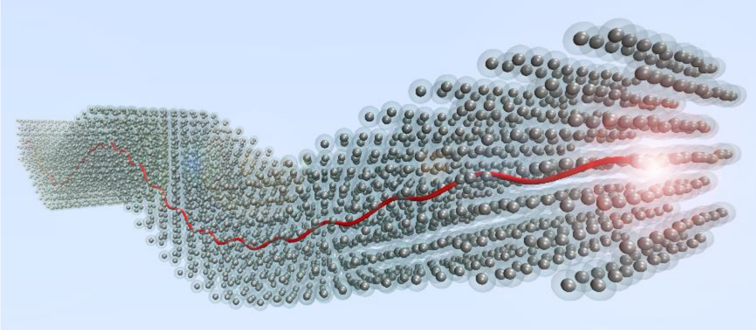
Atomistic modelling of electron and positron propagation and radiation emission in crystals by means of MBN Explorer

Andrei Korol

MBN Research Center, Frankfurt am Main, Germany



Annual Workshop of TECHNO-CLS, Ferrara, October 5-6, 2023

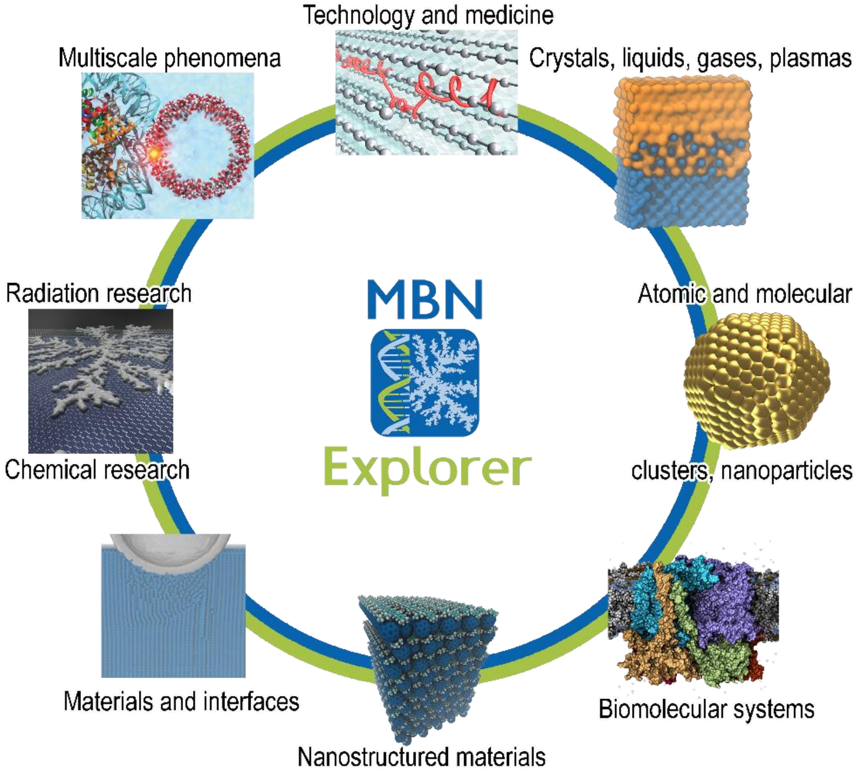
Outline

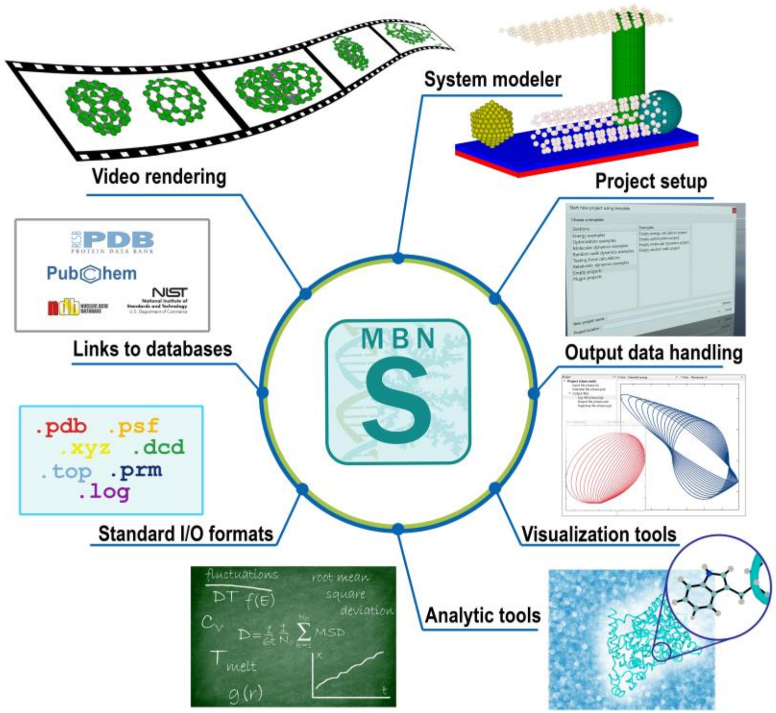
- Characterization of CLS: case study
- Emission spectra from thin Si and Ge crystals
- Channeling in a diamond-boron hetero-crystal
- Channeling process with account for radiation reaction force
- Ongoing and future work

MBN Explorer and MBN Studio 5.0

MBN Research Center

- **MBN Explorer & Studio software 5.0** are the powerful instruments for advanced theoretical and computational research and **multiscale modelling** of structure and dynamics of complex Meso-Bio-Nano (MBN) systems.
- **MBN Explorer & Studio software** can be utilised for teaching of many disciplines
- **MBN Explorer & Studio** are being developed by the **MBN Research Center** in Frankfurt, www.mbnresearch.com. **You are welcome to contact us!**





Characterization of CLS based on Small-Amplitude Small-Period (SASP) periodically bent crystals*

SASP bending:
- Bending amplitude << inter-planar distance: $a \ll d$
- Bending period << period of channeling oscillations: $\lambda \ll \lambda_{ch}$

* G.B. Sushko, A.V. Korol, A.V. Solov'yov. *Nuclear Instrum. Meth. B* **535** (2023) 117

Characterization of a CLS

Main characteristics of Crystal-based Light Sources (CLS):

- Spectral and spectral angular distributions of radiation: $$\frac{\mathrm{d}E(\theta \le \theta_0)}{\mathrm{d}(\hbar\omega)} = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\theta_0} \frac{\mathrm{d}^3 E}{\mathrm{d}(\hbar\omega)\,\mathrm{d}\Omega}\,\theta \mathrm{d}\theta$$

- Number of photons per second: $$\mathcal{N}_\omega\,[\mathrm{s}^{-1}] = \frac{\mathrm{d}E(\theta \le \theta_0)}{\mathrm{d}(\hbar\omega)}\,\frac{\Delta\omega}{\omega}\,\frac{I\,[\mathrm{A}]}{e} = 6.25 \times 10^{21}\,\frac{\mathrm{d}E(\theta \le \theta_0)}{\mathrm{d}(\hbar\omega)}\,\frac{\Delta\omega}{\omega}\,I\,[\mathrm{kA}]$$

- Power of radiation: $$P_\omega\,[\mathrm{W}] = \frac{\mathrm{d}E(\theta \le \theta_0)}{\mathrm{d}(\hbar\omega)}\,\hbar\Delta\omega\,\frac{I\,[\mathrm{A}]}{e} = 10^{12}\,\frac{\mathrm{d}E(\theta \le \theta_0)}{\mathrm{d}(\hbar\omega)}\,\frac{\Delta\omega}{\omega}\,\hbar\omega\,[\mathrm{GeV}]\,I\,[\mathrm{kA}]$$

$\Delta\omega$ – bandwidth /BW)

I – electric current

- Brilliance of radiation: $$B = \frac{\mathrm{d}E(\theta \le \theta_0)}{\mathrm{d}(\hbar\omega)}\,\frac{1.58 \times 10^{14}}{\mathcal{E}_x \mathcal{E}_y}\,I\,[\mathrm{A}]$$

$$\mathcal{E}_{x,y} = \sqrt{\sigma^2 + \sigma_{x,y}^2}\,\sqrt{\phi^2 + \phi_{x,y}^2}$$

$\sigma_{x,y}$, $\sigma_{\varphi x,y}$ – beam sizes and angular divergencies

σ, φ – photon source size and emission angle

Parameters used in the simulations

MBN Research Center

- **10 GeV electron and positron beams**

The rms beam sizes $\sigma_{x,y}$, normalized emittances $\gamma\epsilon_{x,y} = \gamma\sigma_{x,y}\phi_{x,y}$ and peak current I_{peak} for the 10 GeV electron and positron FACET-II beams [4]. The beam divergencies $\phi_{x,y}$ correspond to the indicated values of $\sigma_{x,y}$ and $\gamma\epsilon_{x,y}$.

