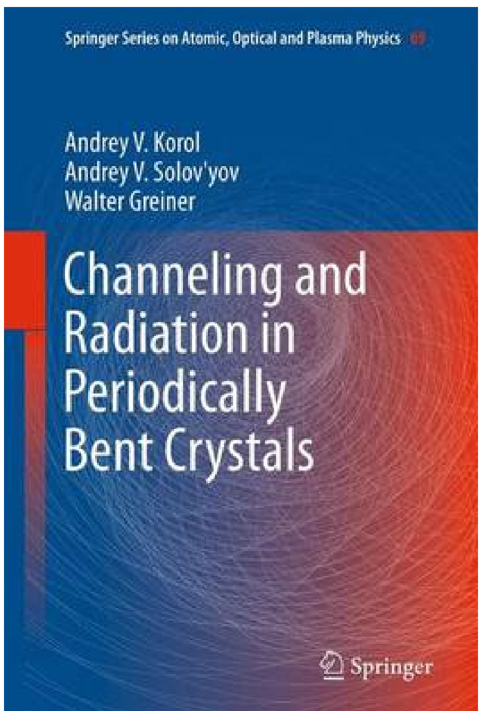
MBN Research Center

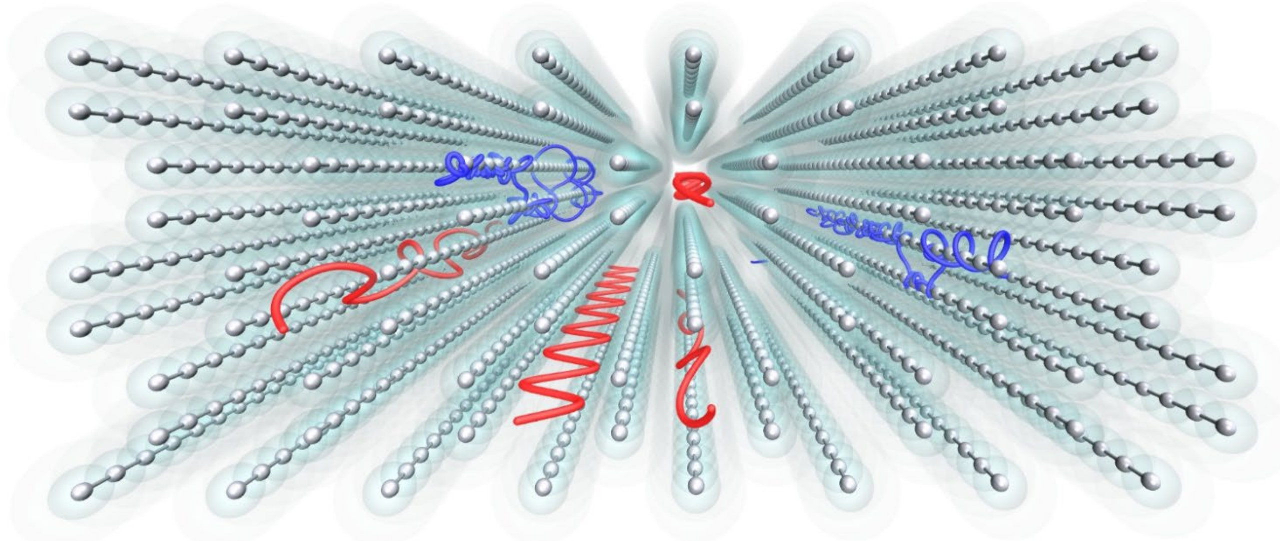
Simulation of motion of relativistic particles in MBN Explorer is based on relativistic equations of motion.

$$\begin{cases} \dot{\mathbf{v}} = \dfrac{1}{m\gamma}\left(\mathbf{F} - \mathbf{v}\dfrac{(\mathbf{F}\cdot\mathbf{v})}{c^2}\right) \\ \dot{\mathbf{r}} = \mathbf{v} \end{cases}$$

This system of equations is strongly nonlinear and requires the use of high-order integrator in order to be solved correctly

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}}\,.$$



The developed approach (G.B. Sushko, V.G. Bezchastnov, I.A. Solov'yov, A.V. Korol, W. Greiner, A.V. Solov'yov, Journal of Computational Physics, 252, 404 (2013) is not restricted to the crystalline medium and is applicable to describe the propagation of ultra-relativistic projectile in an arbitrary medium.

A.V. Korol, G.B. Sushko, and A.V. Solov'yov, All-atom relativistic molecular dynamics simulations of channeling and radiation processes in oriented crystals (Topical Review), Eur. Phys. J. D, vol. 75, 107 (2021)

# Modular structure of MBN Explorer 5.0

MBN Research Center

**MBN Explorer**

**Energy calculation**

**System optimisation**

**Dynamic tasks**

**Molecular dynamics (MD):**
nonrelativistic, Euler, relativistic, reactive (RMD), irradiation driven (IDMD)

**Stochastic dynamics:**
random walks in 2D and 3D, homogeneous and heterogeneous systems, random transformations

**Multiscale approach**

Input

- Potentials (pairwise, many-body)
- Molecular force fields
- Reactive force fields
- External fields
- System geometry and initial conditions

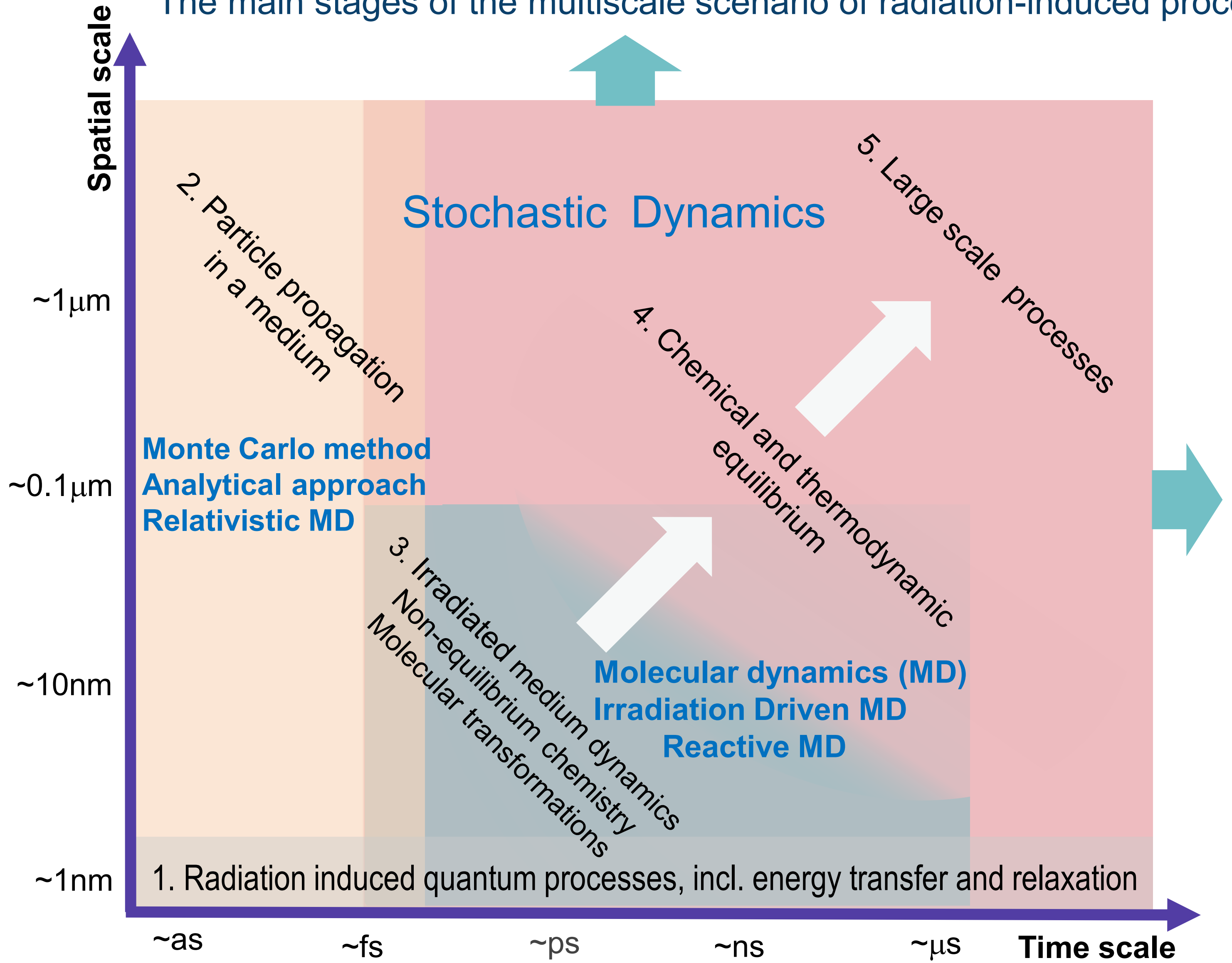
Input

- Diffusion, coalescence, dissociation probabilities
- Creation, annihilation and reaction (fission, fusion, substitution) rates
- System geometry and initial conditions

# Multiscale theory of irradiated MesoBioNano (MBN) systems

MBN Research Center

The main stages of the multiscale scenario of radiation-induced processes




A.V. Solov'yov, A.V. Verkhovtsev, N Mason, I.A. Solov'yov, et al, *Condensed matter systems exposed to radiation: the multiscale theory, simulations and experiment, Roadmap paper*, arXiv:2311.13402 [physics.chem-ph], Chemical Reviews (2024, online ahead of print, https://pubs.acs.org/doi/10.1021/acs.chemrev.3c00902 ) (impact factor 62);

