



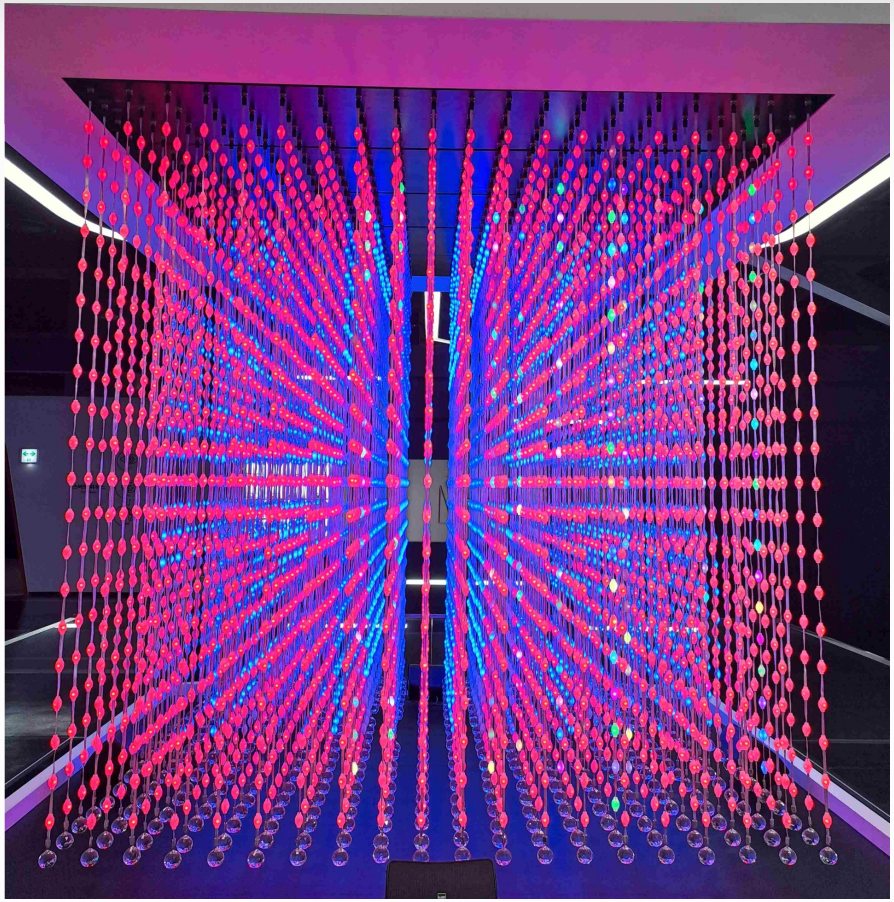



# Modelling of channeling in crystals and nanostructures

**A. Sytov**
**sytov@fe.infn.it**

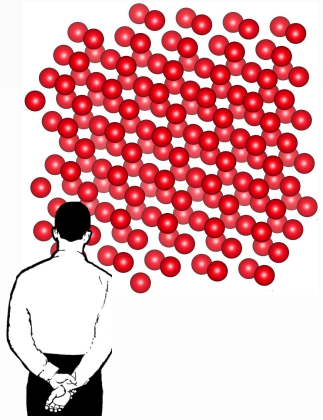
**NanoAc 2024, Valencia, 18/09/24**

# How an oriented crystal looks like

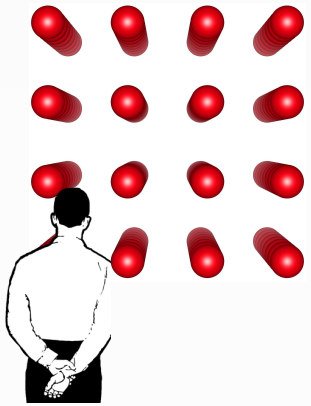


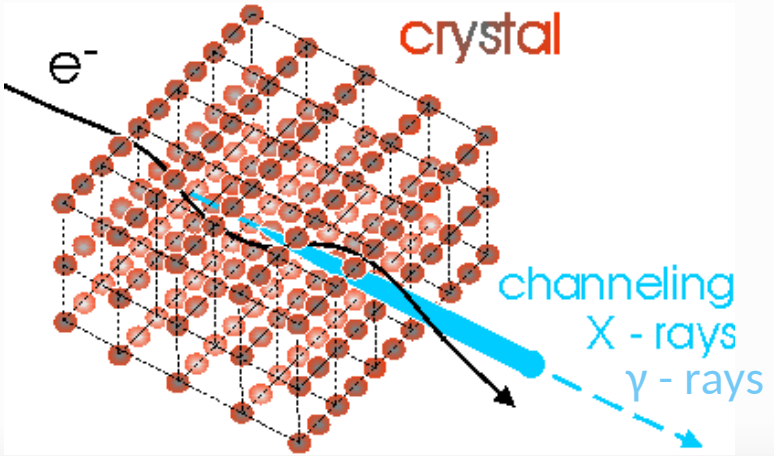
**from National Science Museum, Daejeon, Korea**

**Non-oriented crystal**



**Oriented crystal**





# Marie Sklodowska-Curie Action Global Individual Fellowships by A. Sytov in 2021-2025, Project TRILLION GA n. 101032975

**Main goal:** The **implementation** of both physics of **electromagnetic processes in oriented crystals** and the design of specific applications of crystalline effects into **Geant4** simulation toolkit as Extended Examples to bring them to a large scientific and industrial community and under a free Geant4 license.

**Group:**

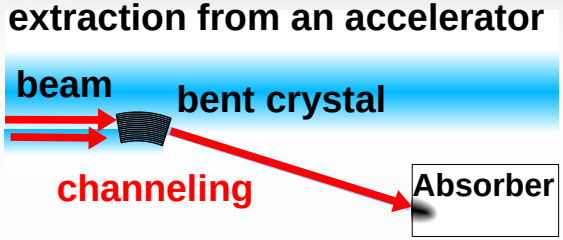
- **A. Sytov** – project coordinator
- **L. Bandiera** – INFN supervisor
- **K. Cho** – KISTI supervisor
- **G. Kube** – DESY supervisor
- **I. Chaikovska** – IJCLab Orsay supervisor

**Location:**

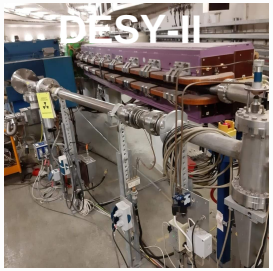
- 2 years at **KISTI** (partner organization)
- 1 year at **INFN Section of Ferrara** (host organization)
- 1 month of secondment at **DESY** (partner organization)
- 1 month of secondment at **IJCLab Orsay** (partner organization)

# Applications*

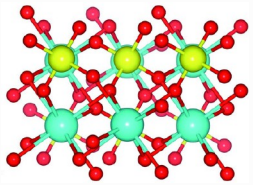
**Crystal-based collimation or beam extraction from an accelerator**





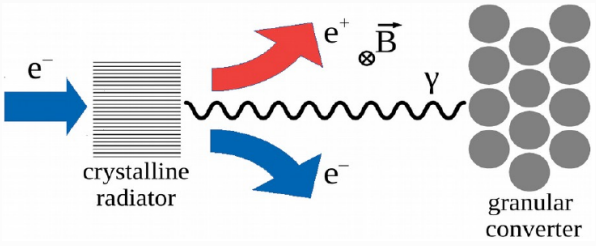


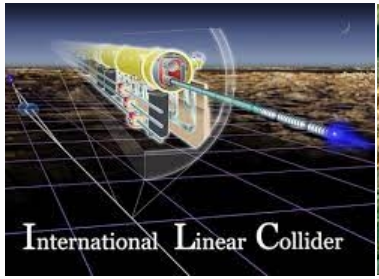

**Ultrashort crystalline calorimeter**



**Gamma-ray Space Telescope**

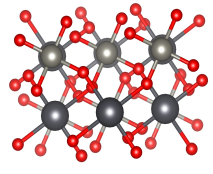
**Positron source for future e+/e- and muon colliders**