	$\gamma\epsilon_x$ (μm-rad)	$\gamma\epsilon_y$ (μm-rad)	σ_x (μm)	σ_y (μm)	σ_{ϕ_x} (μrad)	σ_{ϕ_y} (μrad)	I_{peak} (kA)
Electron	4.0	3.2	6.8	16.3	30	10	64
Positron	10	12	17	61	30	10	5.8

[4] SLAC Site Office: Technical Design Report for the FACET-II Project at SLAC National Accelerator Laboratory, Report SLAC-R-1072, SLAC, 2016.

- **Crystals:** diamond, silicon, germanium (d_{110}=1.26, 1.92, 2.00 Å)

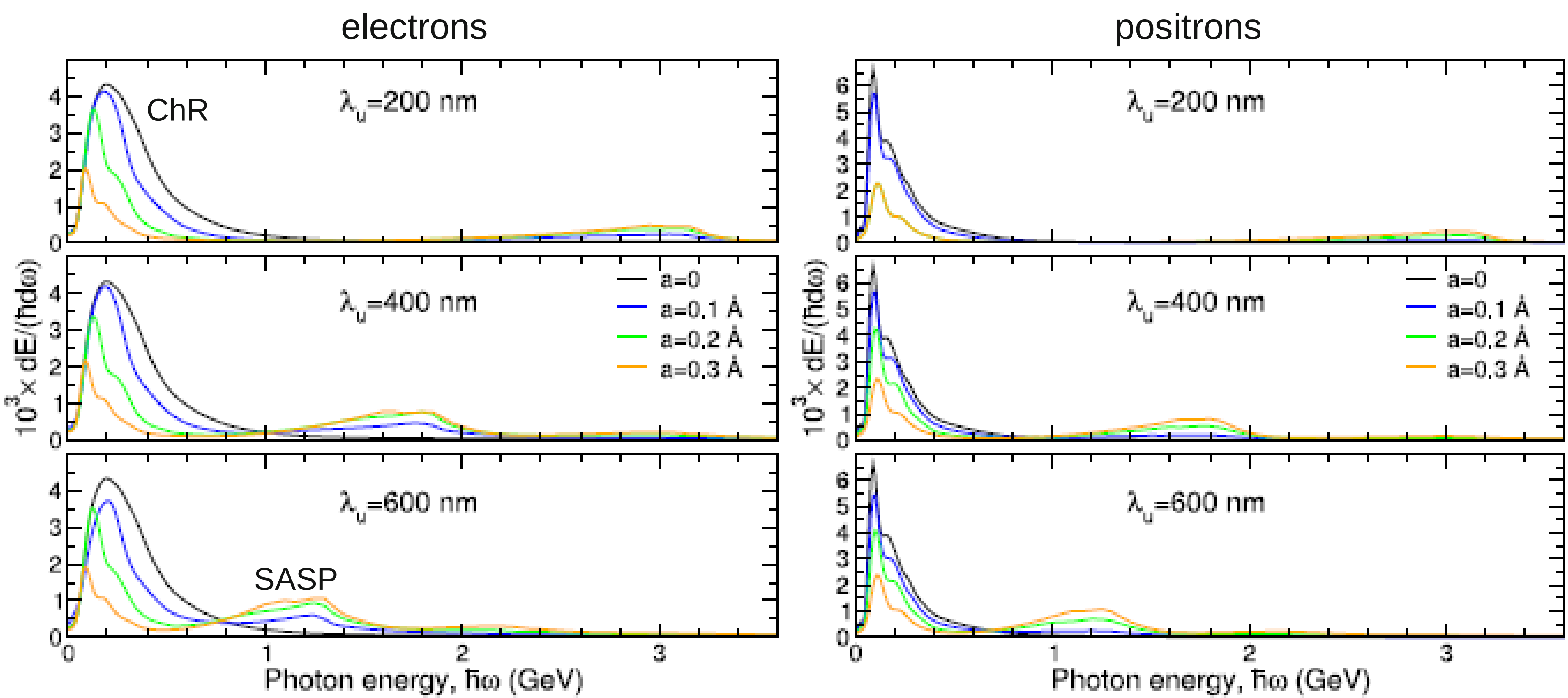
  Thickness: L=6-100 microns

  SASP bending: a=0.1-0.3 Å, λ= 200-600 nm (λ_{ch}≈10 microns)

G.B. Sushko, A.V. Korol, A.V. Solov'yov. *Nuclear Instrum. Meth. B* **535** (2023) 117

Emission spectra

Case study: Diamond(110), L = 12 μm, $\theta = \gamma^{-1} \approx$ 50 μrad; **varying a and λ**

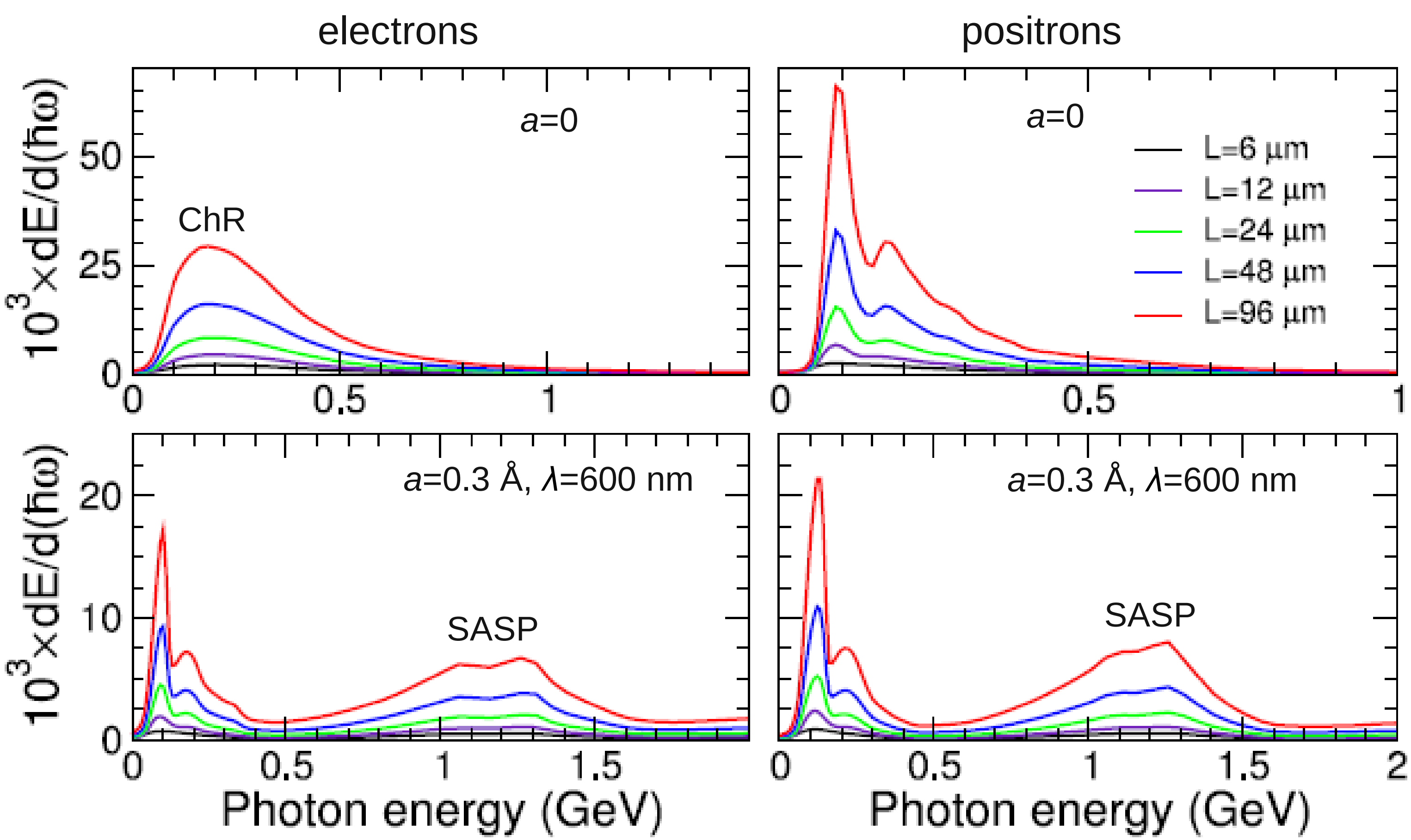


Bremsstrahlung background ≈ 0.016×10^{-3}

G.B. Sushko, A.V. Korol, A.V. Solov'yov. *Nuclear Instrum. Meth. B* **535** (2023) 117