A.V. Solov'yov (ed.), *Advances in Atomic and Molecular Physics at the interfaces with Natural Sciences, Technology and Medicine*, World Scientific, in preparation, 2024

# Roadmap paper for the CA MultIChem

MBN Research Center


ACS Publications
Most Trusted. Most Cited. Most Read.

www.acs.org

CHEMICAL REVIEWS

(2024), online ahead of print, https://pubs.acs.org/doi/10.1021/acs.chemrev.3c00902

pubs.acs.org/CR

Review

## Condensed Matter Systems Exposed to Radiation: Multiscale Theory, Simulations, and Experiment

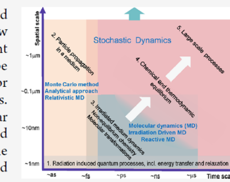
Andrey V. Solov'yov,* Alexey V. Verkhovtsev, Nigel J. Mason, Richard A. Amos, Ilko Bald, Gérard Baldacchino, Brendan Dromey, Martin Falk, Juraj Fedor, Luca Gerhards, Michael Hausmann, Georg Hildenbrand, Miloš Hrabovský, Stanislav Kadlec, Jaroslav Kočišek, Franck Lépine, Siyi Ming, Andrew Nisbet, Kate Ricketts, Leo Sala, Thomas Schlathölter, Andrew Wheatley, and Ilia A. Solov'yov*

Cite This: https://doi.org/10.1021/acs.chemrev.3c00902

Read Online



**ABSTRACT:** This roadmap reviews the new, highly interdisciplinary research field studying the behavior of condensed matter systems exposed to radiation. The Review highlights several recent advances in the field and provides a roadmap for the development of the field over the next decade. Condensed matter systems exposed to radiation can be inorganic, organic, or biological, finite or infinite, composed of different molecular species or materials, exist in different phases, and operate under different thermodynamic conditions. Many of the key phenomena related to the behavior of irradiated systems are very similar and can be understood based on the same fundamental theoretical principles and computational approaches. The multiscale nature of such phenomena requires the quantitative description of the radiation-induced effects occurring at different spatial and temporal scales, ranging from the atomic to the macroscopic, and the interlinks between such descriptions. The multiscale nature of the effects and the similarity of their manifestation in systems of different origins necessarily bring together different disciplines, such as physics, chemistry, biology, materials science, nanoscience, and biomedical research, demonstrating the numerous interlinks and commonalities between them. This research field is highly relevant to many novel and emerging technologies and medical applications.



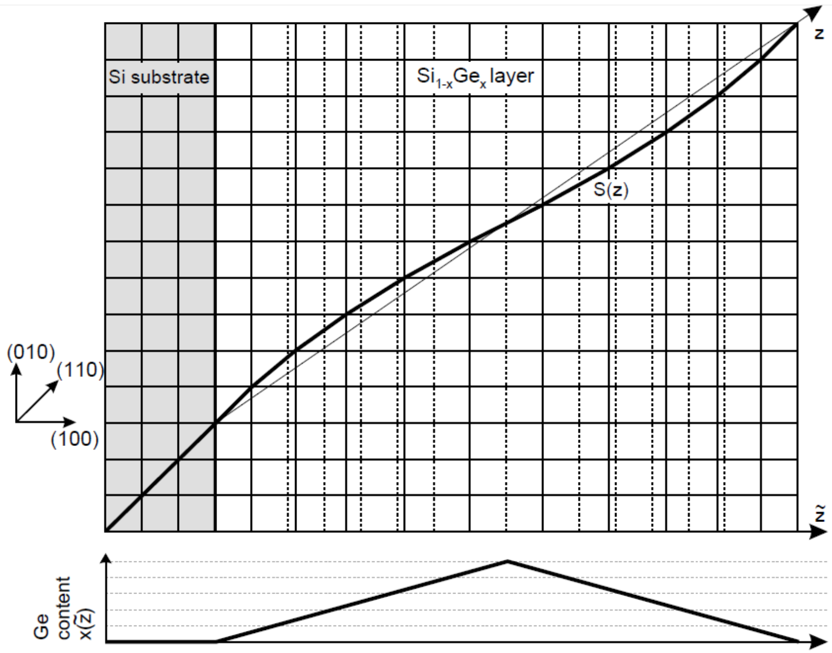

CONTENTS



Received: December 6, 2023
Revised: May 2, 2024
Accepted: May 10, 2024

ACS Publications

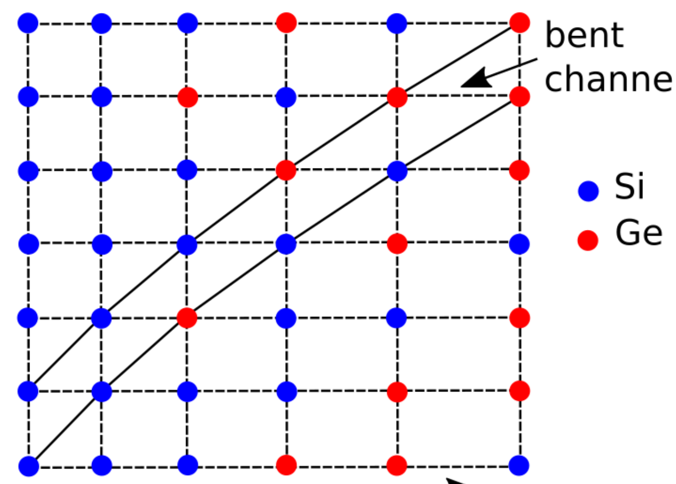
# Channeling in binary crystalline structures




Bending can be achieved by variation of the dopant content in binary crystals [1].

Scheme of $Si_{1-x}Ge_x$ crystal bending due to variation of Ge content [3].

Ge and Si have different lattice parameters which leads to a deformation in $Si_{1-x}Ge_x$ [3]

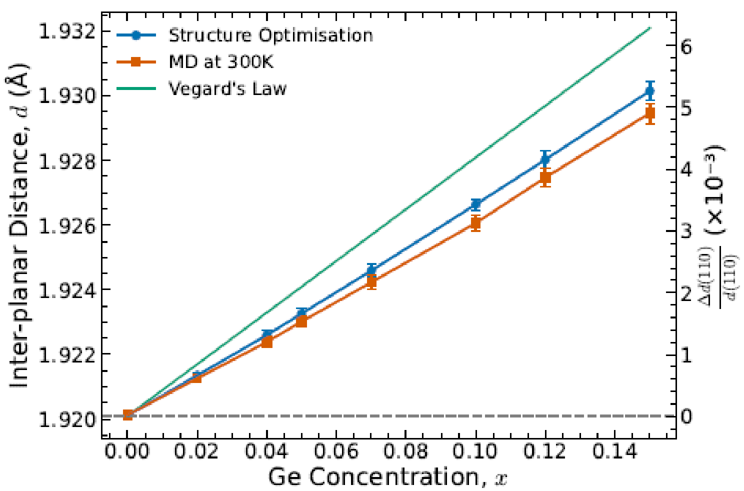


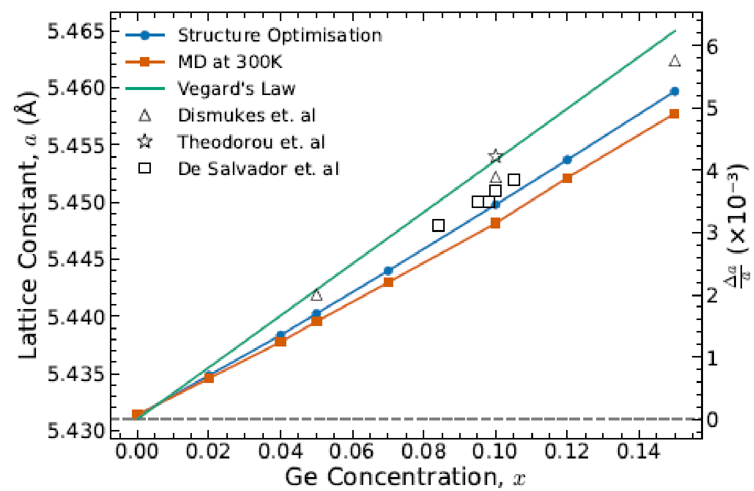

By means of MBN Explorer one can model $Si_{1-x}Ge_x$, diamond-boron etc binary systems using the MD methods.


[1] Mikkelsen & Uggerhøj, NIMB **160** (2000) 435
[2] Krause, Korol, Solov'yov, & Greiner, *NIMB*, **483** (2002) 455
[3] Korol, Solov'yov, Greiner, "Channeling and radiation in periodically bent crystals", Springer (2014)

# Effect of doping on crystalline structure

- We have conducted a systematic analysis of the inter-planar distance change as a result of the introduction of dopant Ge atoms to a Si crystal at concentrations of $0 < x < 0.15$ ($Si_{1-x}Ge_x$) using MD simulations.
- A linear increase in inter-planar distance with Ge concentration has been observed.
- Our results are in agreement with those of experiments




Plots of the average inter-planar distance (left) and lattice constant (right) as functions of the dopant concentration. In each plot a second y axis shows the relative change in lattice constant Δa/a or inter-planar distance Δd/d. The lattice constant is compared to experimental data (symbols) as well as the empirical Vegard's Law (the green line). The grey dashed lines show the nominal values in single Si crystals.