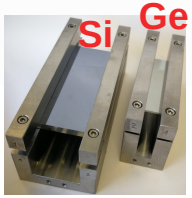





**Oriented crystals**



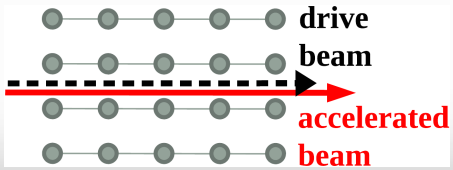
**Measurement of dipole magnetic and electric moments of exotic particles**



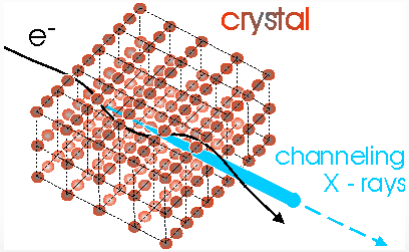


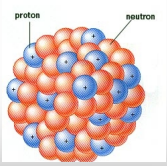


**Plasma acceleration**




**X and γ-ray source for nuclear and medical physics**

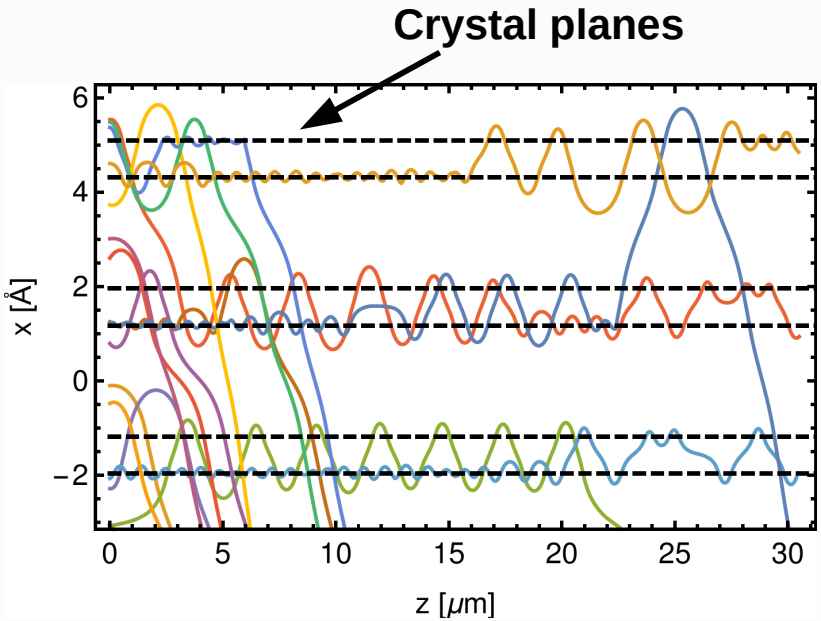



*A. Sytov et al. arXiv: 2303.04385, Accepted for publication in JKPS

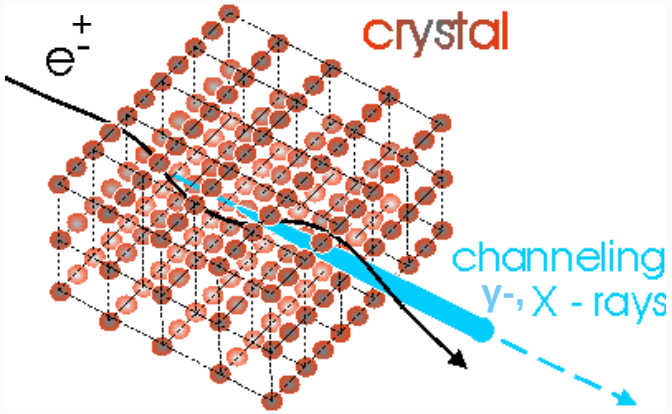
# Baseline channeling simulation technique: CRYSTALRAD Monte Carlo simulation code

**Main conception** – simulation of classical trajectories of charged particles in a crystal in averaged atomic potential of planes or axes. Multiple and single **scattering simulation** at every step




**channeling***

**New 2024: ionization losses in channeling**




**Baier-Katkov formula:**

integration is made over the classical trajectory

$$\frac{dE}{d^3k} = \omega \frac{dN}{d^3k} \frac{\alpha}{4\pi^2} \iint dt_1 dt_2 \frac{\left[(E^2+E'^2)(v_1 v_2 - 1) + \omega^2/\gamma^2\right]}{2E'^2} e^{-ik'(x_1 - x_2)}$$


A.I. Sytov, V.V. Tikhomirov. NIM B 355 (2015) 383–386.

L. Bandiera, et al., Nucl. Instrum. Methods Phys. Res., Sect. B 355, 44 (2015)

*A. Sytov et al. Journal of the Korean Physical Society 83, 132–139 (2023)

A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. PRAB 22, 064601 (2019)

# Main concept of full ab-inition G4BaierKatkov

$$\frac{dE}{d^3k} = \omega \frac{dN}{d^3k} \frac{\alpha}{4\pi^2} \iint dt_1 dt_2 \frac{[(E^2+E'^2)(v_1v_2-1)+\omega^2/\gamma^2]}{2E'^2} e^{-ik'(x_1-x_2)}$$

Monte Carlo integration by photon **3 components of momentum**

$\vec{k}$

**Radiation probability** calculated **per photon**

Monte Carlo integration by photon **energy** and **angles**

$\omega$, $\theta x$, $\theta y$

$$\vec{k}_i \Rightarrow P_i$$

If radiation happens, **select a photon** from using ***Pi*** as their **weight** and generate it

Photon **energy** and **angular distribution** naturally comes **from Baier-Katkov**

# How to implement an external code into Geant4? Geant4 FastSim interface, solution to most of challenges

**FastSim model:**

- **Physics list independent**
- Declared in the **DetectorConstruction** (just **few lines of code**)
- Is activated **only** in a **certain G4Region** at a **certain condition** and only for **certain particles**
- **Stops Geant processes** at the step of FastSim model and then resumes them

```
71  G4bool TestModel::IsApplicable(const G4ParticleDefinition& particleType)
72  {
73    return
74      &particleType == G4Proton::ProtonDefinition()||
75      &particleType == G4AntiProton::AntiProtonDefinition()||
76      &particleType == G4Electron::ElectronDefinition() ||
77      &particleType == G4Positron::PositronDefinition();// ||
78      //&particleType == G4Gamma::GammaDefinition();
79  }
80
81  //....oooOOOOOooo........oooOOOOOooo........oooOOOOOooo........oooOOOOOooo......
82
83  G4bool TestModel::ModelTrigger(const G4FastTrack& fastTrack)
84  {
102 }
103
104 //....oooOOOOOooo........oooOOOOOooo........oooOOOOOooo........oooOOOOOooo......
105
106 void TestModel::DoIt(const G4FastTrack& fastTrack,
107                      G4FastStep& fastStep)
108 {
```

Insert particles for which the model is applicable

Insert the condition to enter the model

Insert what the model does

# How to use the Geant4 channeling model in your example?

- **Add to DetectorConstruction::Construct()**

```
//crystal volume
G4Box* crystalSolid = new G4Box("Crystal",CrystalSizeX/2,CrystalSizeY/2,CrystalSizeZ/2.);
crystalLogic = new G4LogicalVolume(crystalSolid,crystalMaterial,"Crystal");
            new G4PVPlacement(xRot,posCrystal,crystalLogic,"Crystal",logicWorld,false,0);
//crystal region (necessary for the FastSim model)
fRegion = new G4Region("Crystal");
fRegion->AddRootLogicalVolume(crystalLogic);
```

Volume declaration (completely standard)