Emission spectra

Case study: Diamond(110), $\theta = \gamma^{-1} \approx 50$ μrad; **varying L**

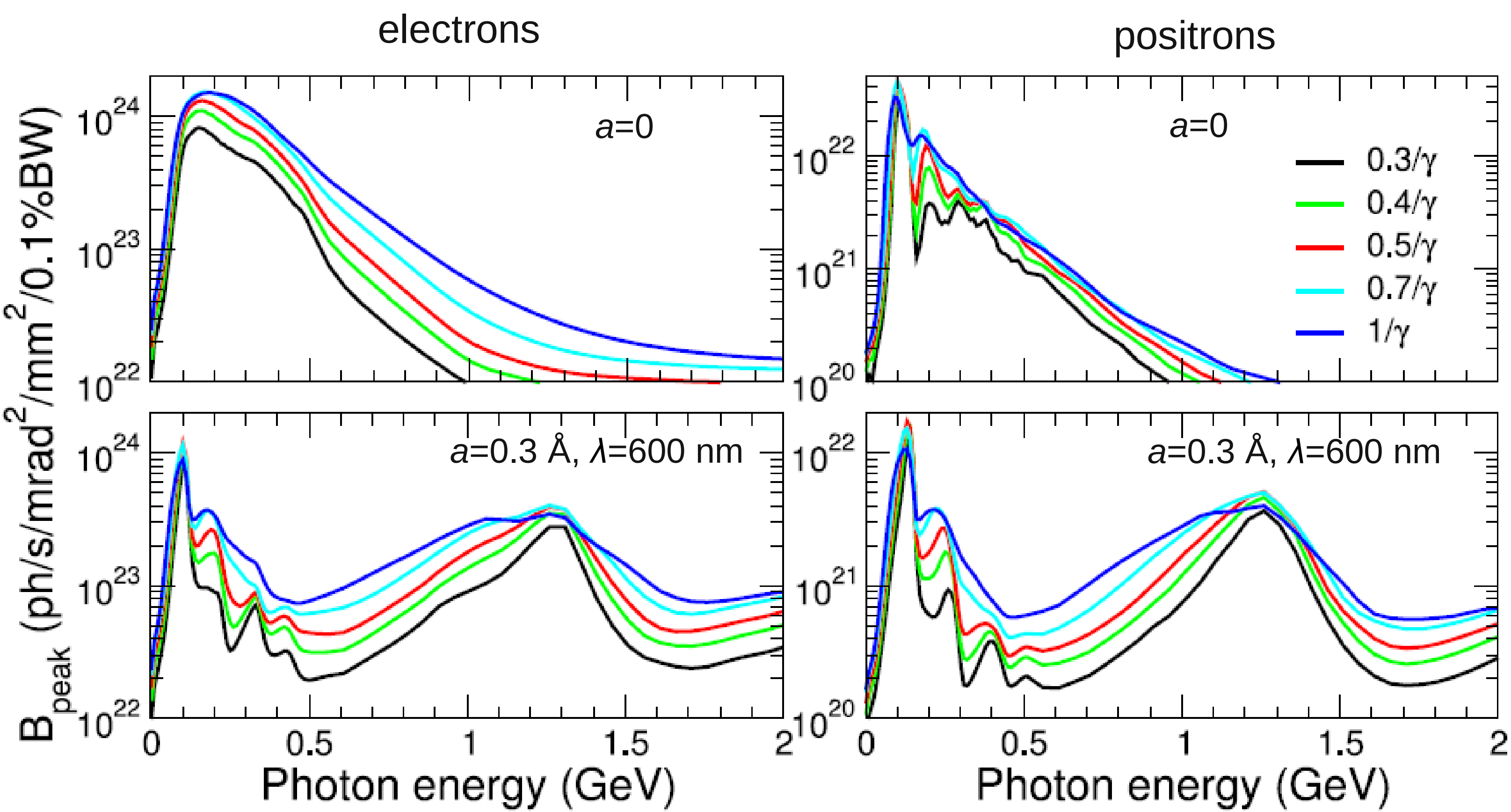


G.B. Sushko, A.V. Korol, A.V. Solov'yov. *Nuclear Instrum. Meth. B* **535** (2023) 117

Peak brilliance, B_{peak}

MBN Research Center

Case study: Diamond(110), a=0.3 Å, λ=600 nm, L=96 µm; **varying θ**

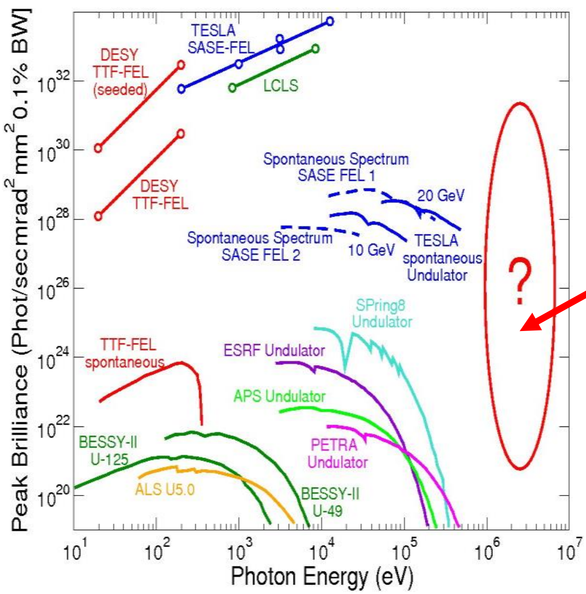


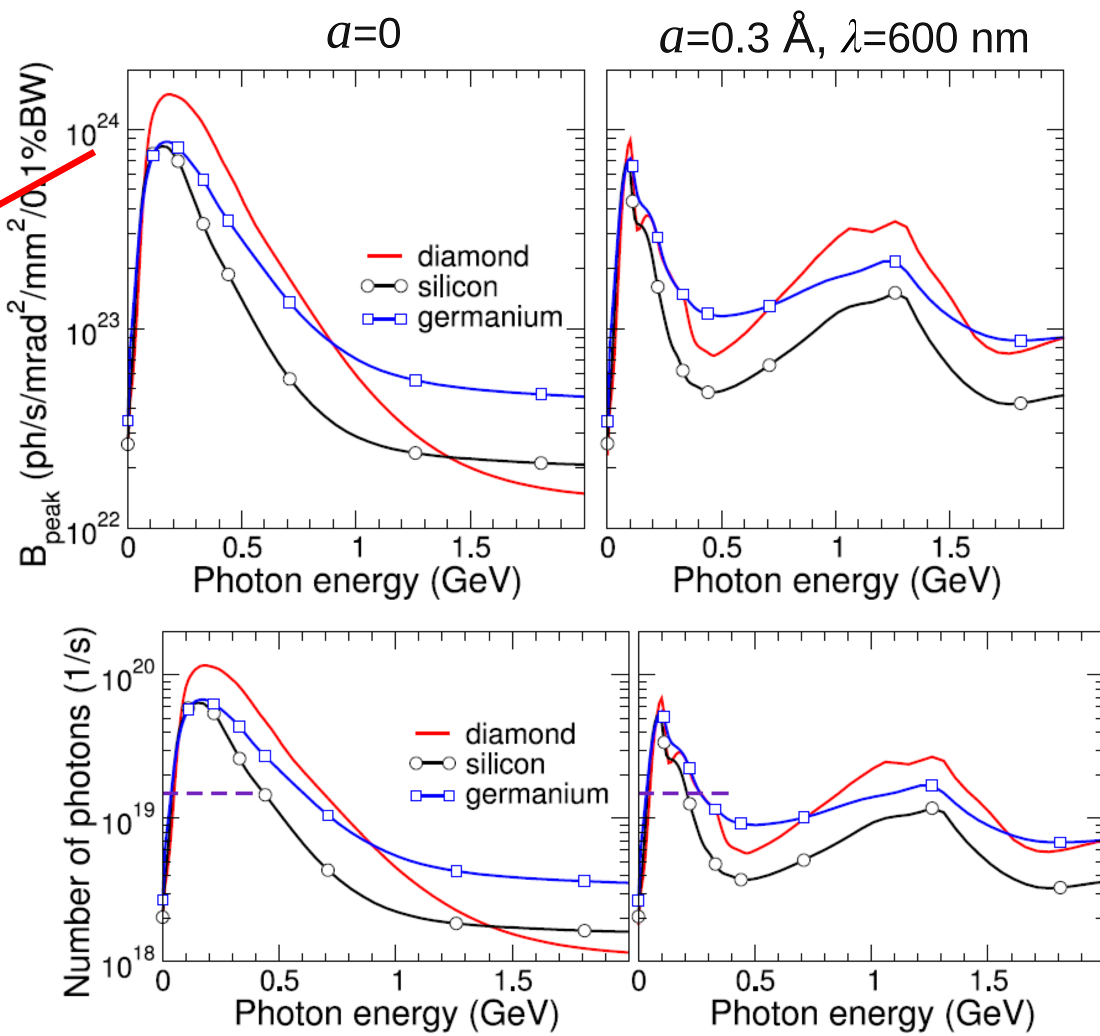
$\gamma^{-1} \approx 50$ µrad

G.B. Sushko, A.V. Korol, A.V. Solov'yov. *Nuclear Instrum. Meth. B* **535** (2023) 117