M. D. Dickers, G. B. Sushko, A. V. Korol, N. J. Mason, F. Fantuzzi, A. V. Solov'yov. *Dopant concentration effects on $Si_{1-x}Ge_x$ crystals for emerging light-source technologies: A molecular dynamics study*. arXiv:2402.10120v1; EPJD (in print, doi: 10.1140/epjd/s10053-024-00870-2)

# Experimental and computational characterisation of PBCs



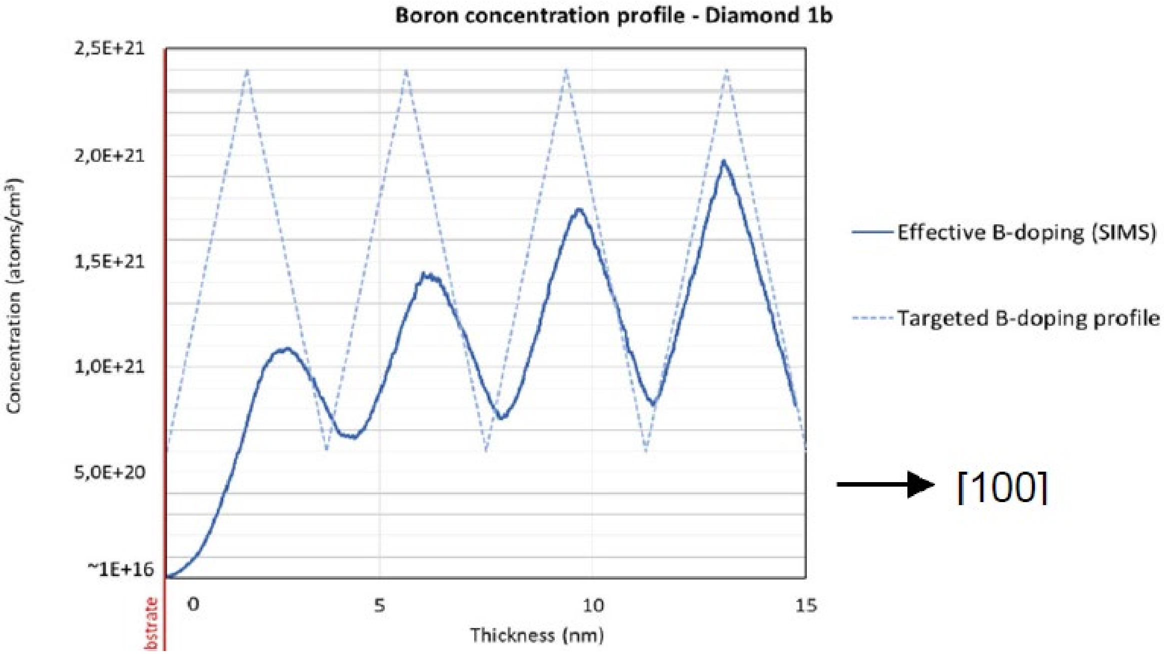



**Figure 2.2.1**: Boron-doping profile for diamond sample 1b.

Ref.: ESRF, 2nd year TECHNO-CLS Report.

Work in progress:
ESRF & Uni-Mainz.

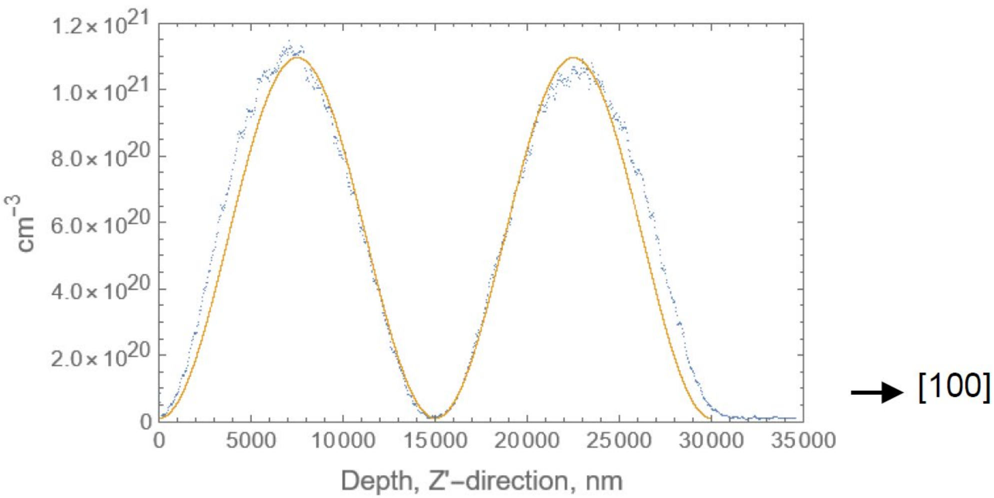



**Figure 2.2.4**: Comparison of the experimentally measured boron-doping for diamond sample 2a[3]

Ref.: ESRF and MBN RC, 2nd year TECHNO-CLS Report.

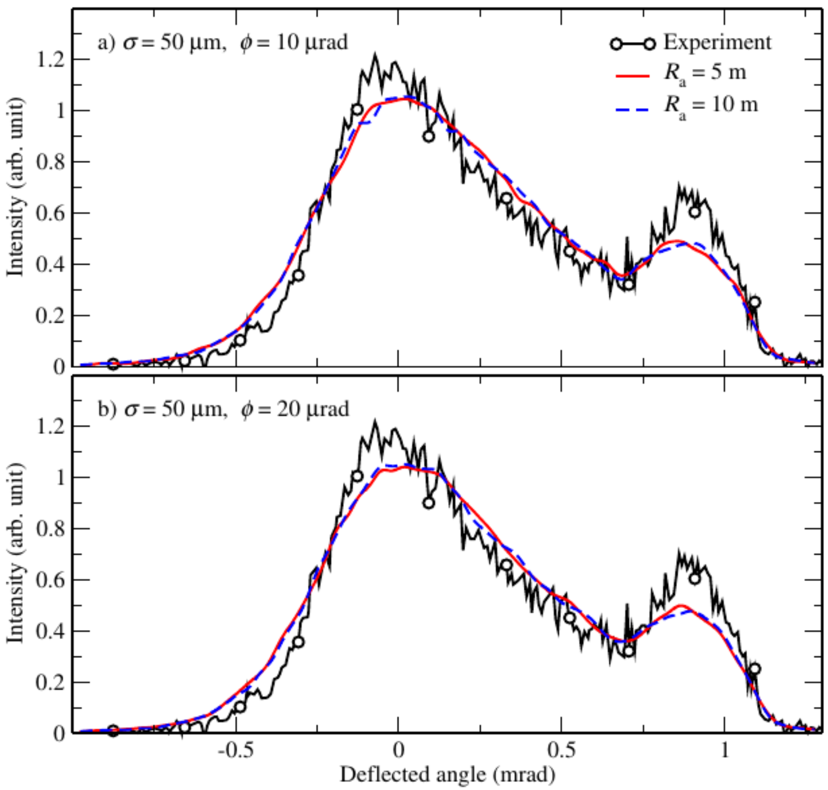
Work in progress:
ESRF & MBN-RC.

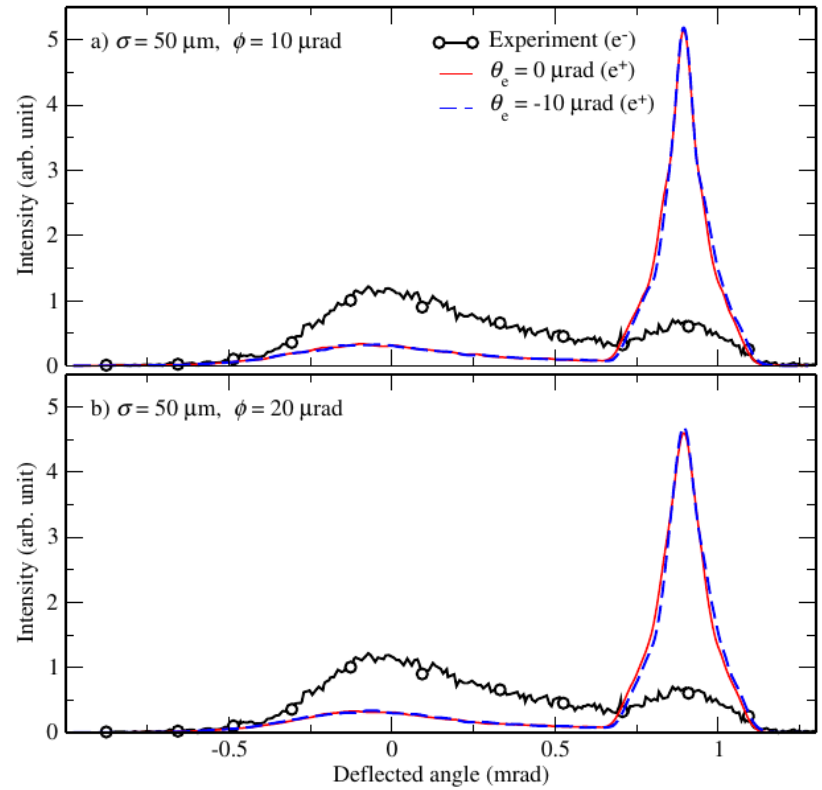
**T2.3 (MBN-RC, INFN, UNIFE, Uni-Mainz)**

- **Multiscale simulations of *particles propagation in LCs, BCs & PBCs* for various experimental conditions.**
- Atomistic level assessment of *related phenomena* (multiple scattering, volume reflection & capture, energy loss).
- Verification of the results with available experimental data and theoretical benchmarking for future experiments.

# Simulation of e- / e+ deflection by bent Si crystal (@ MAMI energies)

MBN Research Center




***Left:*** Angular distribution of deflected 855 MeV *electrons* simulated for different values of the beam divergence (φ = 10 and 20 μrad in the top and bottom graphs, correspondingly) and for two values of the anticlastic curvature radii $R_a$ as indicated in the common legend shown in the top graph. All dependencies shown correspond to the beam transverse size σ = 50 μm. Solid line with open circles corresponds to the experimental data from Mazzolari et al, *Phys. Rev. Lett.* 112 (2014) 135503.