G4Region declaration

- **Add to DetectorConstruction::ConstructSDandField()**

```
void DetectorConstruction::ConstructSDandField()
{
    // --------------- fast simulation ---------------------------
    //extract the region of the crystal from the store
    G4RegionStore* regionStore = G4RegionStore::GetInstance();
    G4Region* RegionCh = regionStore->GetRegion("Crystal");

    //create the channeling model for this region
    G4ChannelingFastSimModel* ChannelingModel =
        new G4ChannelingFastSimModel("ChannelingModel", RegionCh);
    //activate the channeling model
    ChannelingModel->Input(crystalMaterial, Lattice);
    //setting bending angle of the crystal planes (default is 0)
    ChannelingModel->GetCrystalData()->
            SetBendingAngle(BendingAngle,crystalLogic);

    //activate radiation model
    if (ActivateRadiationModel) ChannelingModel->RadiationModelActivate();
}
```

Get crystal region

Channeling FastSim model declaration

Model activation and input

Optional

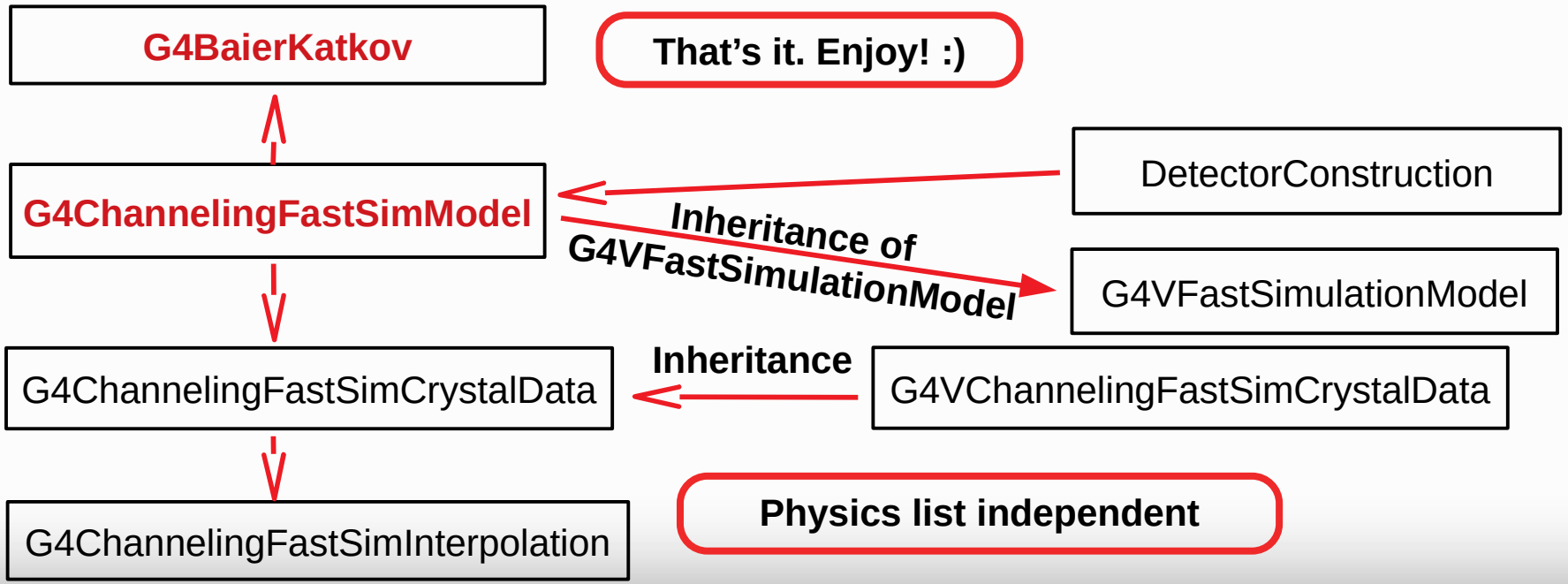
Radiation model activation

# How to use the Geant4 channeling model in your example?

- **Add to main:**

**Register FastSimulationPhysics**

```
G4FastSimulationPhysics* fastSimulationPhysics = new G4FastSimulationPhysics();
fastSimulationPhysics->BeVerbose();
// -- activation of fast simulation for particles having fast simulation models
// -- attached in the mass geometry:
fastSimulationPhysics->ActivateFastSimulation("e-");
fastSimulationPhysics->ActivateFastSimulation("e+");
// -- Attach the fast simulation physics constructor to the physics list:
physicsList->RegisterPhysics( fastSimulationPhysics );
```



# Current status

**In Geant4 since geant4-11.2.0 !**

**geant4-v11.2.0/source/parameterisations/channeling/**

**Please use it!**

**https://geant4.web.cern.ch/download**

**Don't hesitate to contact me in the case of any problems/issues/suggestions**

**sytov@fe.infn.it**

**Geant4 Physics Reference Manual:**

**https://geant4-userdoc.web.cern.ch/UsersGuides/PhysicsReferenceManual/html/solidstate/channeling/channeling_fastsim.html**

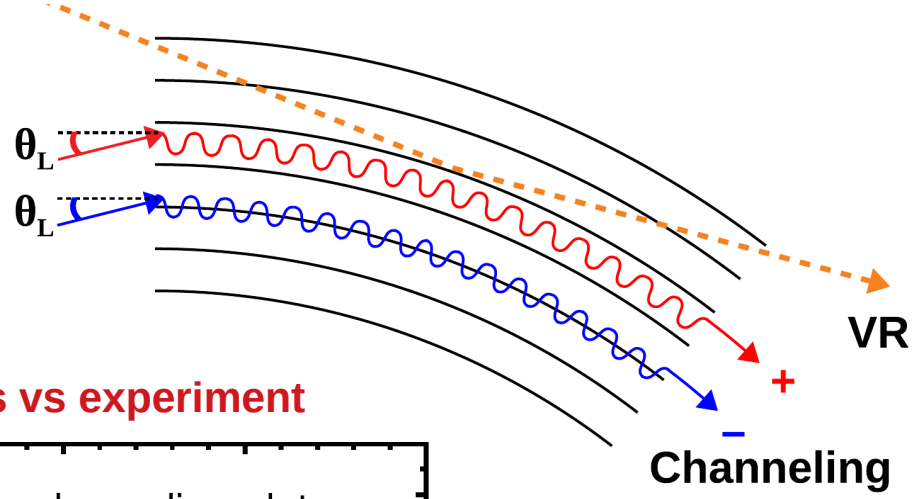
**Please cite our papers if you use our model:**

1. A. Sytov et al. Journal of the Korean Physical Society 83, 132–139 (2023)
2. A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. PRAB 22, 064601 (2019)