B_{peak} and number of photons

Case study: electron beam, **varying crystals**





G.B. Sushko, A.V. Korol, A.V. Solov'yov. *Nuclear Instrum. Meth. B* **535** (2023) 117

Channeling and synchrotron-like radiation in bent Si and Ge crystals

Experiment:
(IFNF,UNIFE,
UniMainz)

A. I. Sytov, L. Bandiera, D. De Salvador, et al. *Eur. Phys. J. C* **77** (2017) 901

L. Bandiera, A. Sytov, D. De Salvador, et al. *Eur. Phys. J. C* **81** (2021) 284

Atomistic
modelling:
(MBN-RC)

V. V. Haurylavets, V. K. Ivanov, A. V. Korol, A.V. Solov'yov. arXiv: 2309.09716
(*NIMA submitted,* 2023)

Parameters used in the simulations

MBN Research Center

- **855 MeV electron beam (MAMI)**
- **Crystals:** Si, Ge. **Thickness:** L=15 μm along the beam direction, $\mathbf{v}_0$.
  Quasi-mosaic bending: R=47.6, 27.3, 20.0, 13.9 mm for Si; R=18.3, 12.5, 10.5 mm for Ge
- **Beam–crystal alignments:**
  - *Planar channeling (Ch) alignment* : $\mathbf{v}_0 \uparrow\uparrow$ (11-1) plane, Figure b
  - *Volume reflection (VR) alignment*: $\mathbf{v}_0$ at angle α to (11-1) plane, Figure c

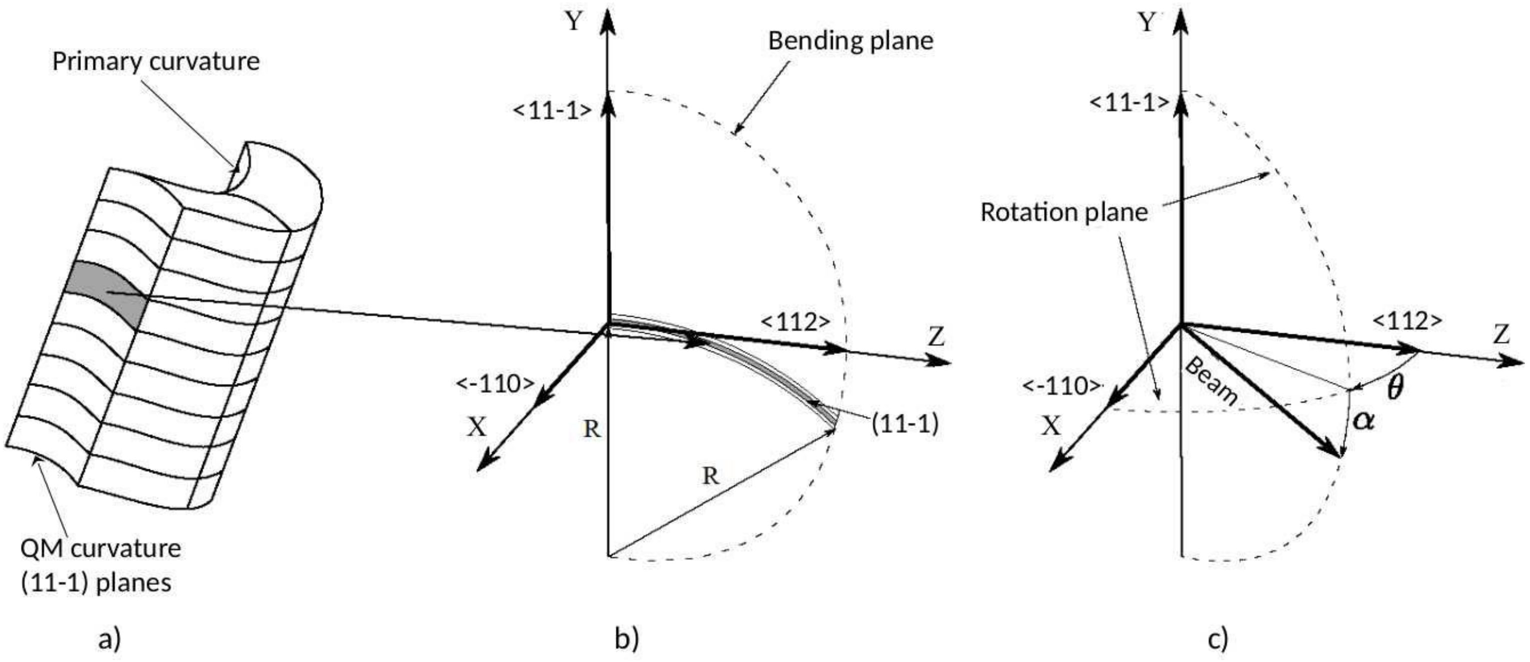
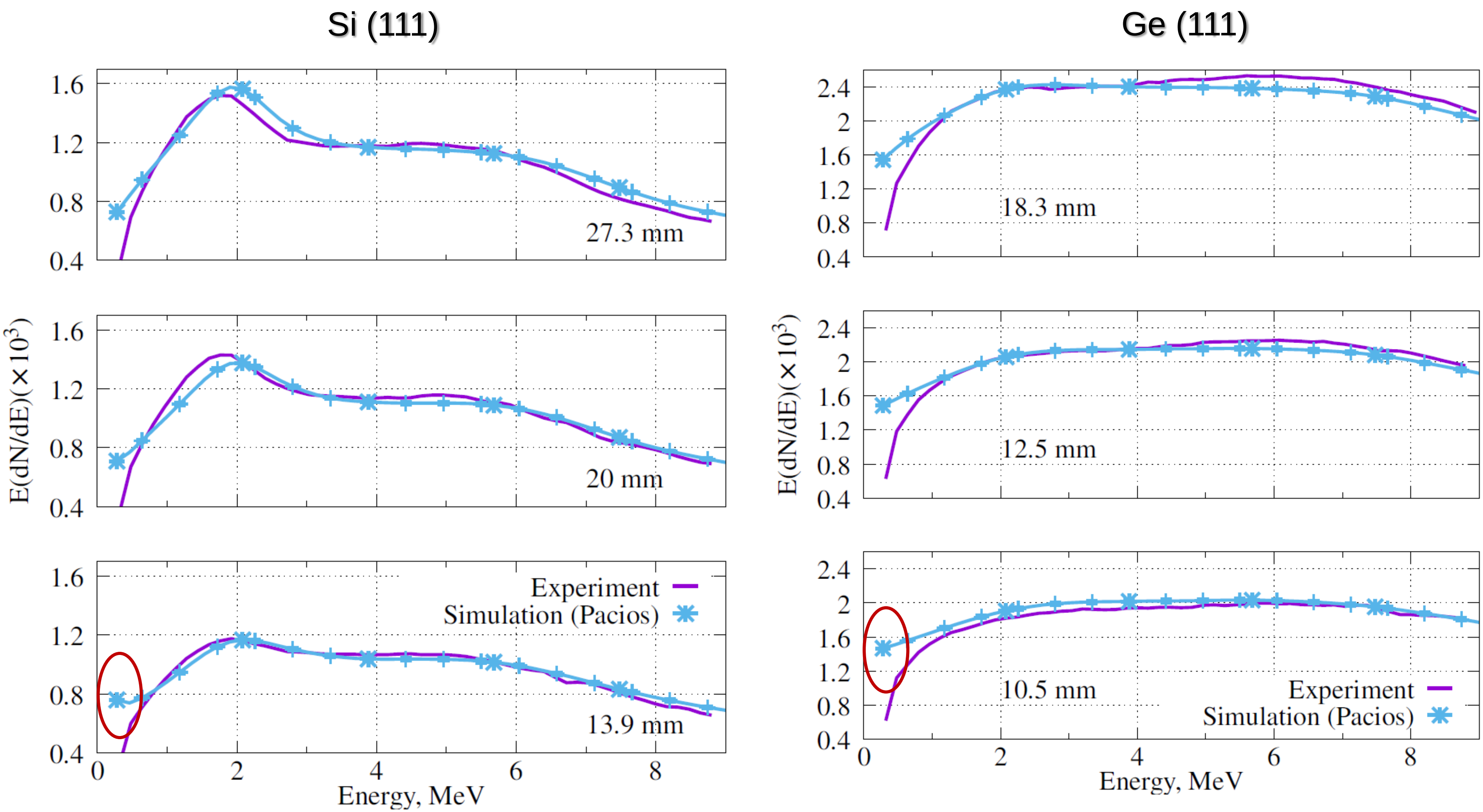