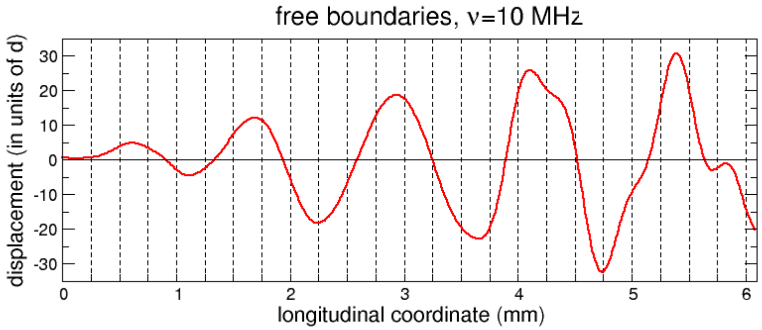
***Right:*** Same as on the left panel but for a 855 MeV *positron* beam incident on the quasi-mosaic Si(111) crystal. All simulated distributions refer to the anticlastic curvature radius Ra = 5 m. For the sake of comparison. The experimental data for electrons are also shown.

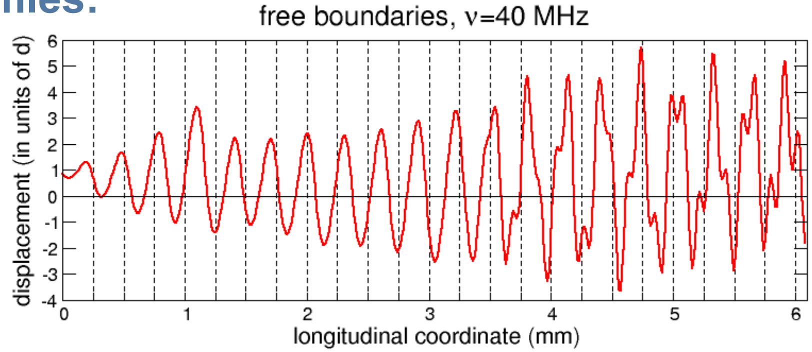
P.E Ibanez-Almaguer, G. Rojas-Lorenzo, M. Marquez-Mijares, J. Rubayo-Soneira, G.B. Sushko, A.V. Korol, A.V. Solov'yov, arXiv:2312.09927 (https://arxiv.org/abs/2312.09927) (15 Dec 2023).

# Multiscale simulations of 20 GeV $e^+$ in 2-6 mm thick Si crystals bent by AW

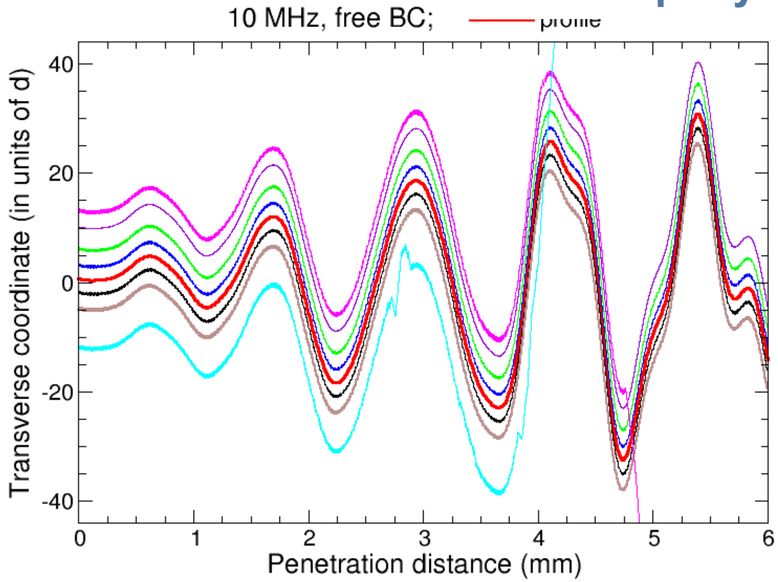
MBN Research Center

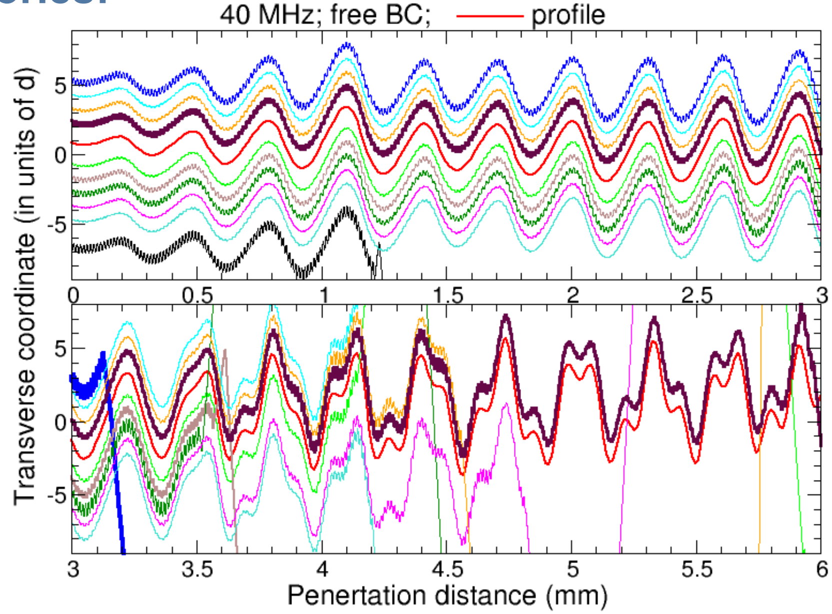
## Bending profiles:




## Exemplary trajectories:



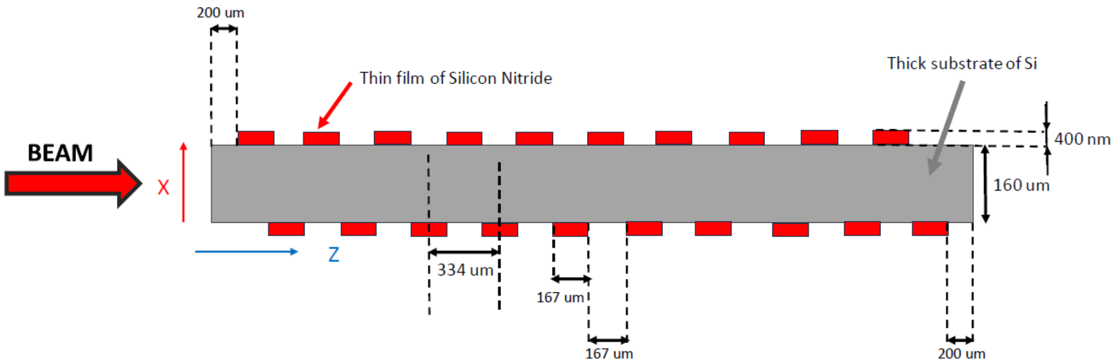

In the right figure the trajectories are shown in two segments: 0-3 mm(top) and 3-6 (bottom)

MBN-RC & HMU teams: work in progress.

# Simulations of 5-20 GeV $e^+$ in Si PBC

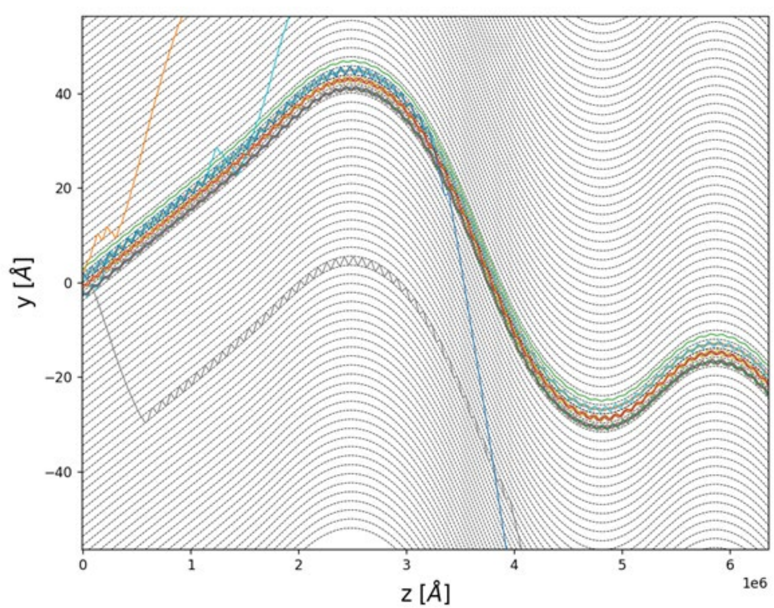
MBN Research Center

## PBC Si crystal manufactures by means of surface patterning technology (UNIFE & INFN):




## Exemplary trajectories:

MBN-RC, INFN & UNIFE teams: work in progress.



MBN Research Center

**T2.4 (MBN-RC, INFN, Uni-Mainz, UNIFE, HMU)**

- **Theoretical and computational *characterisation of radiation emitted in CLSs*** based on different (i) manufactured crystal structures, (ii) propagation regimes, (iii) beam parameters.
- **Comparative characterisation/description and computational design of novel CLSs** which can be tuned for the beams available at existing and future facilities.