# Geant4 channeling model validation: beam deflection by a bent crystal

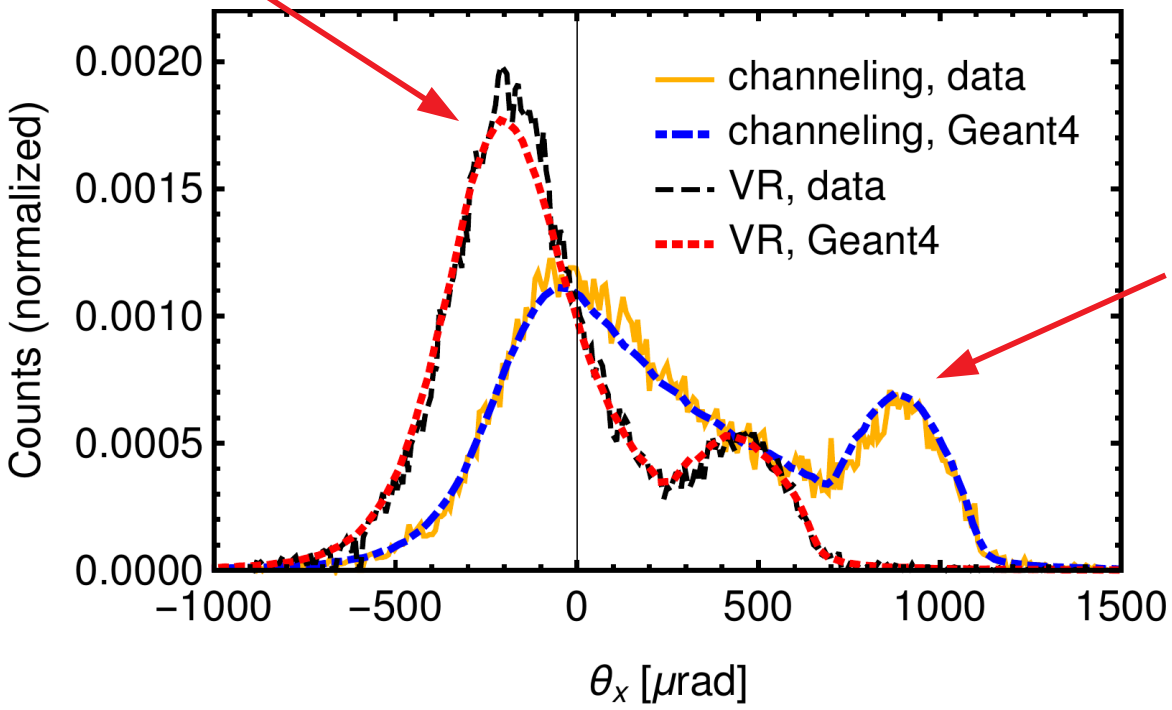
**855 MeV electrons**

**15 µm thick bent crystal**




**volume reflection (VR)**

**Geant simulations vs experiment**

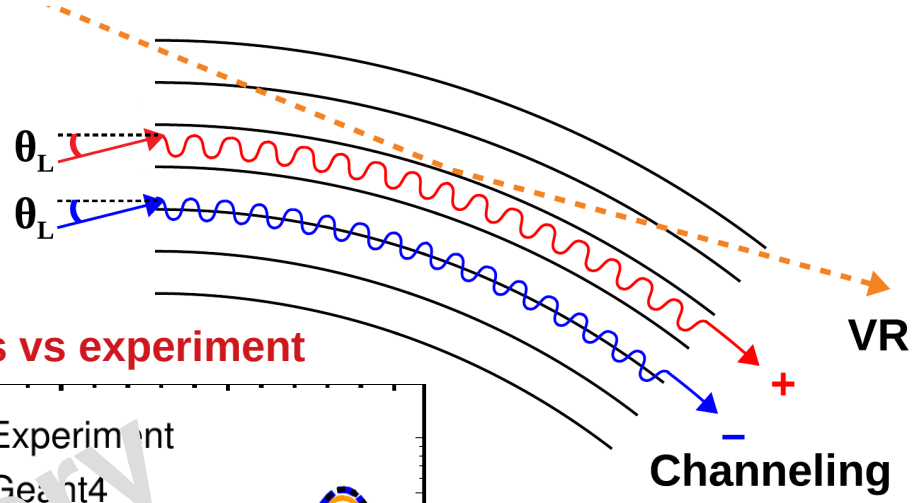



**channeling**

# More Geant4 channeling model validation: quasichanneling oscillations* at SLAC FACET Facility

**20.35 GeV positrons**

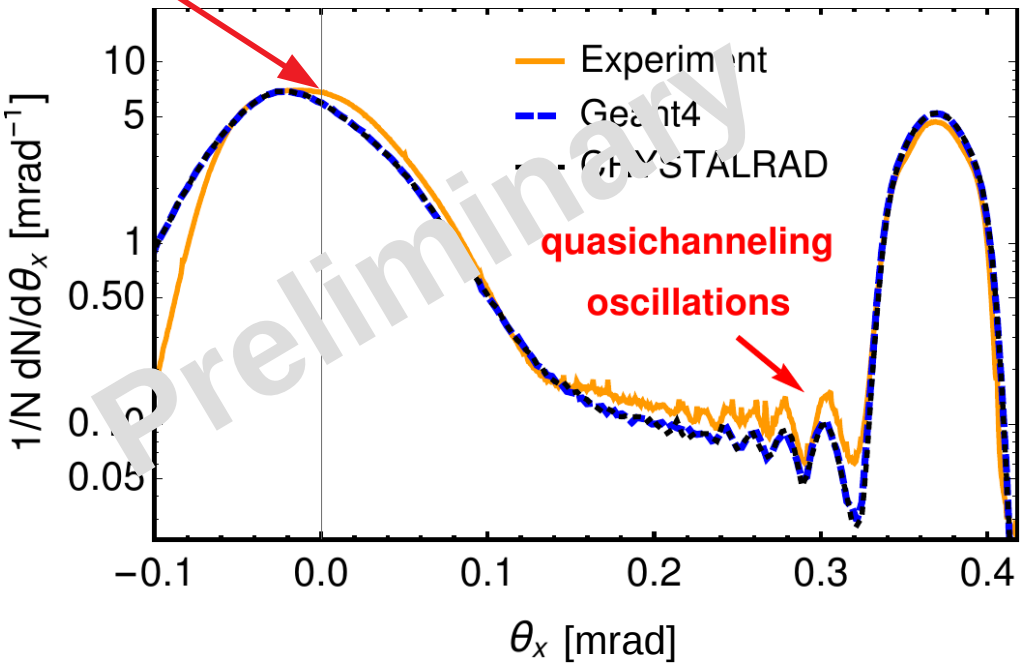
**60 μm thick bent crystal**




**volume reflection (VR)**

**channeling**

**Geant simulations vs experiment**




**To be submitted for publication soon**

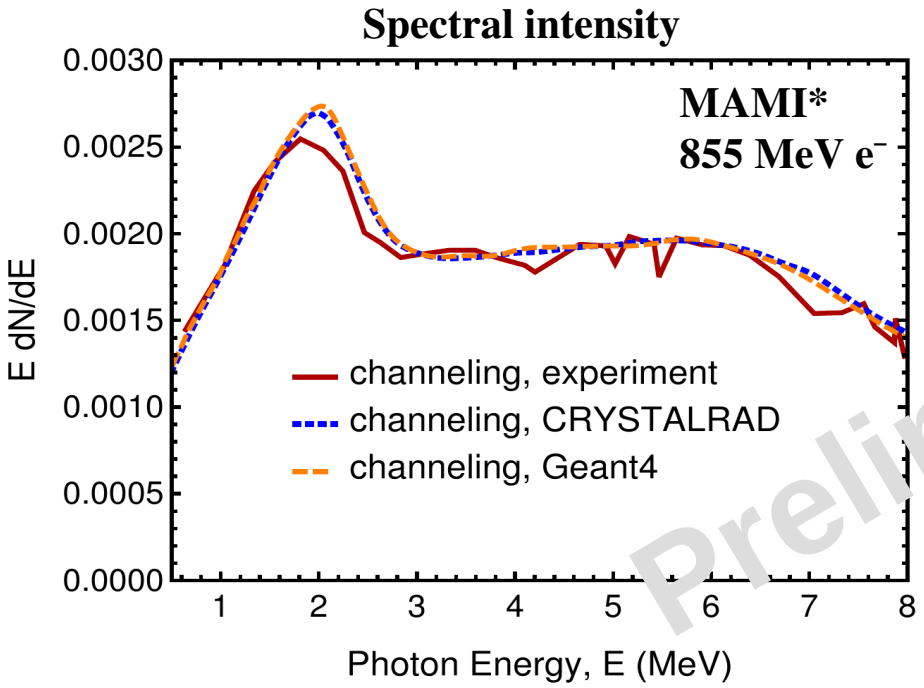
*T. N. Wistisen, …, and A. Sytov, Phys. Rev. Lett. 119, 024801 (2017)