Figure from Haurylavets et al. arXiv: 2309.09716 (*NIMA submitted,* 2023)

Emission spectra: Channeling alignment

MBN Research Center



Experiment: Bandiera et al. *EPJC* **81** (2021) 284

Figures from Haurylavets et al. arXiv: 2309.09716 (*NIMA submitted,* 2023)

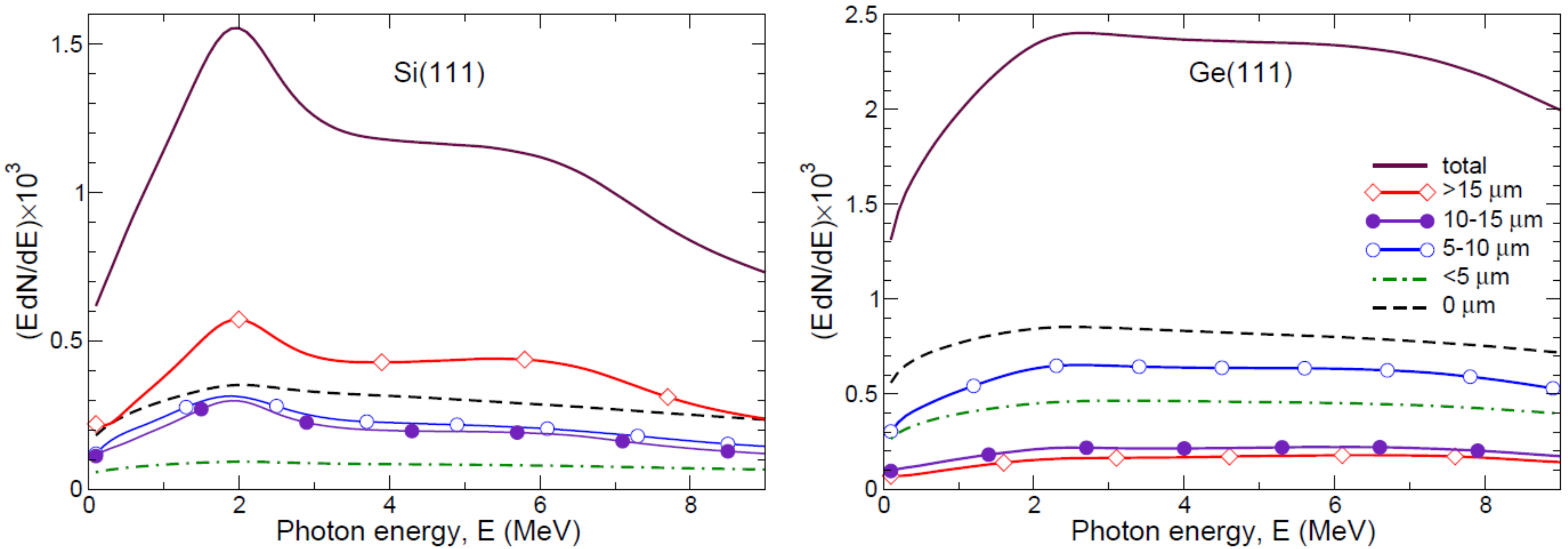
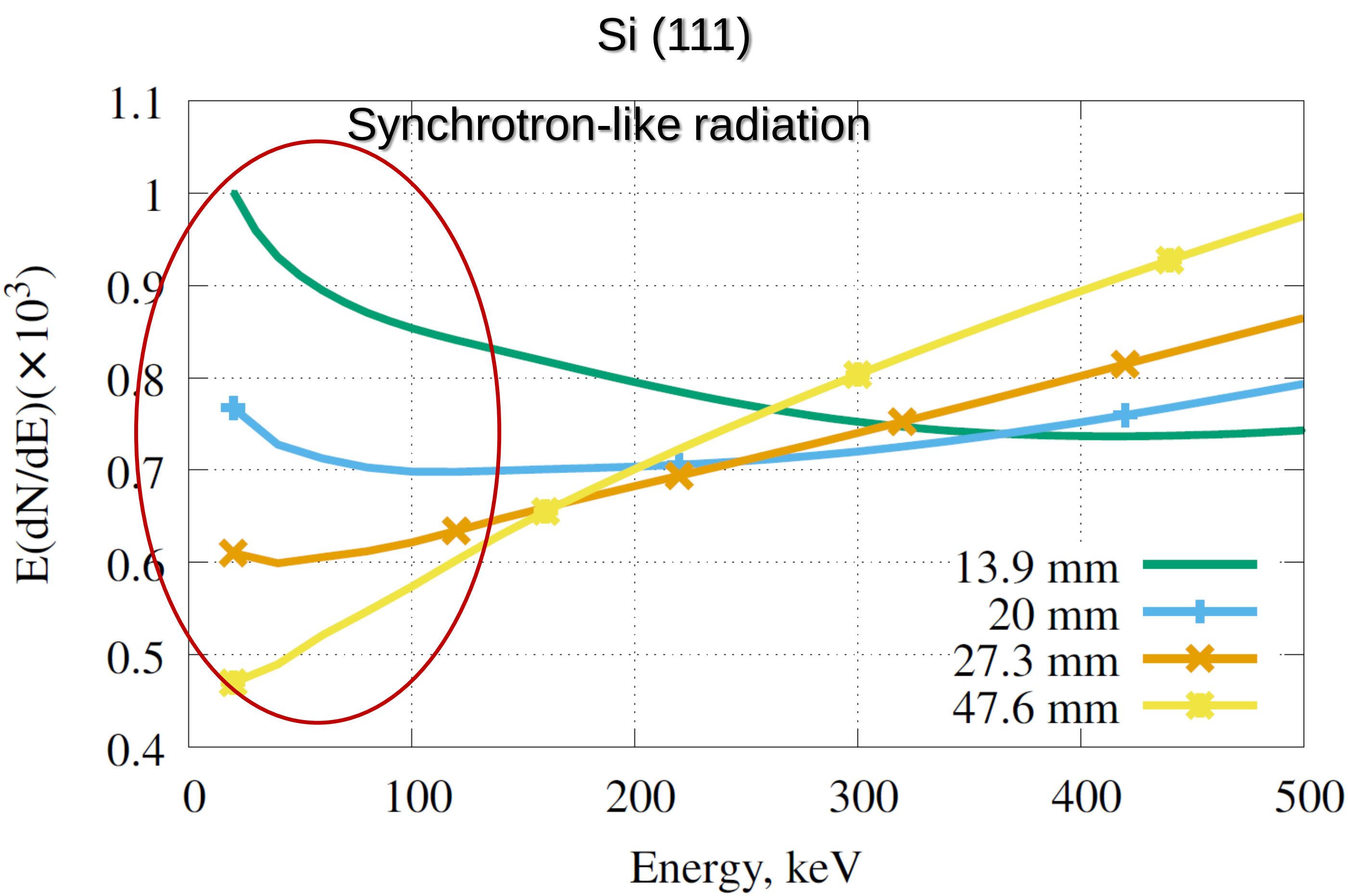


Figure 8. Spectral distribution of radiation in Si ($R = 27.3$ mm, left graph) and Ge (18.3 mm, right graph) bent crystals with explicit contributions from different group of particles as indicated in the common legend in the right graph. See explanations in the text. The incident beam geometry corresponds to the planar channeling alignment.