# Definition of the term "CLS prototype"

MBN Research Center

CLS Prototype implies full characterization (experimental or/and theoretical and computational) of radiation emitted by a beam of charged projectiles passing through a crystalline target. The following data / parameters are to be specified / calculated / measured:

1) *Data on the radiation emitted:* spectral-angular and spectral distributions, photon flux (i.e. number of photons per second for given aperture), brilliance;
2) *Parameters of the beam:* type of the particles (electrons or positrons), beam energy, divergence, size, emittance, energy spread;
3) *Data on the crystal target:* type of the crystal, orientation, geometry (linear, bent, periodically bent), bending parameters (curvature radius, amplitude and period), thickness, crystal quality (defects concentration, bending homogeneity).

The quantities 1) and 2) are commonly used for the characterisation of other types of gamma-ray light sources (synchrotrons, Compton LS).

# CLS to be compared to modern Compton gamma-ray LS

MBN Research Center

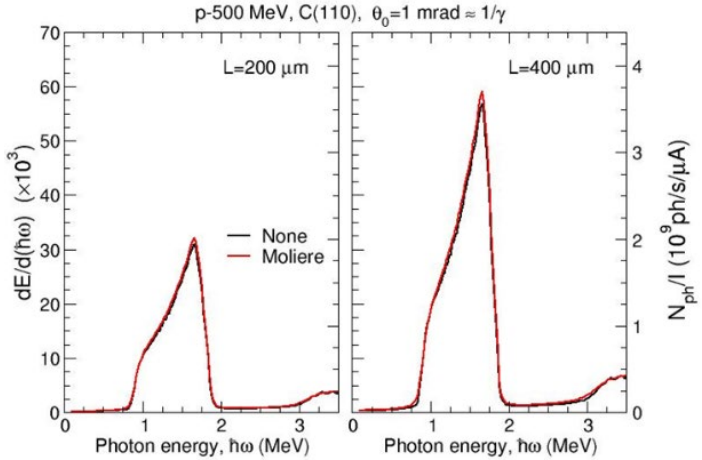
Parameters of several Compton gamma-ray light sources which are either operational or being developed for operation. Listed are: electron beam energy *ε* , average current *I*, gamma photons

| Facility<br>Location | HIGS<br>(US) | LEPS/LEPS2<br>Japan | NewSUBARU<br>Japan | UVSOR-III<br>Japan | SLEGS<br>China | ELI-NP<br>Romania |
|---|---|---|---|---|---|---|
| ε (GeV) | 0.24-1.2 | 8 | 0.5-1.5 | 0.75 | 3.5 | 0.23-0.74 |
| I (mA) | 10-120 | 100 | 300 | 300 | 100-300 | 1 |
| ħω (MeV) | 1-100 | 1300-2900 | 1-40 | 1-5.4 | 0.4-20 | 1-19.5 |
| Δω/ω (%) | 0.8-10 | <15 | 10 | 2.9 | <5 | <0.5 |
| $(N_{ph})_{tot}$ (ph/s) | $10^6$-$3\times10^{10}$ | $10^6$-$10^7$ | (1-4) $\times10^7$ | $10^7$ | $10^6$-$10^8$ | $10^{11}$ |

# Theoretical & computational characterization of CLS Prototypes

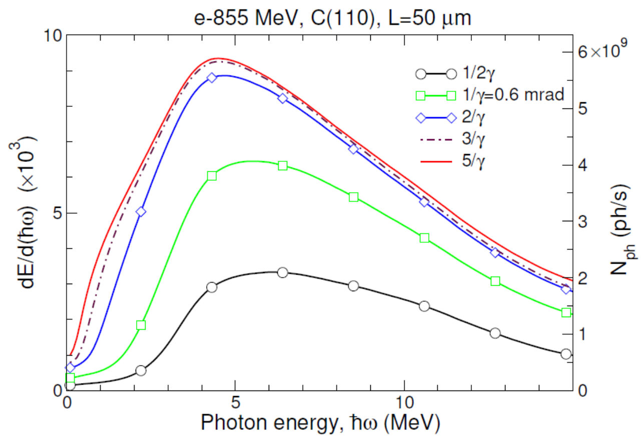
MBN Research Center

## (I) 500 MeV positrons and 855 electrons in single diamond crystals




MBN-RC: work in progress.

Spectral distribution of radiation (left axes) and number of photons per second and **per 1 μA** of the beam current (right axes) emitted by **500 MeV *positrons*** incident along the (110) planar direction in a 200 μm (left figure) and 400 μm (right figure) thick diamond crystals. The emission cone equals to the natural emission cone 1/γ = 1 mrad. The dependences have been calculated without ("None") and with ("Moliere") account for the ionizing collisions. The number of photons is calculated for the bandwidth $\Delta\omega/\omega$ = 0.01.



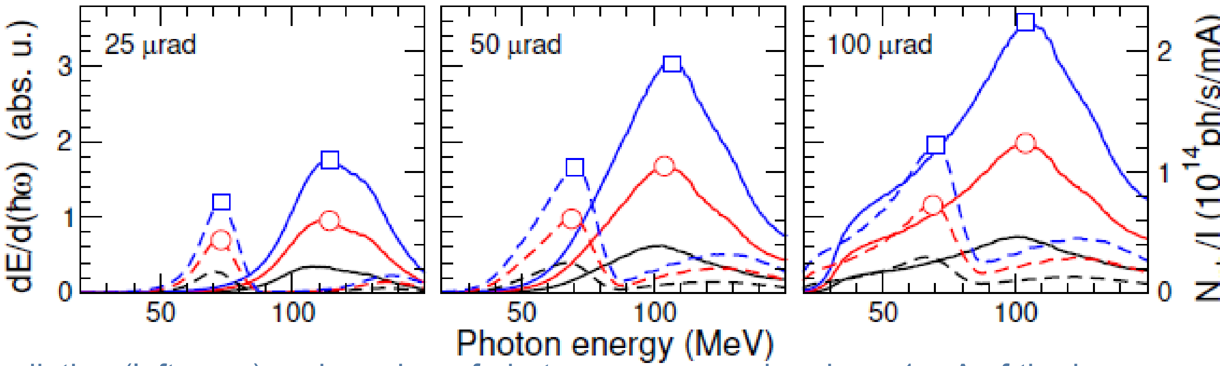

Spectral distribution of radiation (left axes) and number of photons per second and **per 1 μA** of the beam current (right axes) emitted by **500 MeV electrons** incident along the (110) planar direction in a 200 μm (left figure) and 400 μm (right figure) thick diamond crystals. The emission cone equals to the natural emission cone 1/γ = 1 mrad. The dependences have been calculated without ("None") and with ("Moliere") account for the ionizing collisions. The number of photons is calculated for the bandwidth $\Delta\omega/\omega$ = 0.01.

**Work in progress (MBN-RC):** CLS prototypes by means of single diamond crystals are feasible at MAMI energies for both electrons and positrons. **The intensity in the photon energy range 0.5-5 MeV can be up to $10^9$ photons/s/μA thus making the CLS competitors to the existing gamma-ray LS based on the Compton scattering.**

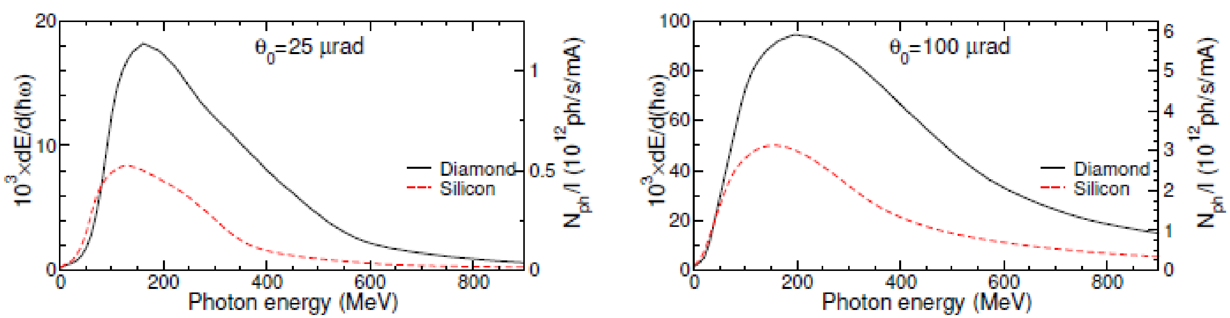
# Theoretical & computational characterization of CLS Prototypes

MBN Research Center

## (II) 10 GeV positrons and electrons in 0.1-6 mm single Si and Diamond crystals




Spectral distribution of radiation (left axes) and number of photons per second and per 1 mA of the beam current (right axes) emitted by **10 GeV *positrons*** incident along the (110) planar direction in diamond (solid lines) and silicon (dashed lines) crystals. The curves without symbols, with open circles and with open squares correspond to the crystal thickness 1, 3, and 6 mm, respectively. Three graphs refer to different emission cones as indicated. The number of photons is calculated for the bandwidth $\Delta\omega/\omega$ = 0.01.