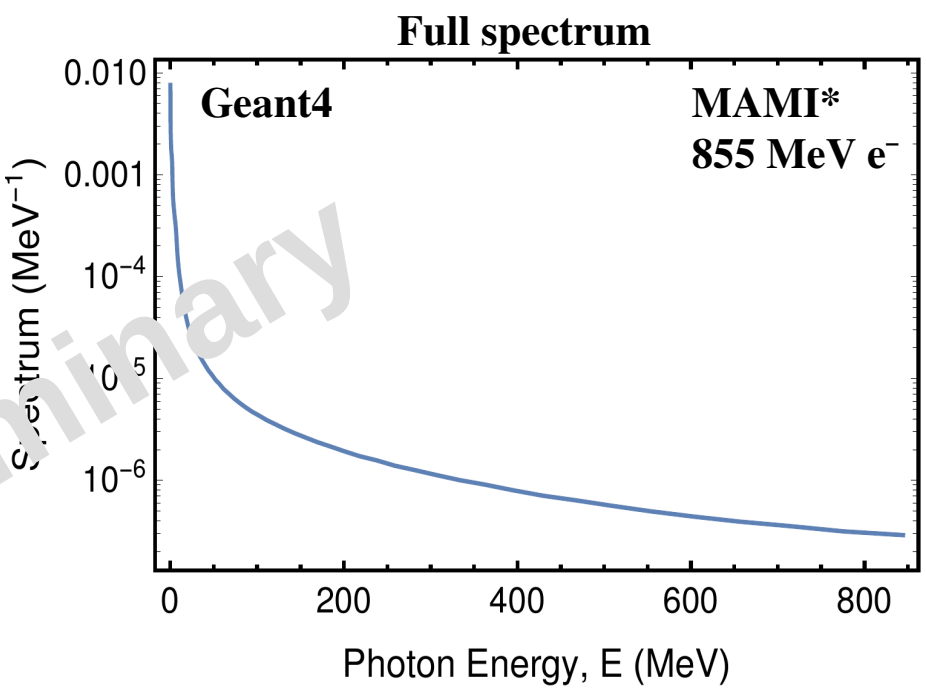
# First Geant4 Baier-Katkov radiation model: radiation by 855 MeV electrons at Mainz Mikrotron MAMI*

**G4BaierKatkov:**

- **Physics list independent**
- Can be used **outside channeling model** within other FastSim model
- Provides **radiation spectrum** for single-photon radiation mode
- Provides generation of **secondary photons**

**Geant simulations vs experiment and CRYSTALRAD simulations**



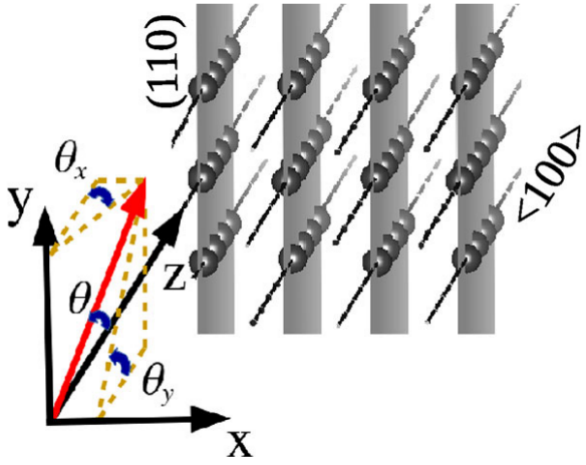

Preliminary

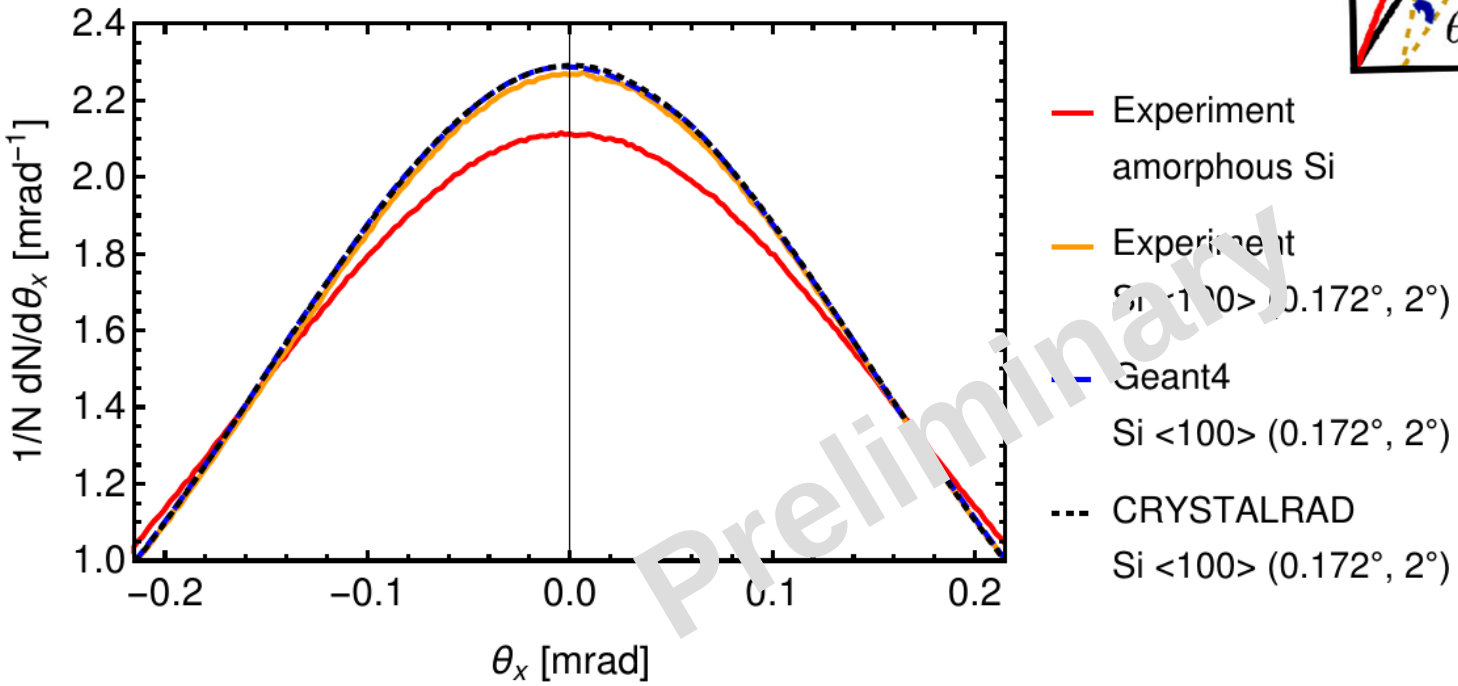
**To be submitted for publication soon**

*L. Bandiera et al. Phys. Rev. Lett. 115, 025504 (2015)

# 2D Geant4 channeling model validation: coherent scattering suppression effect*

**Multiple scattering in crystal and multiple scattering in amorphous material are different!**




**To be submitted for publication soon**

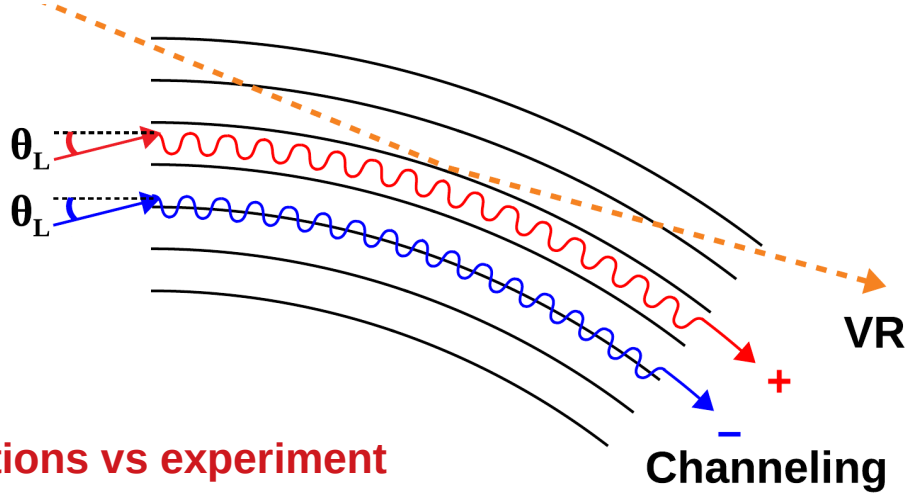
*A. Mazzolari, A. Sytov et al. Eur. Phys. J. C 80, 63 (2020)