Figure from Haurylavets et al. arXiv: 2309.09716 (*NIMA submitted,* 2023)

Synchrotron-like radiation



SR cut-off energy: E_c [MeV]=$2.21\varepsilon^3/R$ with ε in GeV, R in mm

Figures from Haurylavets et al. arXiv: 2309.09716 (*NIMA submitted,* 2023)

Radiation emission from diamond hetero-crystals

Crytal manufacture: ESRF

Channeling experiment: UniMainz

Atomistic modeling*: MBN-RC

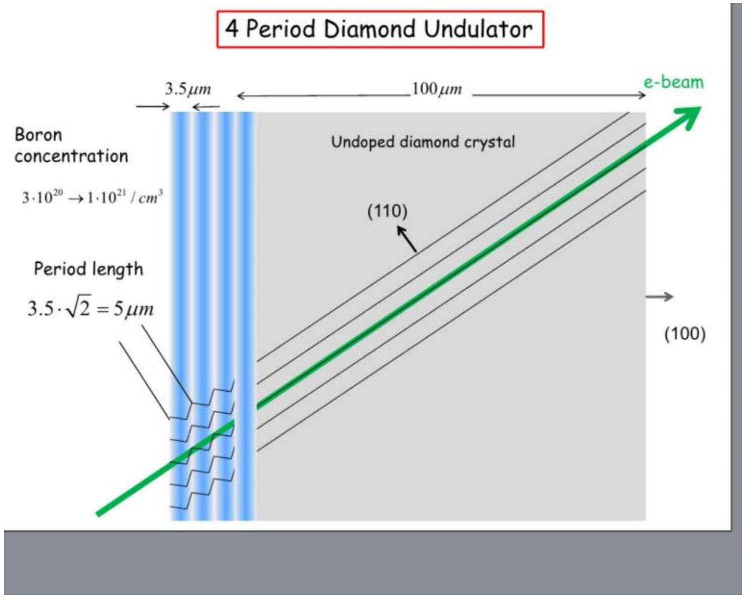
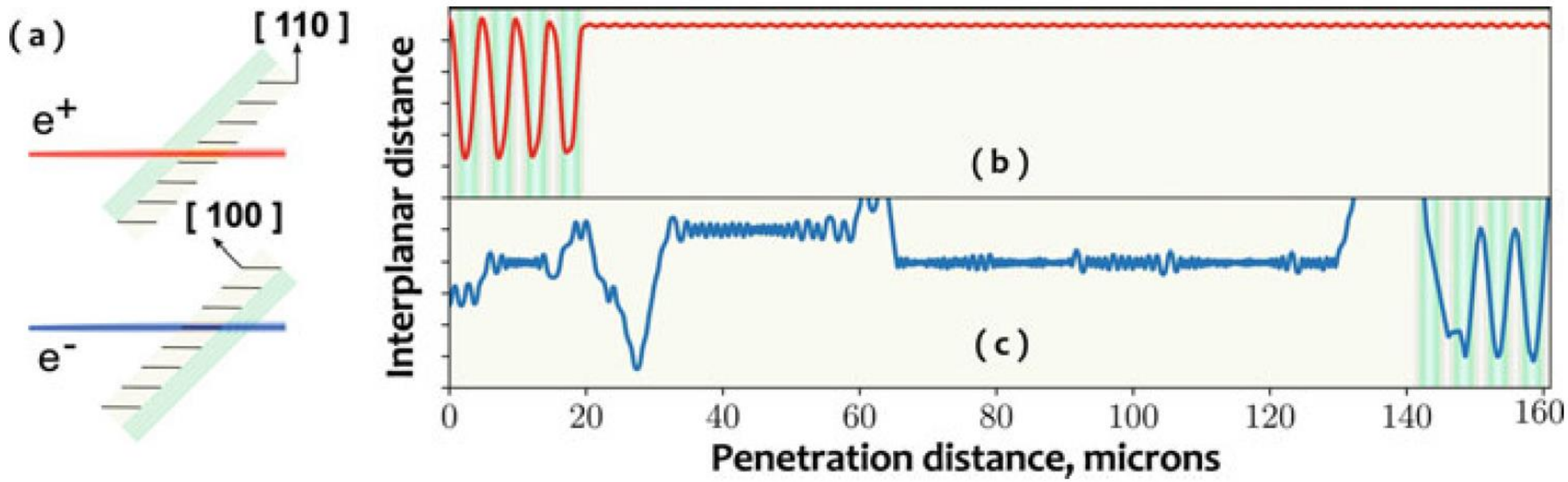


Figure courtesy of W. Lauth and H. Backe (UniMainz)

*A. Pavlov, V. Ivanov, A. Korol, A. Solov'yov. *St. Petersburg Polytech. Uni. J.: Phys. Math*. **14** (2021) 190

Diamond-boron hetero-crystal

MBN Research Center



The hetero-crystal consists of two segments:

(1) a straight (S) L_S = 141 microns thick single crystal substrate,

(2) a boron-doped L_{PB} = 20 microns thick periodically bent (PB) segment with 4 periods.

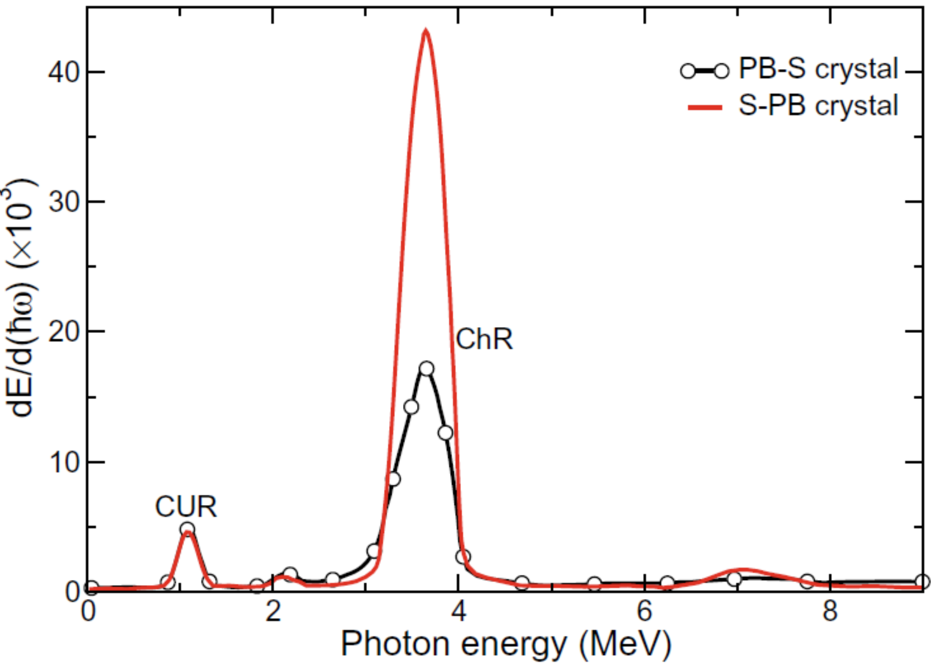
Panel **(b)** shows the PB-S orientation: the beam enters the PB segment,
Panel (**c**) shows the S-PB orientation: the beam enters the S segment.

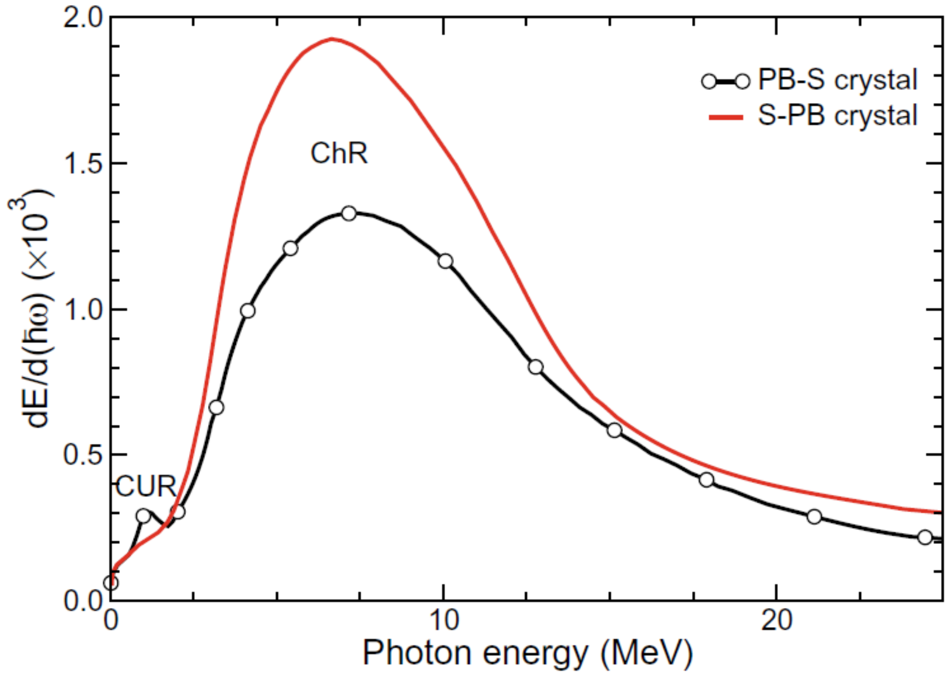
Figure from A.V. Korol, A.V. Solov'yov, *Novel Light Sources beyond FELs*, Springer (2022).

A. Pavlov, V. Ivanov, A. Korol, A. Solov'yov. *St. Petersburg Polytech. Uni. J.: Phys. Math*. **14** (2021) 190

Diamond-boron heterocrystal

MBN Research Center





Spectra of radiation emitted within the cone 0.24 mrad by 855 MeV positrons (left) and electrons (right) in propagating in the oriented PB-S and S-PB hetero-crystals.
The intensity of the background incoherent bremsstrahlung is 2.5 × 10−5 (not indicated in the figure)

Figure from A.V. Korol, A.V. Solov'yov, *Novel Light Sources beyond FELs*, Springer (2022).