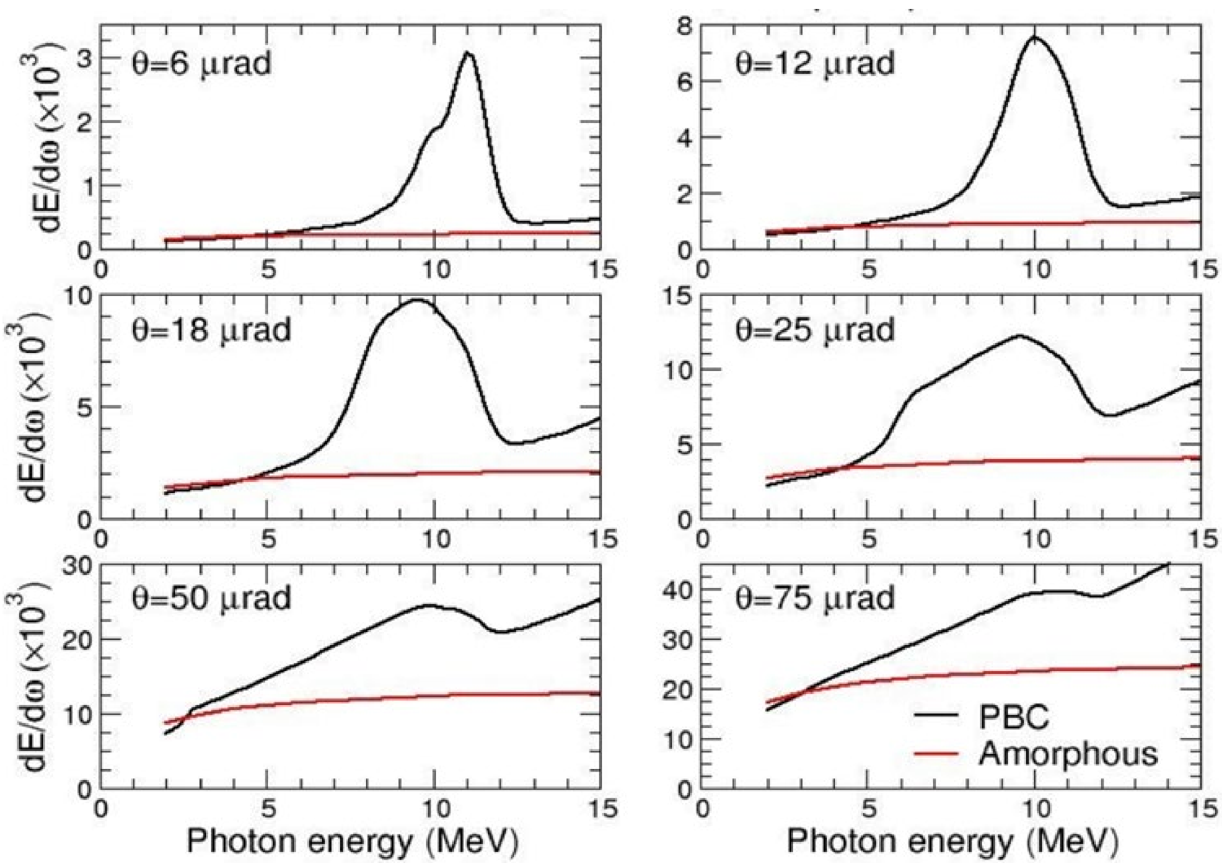

Spectral distribution of radiation (left vertical axes) and number of photons per second and per unit current in mA (right vertical axes) calculated for **10 GeV *electrons*** passing through 0.2 mm thick diamond and silicon crystals along the (110) planar direction. Left and right graphs correspond to the emission cones 25 and 100 $\mu$rad. The number of photons refers to the bandwidth $\Delta\omega/\omega$ = 0.01.

**Summary:** By means of CLS based on single crystals it is possible to achieve average photon fluxes much higher than those available at modern laser-Compton gamma-ray light sources.

G.B. Sushko, A.V. Korol, A.V. Solov‘yov, arXiv:2401.10596 (24 Jan 2024).

# Theoretical & computational characterization of CLS Prototypes

## (III) 20 GeV positrons in acoustically excited Silicon crystals



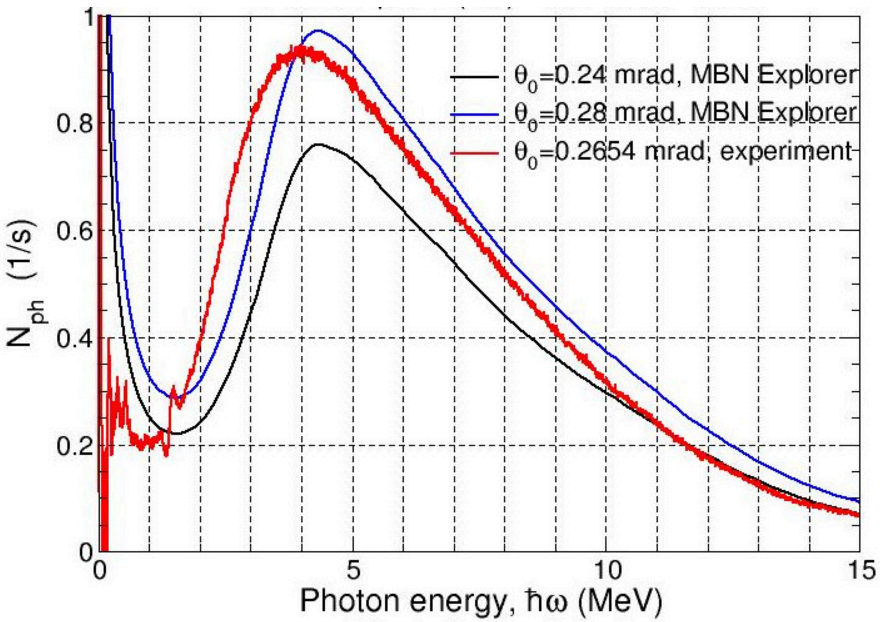

Spectral distribution of CUR (black curves) emitted by 20 GeV positrons in the acoustically excited silicon (110) crystal. Red curves show the distributions in amorphous silicon. Different graphs refer to different emission cones θ as indicated. The data corresponds to the AW frequency of 40 MHz..

Work in progress: MBN-RC & HMU.

# Full characterization of the CLS prototype

MBN Research Center

## 855 MeV electrons in a diamond single crystal




Number of photons (per second) emitted by 855 MeV and $I$=0.166 pA electron beam incident on a 50 microns thick diamond single crystal. In the experiment (Uni-Mainz) the photons were collected within the 0.2654 mrad cone along the incident beam direction. The simulations (MBN-RC) refer to the emission cones as indicated in the legend.

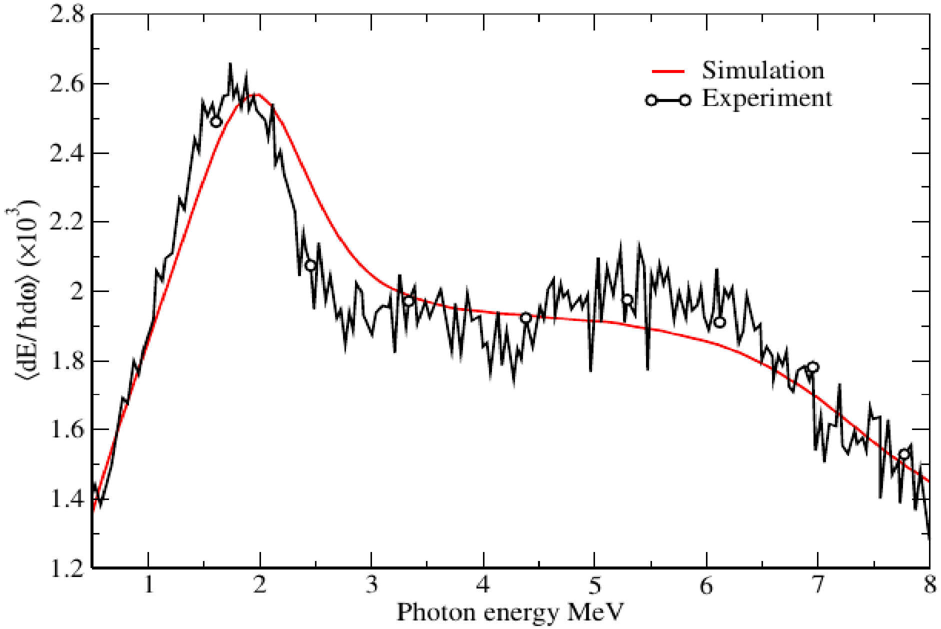
Note that the data on $N_{ph}$ refer to low beam current $I$ and to narrow bandwidth. Increasing the current up to 10 μA (which is achievable at MAMI) and bandwidth by a factor of 25 (this will correspond to $\Delta\omega/\omega=0.01$ in the maximum at $\hbar\omega\approx4$ MeV) the number of photons can be as high as $10^9$ ph/s, thus exceeding $N_{ph}$ achievable at many currently operating Compton gamma-ray LS.

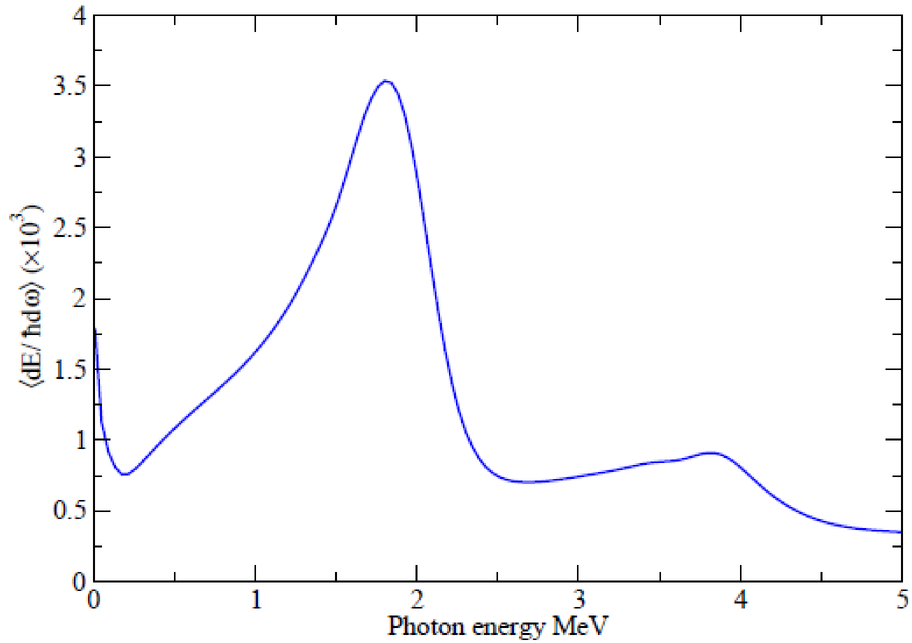
**Summary:** We consider this result as <u>full characterisation</u> of the particular CLS based on the electron beam propagation through a single crystal. This is an important achievement of the Consortium work during the second year of the project.