# Recent experiment
# Channeling of 530 MeV positrons in a bent crystal

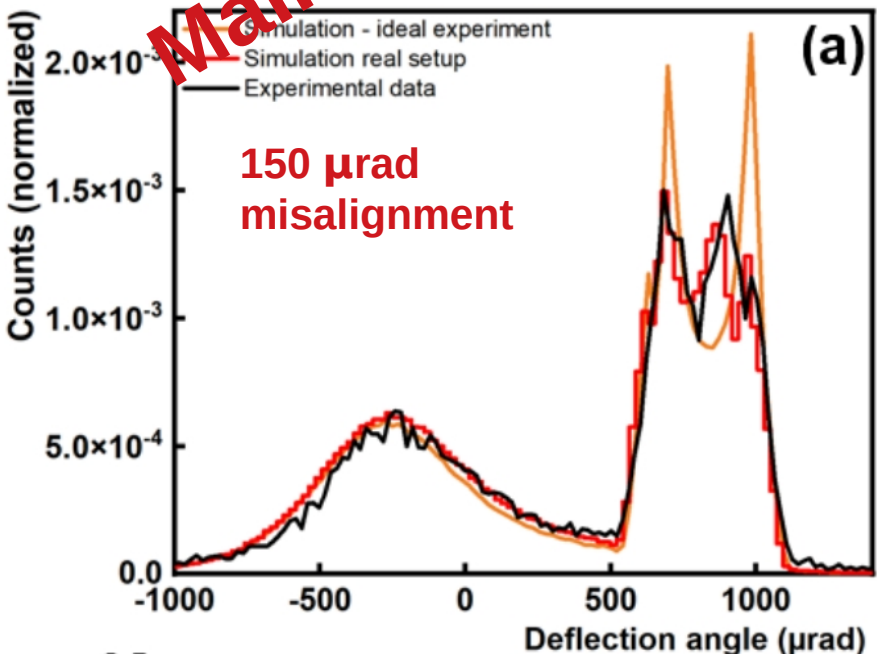
**530 MeV positrons**

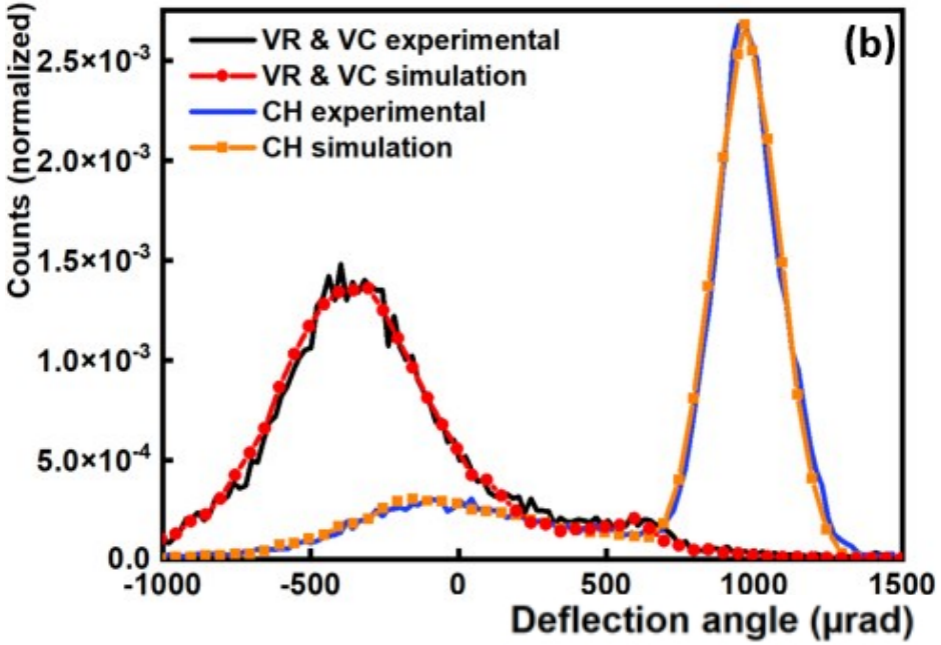
**30 µm thick bent crystal**

**New experiment Mainz Mikrotron 2024**

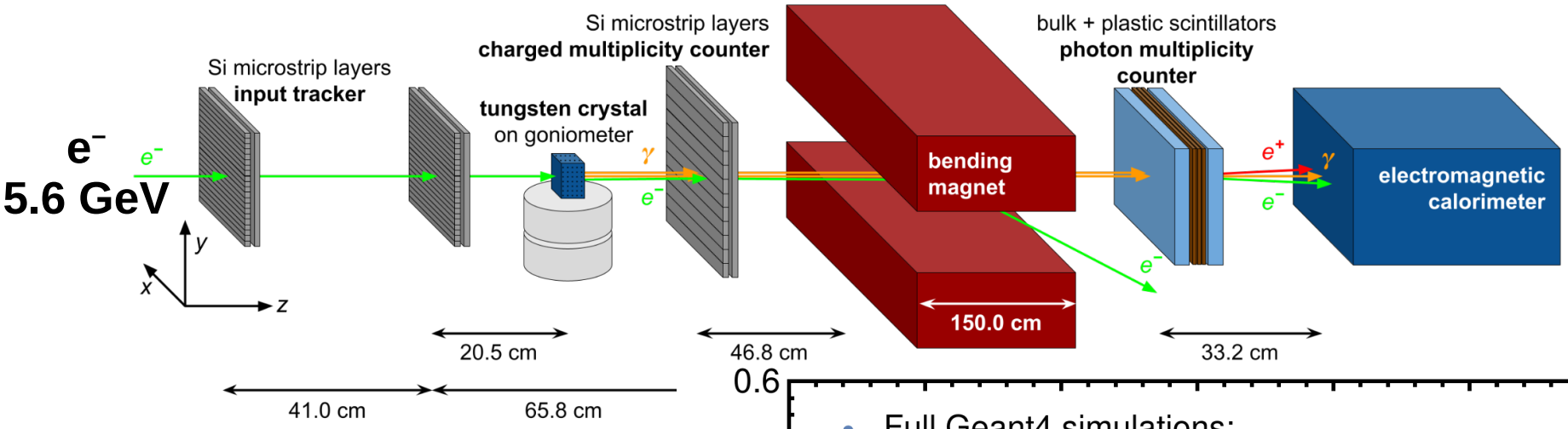


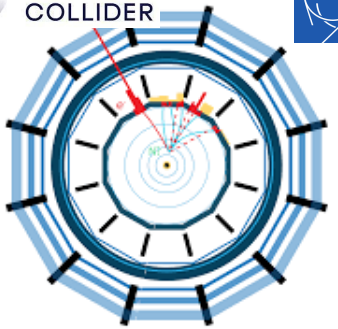

**Geant4 simulations vs experiment**

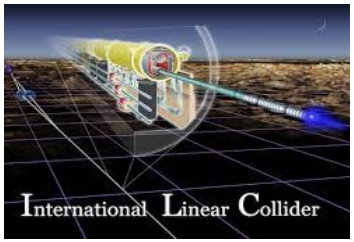


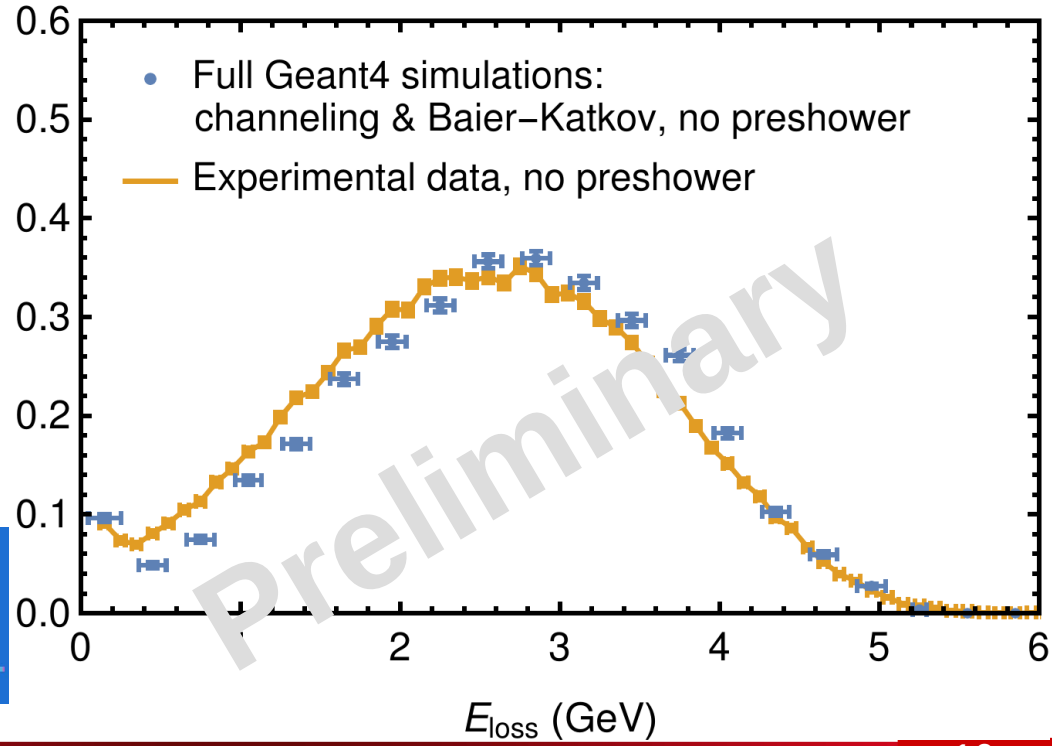



# Full Geant4 simulations of the DESY experiment* for the FCC-ee positron source project



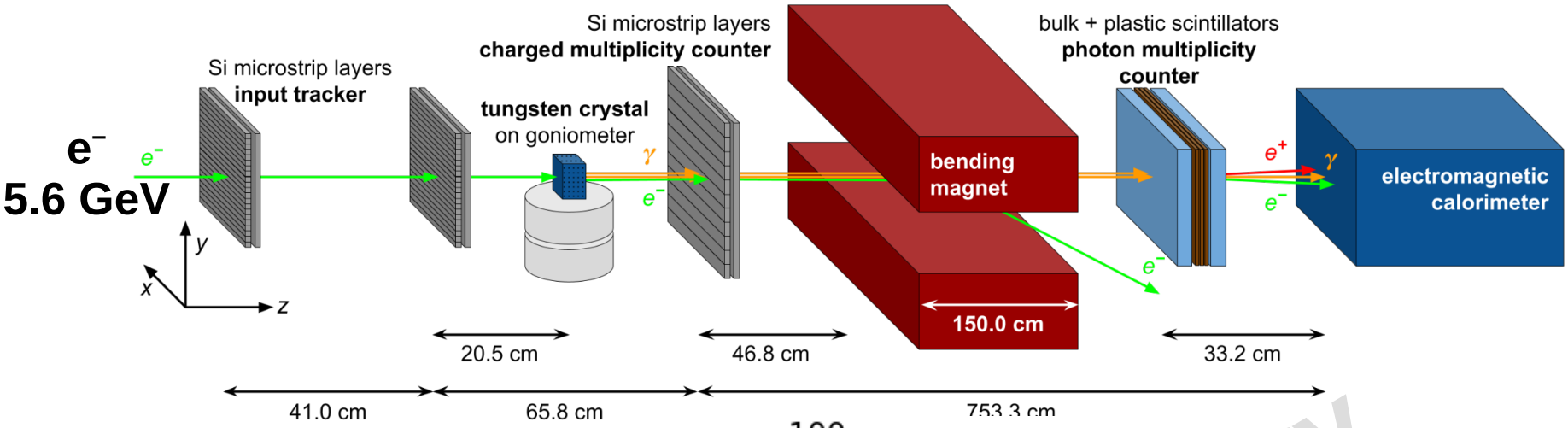



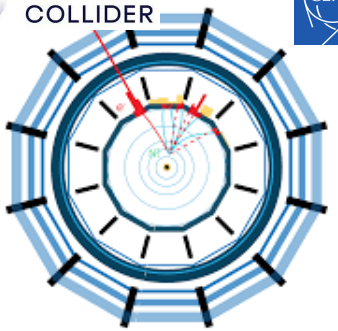



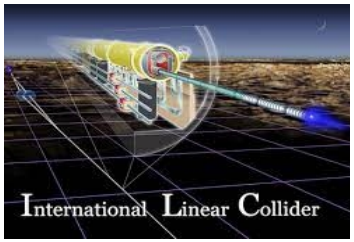



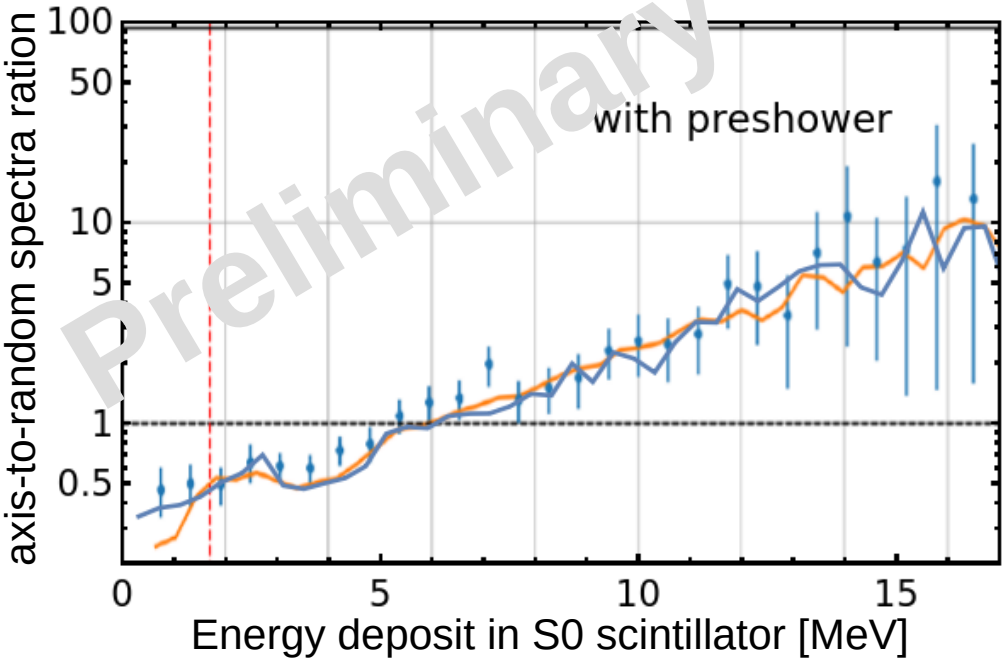

***Intense positron source Based On Oriented crySTals* - e+BOOST**
**(PI L. Bandiera)**
**PRIN2022-2022Y87K7X**
**Financed by Italian Ministry of University and Research - PRIN project**

# Full Geant4 simulations of the DESY experiment* for the FCC-ee positron source project




***Intense positron source Based On Oriented crySTals* - e+BOOST**
**(PI L. Bandiera)**
**PRIN2022-2022Y87K7X**
**Financed by Italian Ministry of University and Research - PRIN project**

Ministero dell'Università e della Ricerca
Bando PRIN 2022
UNIVERSITÀ RICERCA

*L. Bandiera et al. Eur. Phys. J. C 82, 699 (2022)

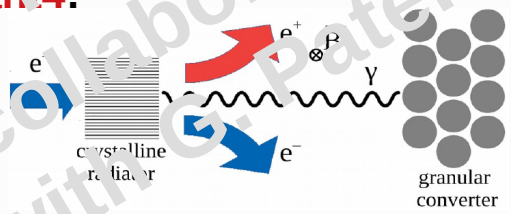
# Approximate list of examples to include in Geant4 in 2024

**Examples:**

- Very **easy example** to demonstrate basic commands to include the channeling model in DetectorConstruction (no input/simple output) — **Done**
- **Complex example** including both channeling and radiation model, input with macro commands, root output and full spectrum of options — **To submit**
- **Pair production model** and dedicated example of electromagnetic shower in a scintillator crystal — **In submission**