A. Pavlov, V. Ivanov, A. Korol, A. Solov'yov. *St. Petersburg Polytech. Uni. J.: Phys. Math*. **14** (2021) 190

Atomistic modeling of the channeling process with radiation reaction force included*

TECHNO-CLS focuses on electron/positron beam energies $\varepsilon \leq 20$ GeV.

At higher beam energies the phenomenon of radiation damping must be accounted for.

Recent experiments with 50 and 150 GeV electrons and positrons:

T. N. Wistisen, A. Di Piazza, H.V. Knudsen, U.I. Uggerhøj, *Nature Commun.* **9** (2018) 1

C.F. Nielsen, J.B. Justesen, A.H. Sørensen, U.I. Uggerhøj, R. Holtzappe, *Phys. Rev. D* **102** (2020) 052004

*G. B. Sushko, A. V. Korol, A.V. Solov'yov. *Nucl. Instrum. Meth. B* **535** (2023) 117–125

Radiation damping

A charged particle moving in a medium/external field *loses energy due to the radiation emission*. This gives rise to *a radiative reaction force acting on a projectile* and leading to *a gradual decrease of the particle's energy*.
For high-energy projectiles (*tens of GeV and above*) this force must be accounted for.

Implemented in MBN Explorer 5.0:

$$\begin{cases} \dot{\mathbf{v}} = \dfrac{1}{m\gamma}\Big(\mathbf{F} - \boldsymbol{\beta}\,(\mathbf{F}\cdot\boldsymbol{\beta})\Big) \\ \dot{\mathbf{r}} = \mathbf{v} \end{cases} \qquad \mathbf{F} = \mathbf{F}_{\rm em} + \mathbf{F}_{\rm rr}$$

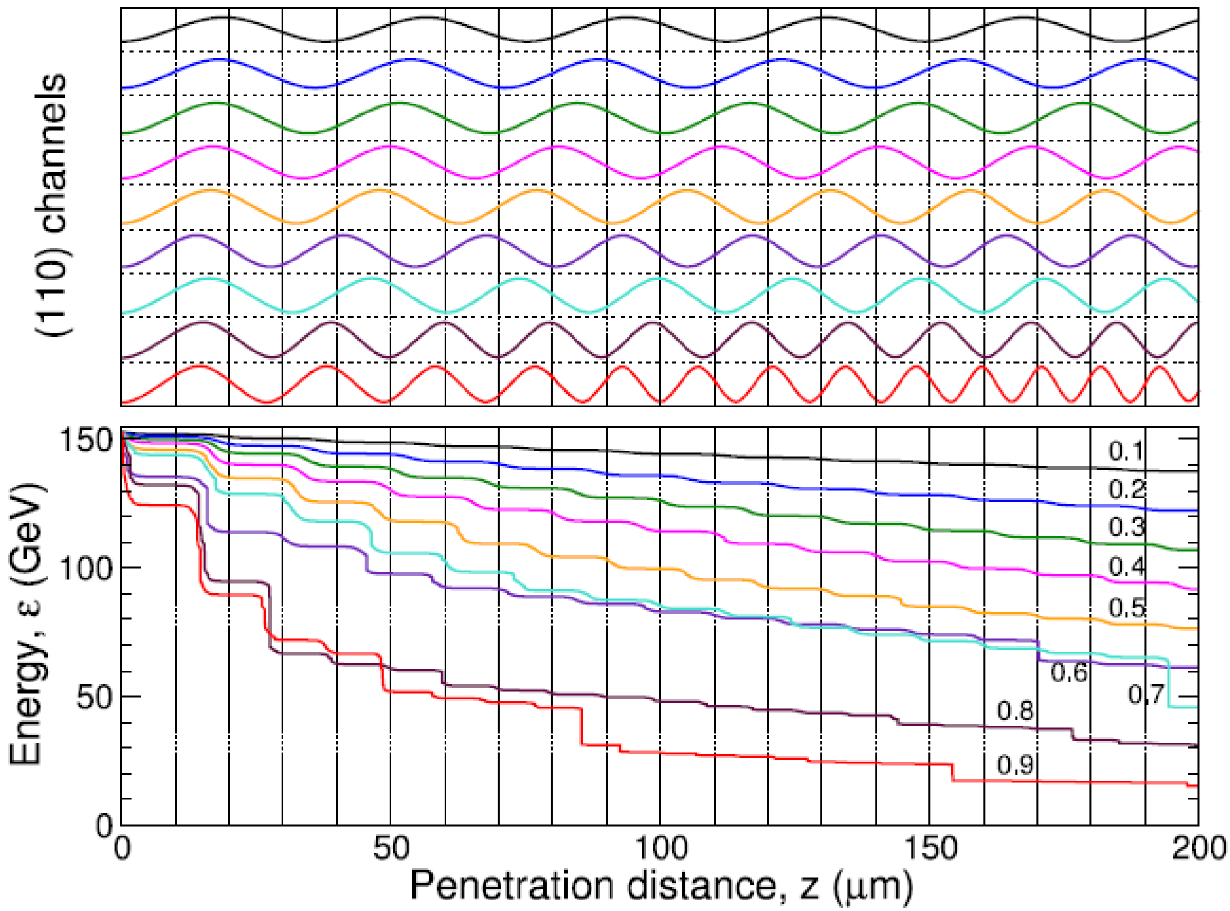
$$\mathbf{F}_{\rm em} = q\,(\mathbf{E} + \boldsymbol{\beta}\times\mathbf{B})$$

$$\mathbf{F}_{\rm rr} = \frac{2q^2}{3\,mc^3}\left\{ q\gamma\left[\frac{\partial\mathbf{E}}{\partial t} + (\mathbf{v}\cdot\boldsymbol{\nabla})\,\mathbf{E} + \boldsymbol{\beta}\times\left(\frac{\partial\mathbf{B}}{\partial t} + (\mathbf{v}\cdot\boldsymbol{\nabla})\,\mathbf{B}\right)\right] + \frac{q}{mc}\Big[\mathbf{F}\times\mathbf{B} + q\,(\boldsymbol{\beta}\cdot\mathbf{E})\,\mathbf{E}\Big] - \frac{\gamma^2}{mc}\Big[\mathbf{F}^2 - q^2\,(\boldsymbol{\beta}\cdot\mathbf{E})^2\Big]\boldsymbol{\beta} \right\}$$

In application to the channeling and photon emission processes, the simulations have been performed for 150 GeV positrons in a 200 μm thick Si(110) crystal*. Several regimes for the decrease in ε have been established and characterized.

*G. B. Sushko, A. V. Korol, A.V. Solov'yov. *Nucl. Instrum. Meth. B* **535** (2023) 117–125