Work in progress: MBN-RC & Uni-Mainz.

# Radiation emission by 855 MeV $e^-/e^+$ in quasi-mosaic bent Si crystal

MBN Research Center



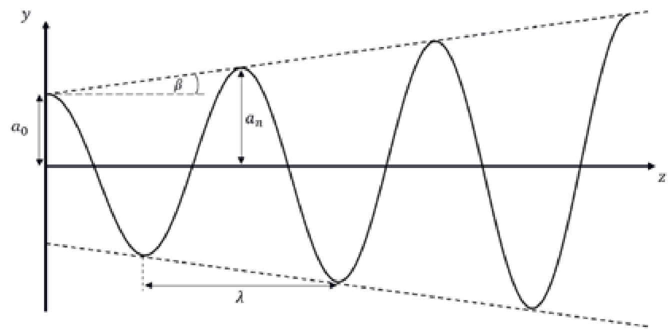



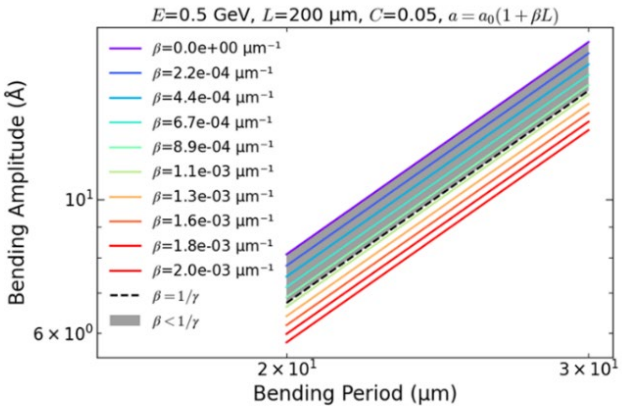

Spectral distribution of radiation emitted by 855 MeV electrons (left) and positrons (right) passing through the ‘quasi-mosaic’ bent Si(111) crystal. Solid (red and blue) curves without symbols stands for the results of the current simulations; solid (black) curve with symbols, shown in the left figure, corresponds to the experimental data reported by Bandiera et al *Phys. Rev. Lett.* 115 (2015) 025504. Note that the values of ⟨dE/d(ħω)⟩ are shown being multiplied by the factor $10^3$. The intensity of the of background radiation due to the incoherent bremsstrahlung is approximately $0.35\times10^{-3}$.


P.E Ibanez-Almaguer, G. Rojas-Lorenzo, M. Marquez-Mijares, J. Rubayo-Soneira, G.B. Sushko, A.V. Korol, A.V. Solov‘yov, arXiv:2312.09927 (https://arxiv.org/abs/2312.09927) (15 Dec 2023).

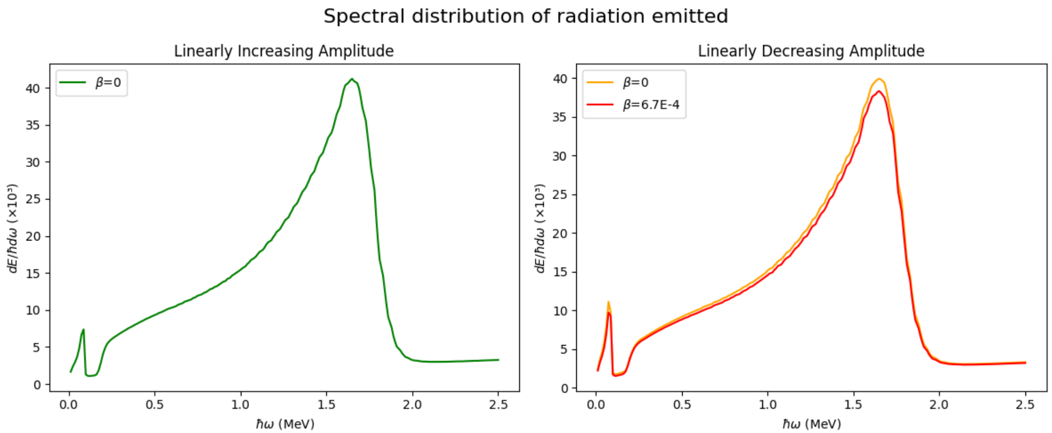
# Computational analysis of radiation emitted by projectiles moving along non-harmonic trajectories

MBN Research Center



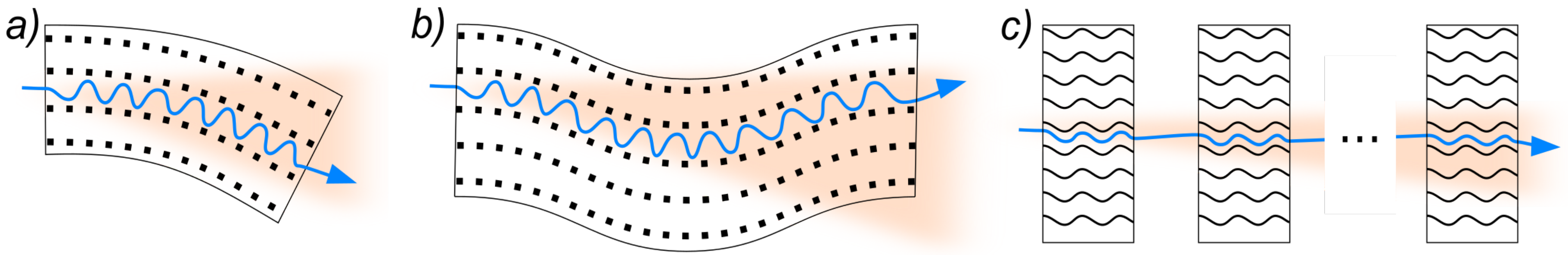

***Left:*** Schematic representation of the linearly increasing bending amplitude where β is the amplitude angle, $a_0$ is the initial amplitude and λ is the period. ***Right:*** Graphical aid for choosing the values of β; Specific scenario considered, with the parameters shown in the figure title. One should aim for the values marked in grey to maintain the coherence of radiation.

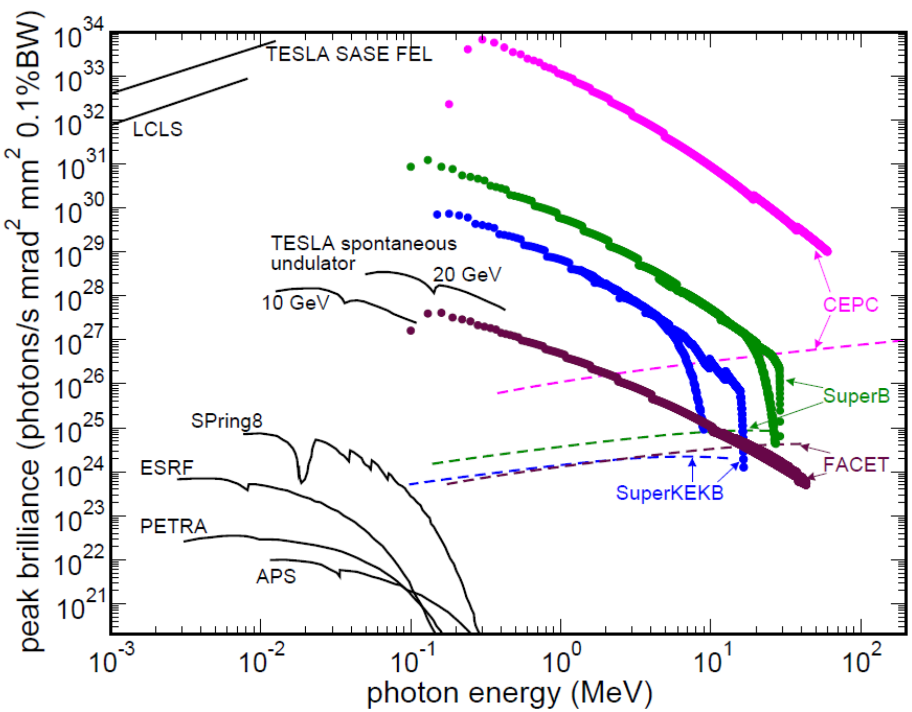


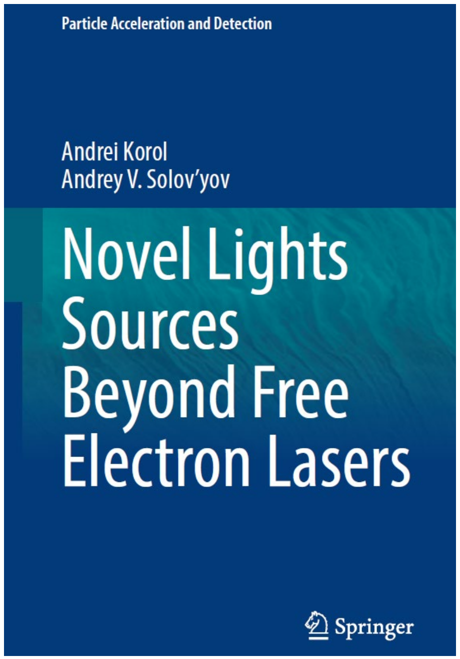

Spectral distribution of radiation emitted by positron channeling in periodically bent diamond (110) crystal with varied bending amplitude. Each plot presents the spectrum for a harmonic bending profile (β =0) as well as non-harmonic profile; The initial values for bending amplitude are 11.2 Å (left) and 14.6 Å (right).