Analysis of the trajectories

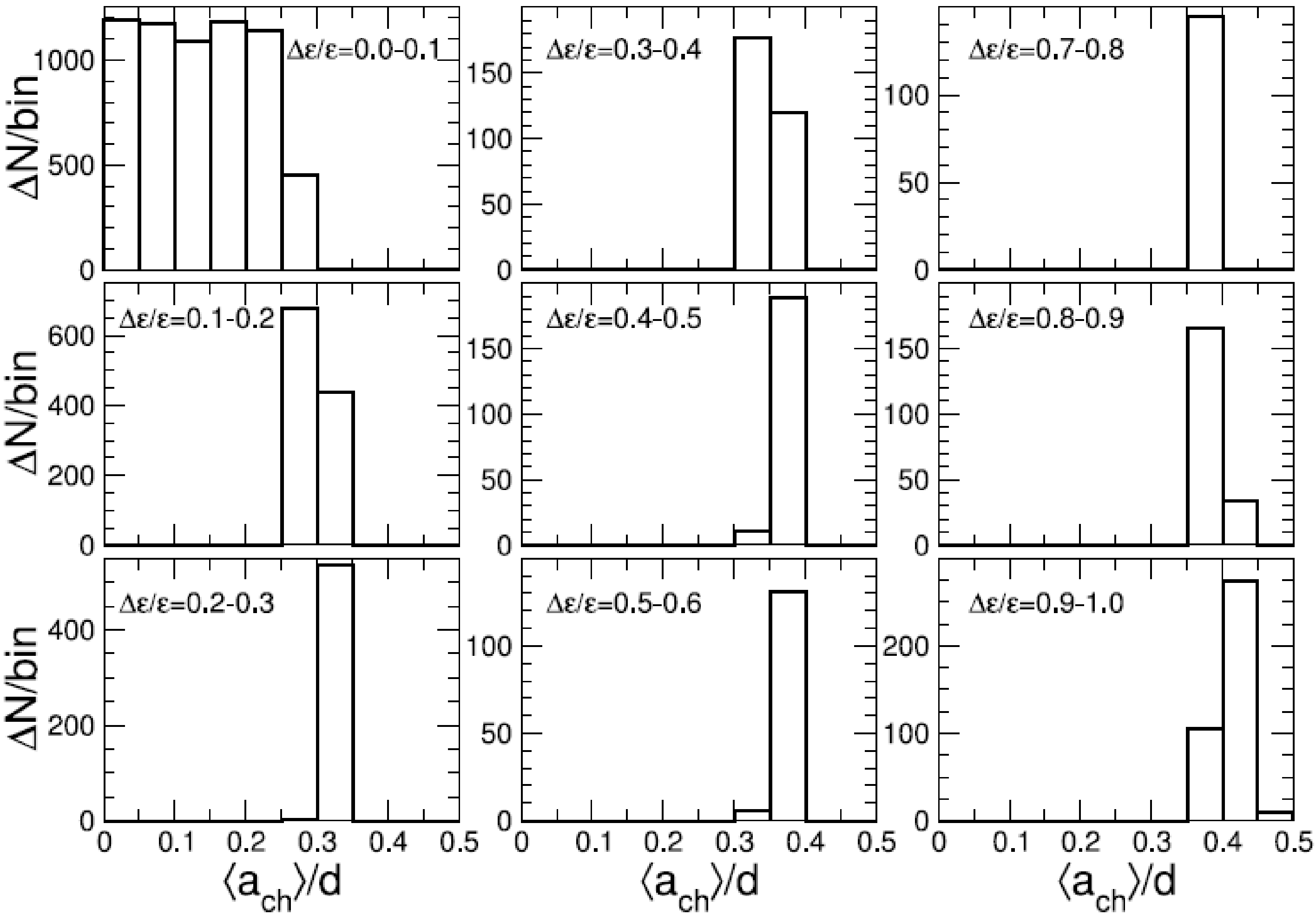


Top: Selected simulated trajectories of 150 GeV positrons in a Si(110) crystal. The trajectories correspond to different values of the relative energy loss: $\Delta\varepsilon/\varepsilon = 0.1$ for the top trajectory up to 0.9 for the lowest trajectory.

Bottom: Dependencies of the projectile energy on the penetration distance for the trajectories from the top graph. The value of $\Delta\varepsilon/\varepsilon$ is indicated for each dependence.

G. B. Sushko, A. V. Korol, A.V. Solov'yov. *Nucl. Instrum. Meth. B* **535** (2023) 117–125

Statistical analysis

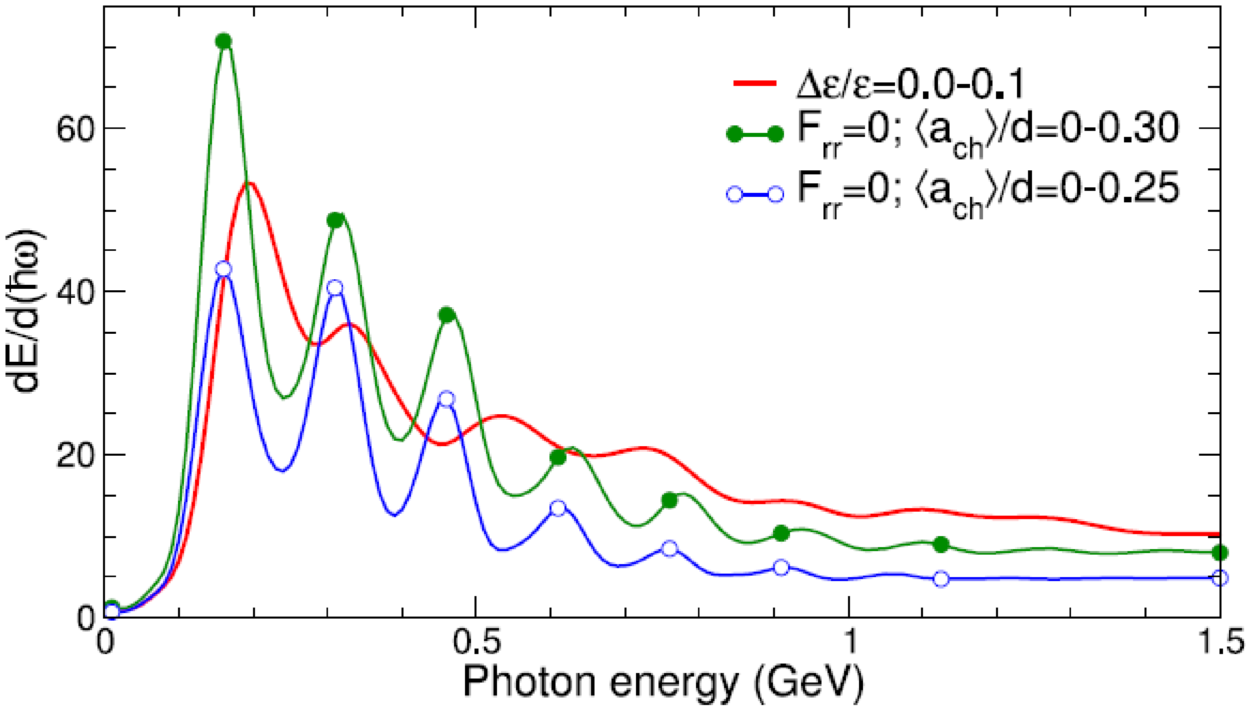


Distribution of projectiles with respect to the average amplitude of channeling oscillations, $\langle a_{ch} \rangle$, along the trajectory. Nine graphs correspond to different intervals of Δε/ε as indicated.

G. B. Sushko, A. V. Korol, A.V. Solov'yov. *Nucl. Instrum. Meth. B* **535** (2023) 117–125

Impact on the emission spectra

Emission spectra by 150 GeV positrons with account for radiation damping



Spectral distribution of radiation emitted by 150 GeV positrons in 200 μm thick Si(110) crystal. Solid (red) curve without symbols presents the dependence calculated for the trajectories that correspond to the interval $\Delta\varepsilon/\varepsilon = 0 - 0.1$ of the relative energy losses due to the radiative reaction force F_{rr}. Solid curves with symbols show the spectra calculated for the trajectories without account for F_{rr} and selected with respect to the ranges for the average amplitude of channeling oscillations, $\langle a_{ch} \rangle$, as indicated in the legend.

G. B. Sushko, A. V. Korol, A.V. Solov'yov. *Nucl. Instrum. Meth. B* **535** (2023) 117–125

Ongoing and future work

MBN Explorer software package allows for:

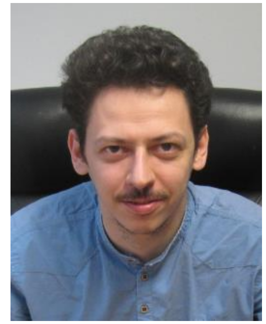
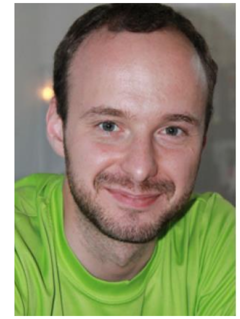
- Atomistic modelling of crystal structure changes due to
  - (i) inserting dopant atoms (ESRF),
  - (ii) surface patterning (INFN),
  - (iii) pulse laser melting (UNIPD)
  - (iv) acoustic excitations (HMU)
- Atomistic modelling of imperfect crystal structures (together with UoK)
- Passage of particles through crystalline structures and characterization of the emitted radiation (together with UoK)
- Characterization of all CLS planned to be probed within the Project.

Acknowledgements to the team

MBN Research Center

Members and visitors:

- Andrei Korol
- Ilia Solov'yov
- Irina Solovyeva
- Gennady Sushko
- Alexey Verkhovtsev
- Alexey Prosvetov
- Matthew Dickers
- Klaudia Cielinska





Former members & visitors: Viktor Beschastnov, Pablo de Vera, Yury Erofeev, Yannick Fortouna, Viktar Haurylavets, Vadim Ivanov, Sergey Kazenyuk, Christian Kexel, Andrey Lyalin, Pavel Nikolaev, Oleg Obolensky, Mikhail Panshenskov, Roman Polozkov, Alexander Pavlov, Veronika Dick/Semenikhina, Eugene Surdutovich, Ilya Volkovetz, Alexander Yakubovich

Current EU projects Consortia: H2020 RISE-RADON, H2020 RISE-N-LIGHT, COST Action MultIChem, EIC Pathfinder Project TECHNO-CLS

Thank you for your attention!