Work in progress: UoK & MBN-RC.

# Conclusions and outlook

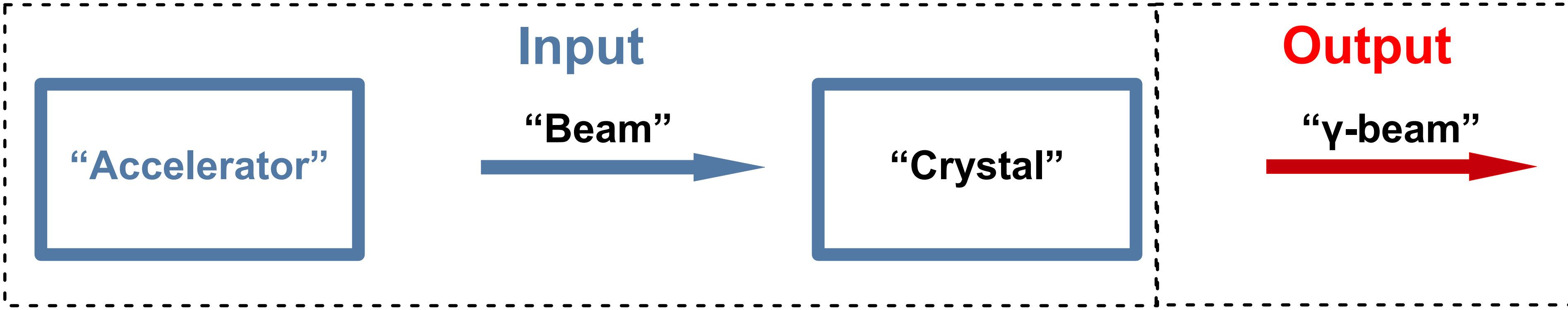


# Realisation of the prototypes of gamma-ray Crystal-based LS (CLS)

MBN Research Center




Work in progress: MBN-RC & HMU.

**Principal elements**:
- Type of accelerator
- Apparatus
- Beam line
- Infrastructure

**Characterisation of the beam:**
- Type of projectile
- Energy and energy spread
- Size
- Emittance
- Current

**Relevant issues:**
- Crystal manufacture;
- Structure characterisation
- Crystal manipulation
- Channeling experiments
- Advanced simulations

**Experimental and theoretical characterisation of the radiation**:
- Spectral-angular distribution
- Number of photons
- Brilliance
- Power

MBN-RC & TECHNO-CLS consortium: TECHNO-CLS report

# Accelerators and beams

**Table 4.5.2 List of suitable accelerator facilities** TECHNO-CLS consortium: TECHNO-CLS report

| Facility | Beam line | projectile | Beam parameters | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | energy (GeV) | size (μm) | divergence (μrad) | repetition rate (pulse/s) | charge (units of *e*) | current peak ave | Already used | Availability |
| MAMI | | $e^-$ | 0.270-0.855 | x:10-1000 y:10-1000 | x:100-1 y:800-8 | CW [1] | | 0.16fA-50μA (average) | Yes | A |
| MAMI | | e+ | 0.530 | x:250 μm [2] y:1500μm | x: [3] y: 60 | CW [1] | | 1.6 fA (peak) | Yes | A |
| CERN | SPS-H2 | e-, e+ | 20-120 | x,y:(2-3)mm @120GeV | x:(325-90) @ (20-120) GeV; y:(230-100) @(20-120)GeV | | $10^4$-$10^5$ per spill [4] | | YES, but parameters can be modified | yes |
| CERN | PS-T9 | e- | 1-15 | x,y: few cm | x:800@6GeV; y:1500@6GeV | | $10^2$-$10^3$ per spill [5] | | YES, but parameters can be modified | yes |
| CERN | PS-T9 | e+ | 1-15 | x,y: few cm | x:800@6GeV; y:1500@6GeV | | $10^2$ per spill [5] | | YES, but parameters can be modified | yes |

■ ■ ■ see report

# Accelerators and beams

MBN Research Center

## Table 4.5.3 Conducted and planned experiments at synchrotrons and accelerators

### a) Experiments conducted at synchrotrons and accelerators during the 1st year of the project

■ ■ ■ see report TECHNO-CLS consortium: TECHNO-CLS report

### b) Experiments conducted at synchrotrons and accelerators during the 2nd year of the project

| Facility | Beam line | Projec tile | energy | Target | Data to be measured | Time | Teams |
|---|---|---|---|---|---|---|---|
| CERN | T9 | e-/e+ | 6 GrV | Tungsten and Iridium single crystals | Radiative energy loss, photon yield | August 2023 | INFN, UNIFE, UNIPD |
| MAMI | X1 | e+ | 530 MeV | Si flat, Bent Si | Beam line tests, Channeling of Positrons, Deflection of Positrons | Several beam times 2023 - 2024 | Uni Mainz, UNIFE, INFN, UNIPD |
| MAMI | X1 | e- | 600MeV - | Diamond, | Radiation Spectra, | Several beam | Uni Mainz, ESRF, |

■ ■ ■ see report TECHNO-CLS consortium: TECHNO-CLS report

### c) Schedule of planned experiments at synchrotrons and accelerators

| Facility | Beam line | Projec tile | energy | Target | Data to be measured | Time | Teams |
|---|---|---|---|---|---|---|---|
| MAMI | X1 | e+ | 530 MeV | Flat Si, PBC SiGe, | Beam line tests, Channeling of | Several beam times 2024 - | Uni Mainz, UNIFE, INFN, UNIPD, |

■ ■ ■ see report TECHNO-CLS consortium: TECHNO-CLS report

# Types of crystals: material, geometry & technologies for crystal manufacturing



**Table 4.5.1 Cumulative list of available crystals and related manufacturing technologies.**

| Silicon (Si) | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Label | Type | Method | Direction | Parameters [1] | | | | Characterisation | Where stored | Availability (A, N/A) |
| | | | | Size | R (cm) | a (nm) | λ (μm) | | | |
| BC-Si-QM1 | BC | QM | (111) | L:15 μm | 3 | - | - | [2] | INFN, UNIFE | A |
| BC-Si-QM0 | BC | QM | (111) | L:30μm | 3 | - | - | [3] | INFN, UNIFE | A |
| BC-Si-St | BC | $Si_3N_4$ | (110) | L=4mm, W=55mm, T=0.5mm | 8000 | - | - | - | INFN, UNIFE | A |
| | PBC | Gr | (111) | L:0.8mm, W:2mm, T:200 μm, UndT:100 μm | - | 0.15 | 80 | [4] | INFN, UNIFE | A |
| PBC-Si-G1 | PBC | Gr | (111) | L:3.2mm, W:10mm, T:200 μm; UndT:160 μm | - | 1.28 | 320 | [4], [5] | INFN, UNIFE | A |
| | PBC | $Si_3N_4$ | (110) | L=10 λ<br>T=160 μm,<br>W to be defined depending on coating homogeneity. Range is to be selected depending on available facility | - | >1<br><br>Dep. on FEM simula-tion | 350<br>500<br>1000 | | To be built at INFN, UNIFE | N/A [9] |

■ ■ ■ see report TECHNO-CLS consortium: TECHNO-CLS report

# Characterisation of Gamma-ray CLSs

MBN Research Center

**Table 4.5.4 List of CLS prototypes (theory, experiment, both) and related manufacturing technologies**

| Linear Crystals | | | | | | |
|---|---|---|---|---|---|---|
| projectile | Beam | Material | Size | Type/ Technology | CLS | |
| | | | | | Spectrum | CLS characteristics |
| **Diamond** | | | | | | |
| e<br>Ref. [1] | E=10 GeV<br>$\sigma_x$=6.8 μm<br>$\sigma_y$=16.3 μm<br>$\gamma\varepsilon_x$=4.0μm-rad<br>$\gamma\varepsilon_y$=3.2μm-rad<br>$I_{peak}$=6.4 kA<br>Ref. [1] | C(110)<br>Ref. [1] | L=6-96 μm<br>Ref. [1] | | PhE=0.1-2 GeV<br>SAD, SD – yes<br>Ref. [1] | PhNo – yes<br>$B_{peak}$ - yes<br>Ref. [1] |
| e<br>Ref. [2] | E=10 GeV<br>$\sigma_{x,y}$=6.8 &16.3 μm<br>$\gamma\varepsilon_x$=4.0μm-rad<br>$\gamma\varepsilon_y$=3.2μm-rad<br>$I$ = 1 mA<br>Ref. [2] | C(110)<br>Ref. [2] | L=200-400 μm<br>Ref. [2] | LC | PhE=50-600 MeV<br>SAD, SD – yes<br>Ref. [2] | PhNo – yes<br>B – yes<br>Ref. [2] |
| e+ | E=10 GeV<br>$\sigma_{x,y}$=6.8 &16.3 μm<br>$\gamma\varepsilon_x$=4.0μm-rad | C(110) | L=1000-6000 μm | LC | PhE=50-150 MeV<br>SAD, SD – yes | PhNo – yes<br>B – yes |

■ ■ ■

see report    TECHNO-CLS consortium: TECHNO-CLS report

# Acknowledgement to the MBN RC team and theTECHNO-CLS Consortium

MBN Research Center

MBN Research Center

INFN
Istituto Nazionale di Fisica Nucleare

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

JG|U

Università degli Studi di Ferrara
- EX LABORE FRUCTUS -

University of Kent

Hellenic Mediterranean University

ESRF

Università degli Studi di Padova

MBN Research Center

# Thank you for your attention !