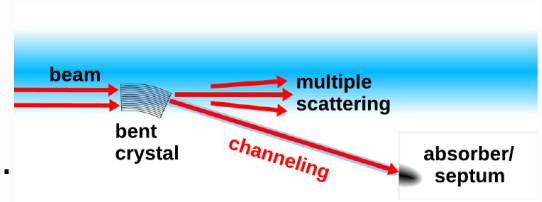
**Specific applications to implement into Geant4:**

- **Crystal-based hybrid positron source for FCC-ee** — **To submit**



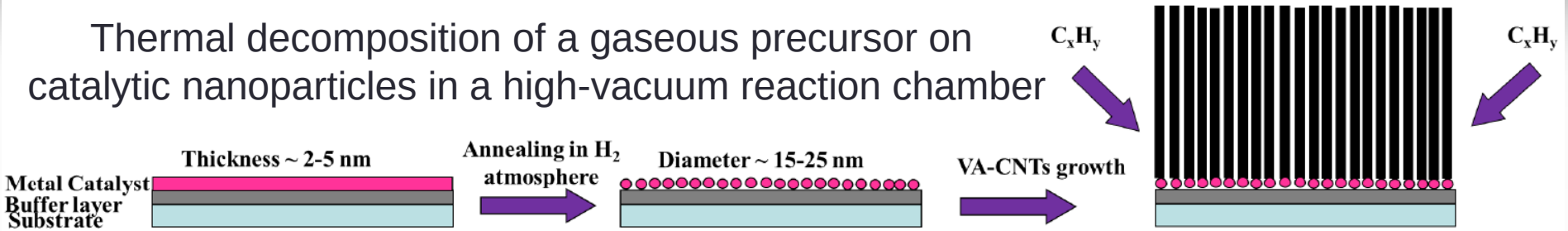

In close collaboration with G. Paternò

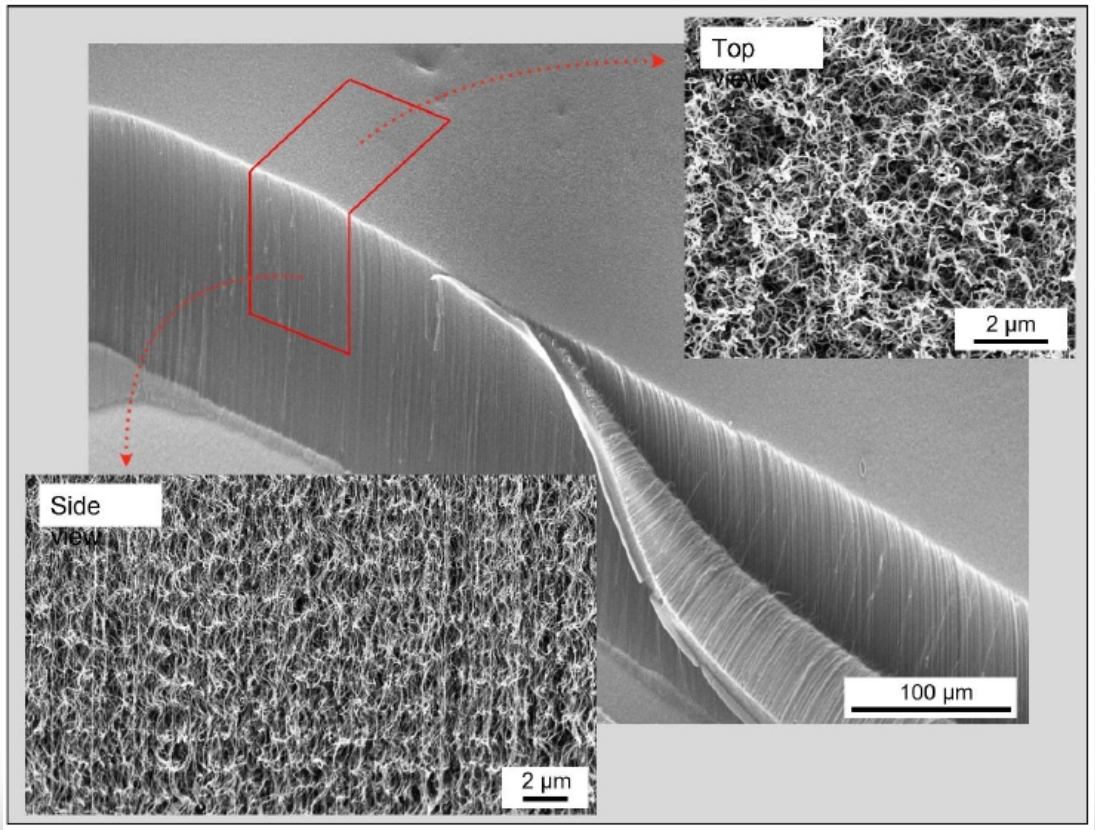
- **Crystalline deflector to extract a charged particle beam from an accelerator** (electron synchrotron, hadron collider) using **BDSim** code. — **Works**

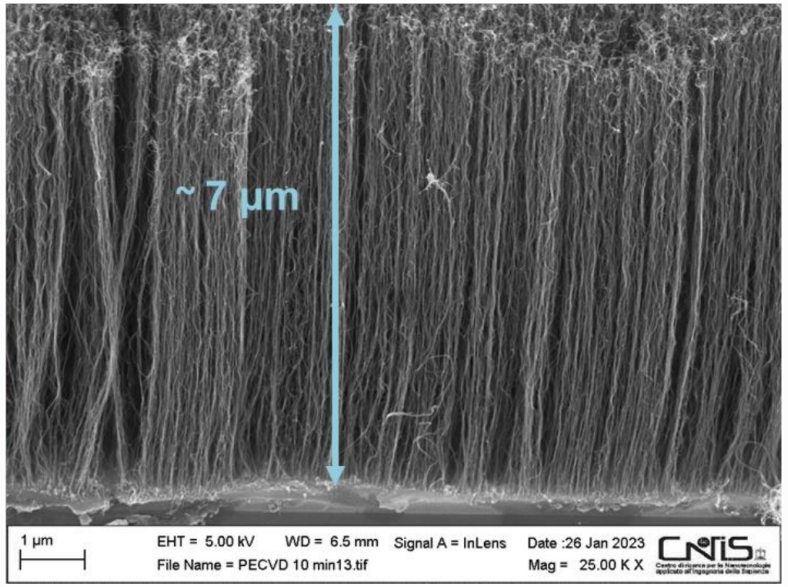


# Future target: carbon nanotubes

Thermal decomposition of a gaseous precursor on catalytic nanoparticles in a high-vacuum reaction chamber



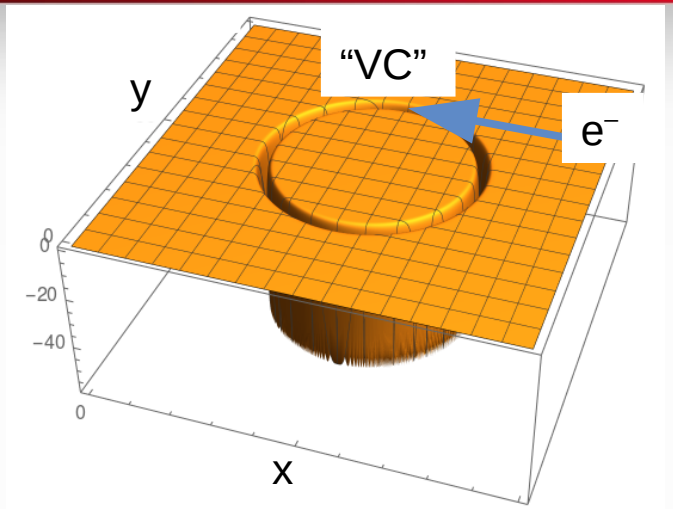

Courtesy of
Prof. Gianluca Cavoto,
Dr. Ilaria Rago

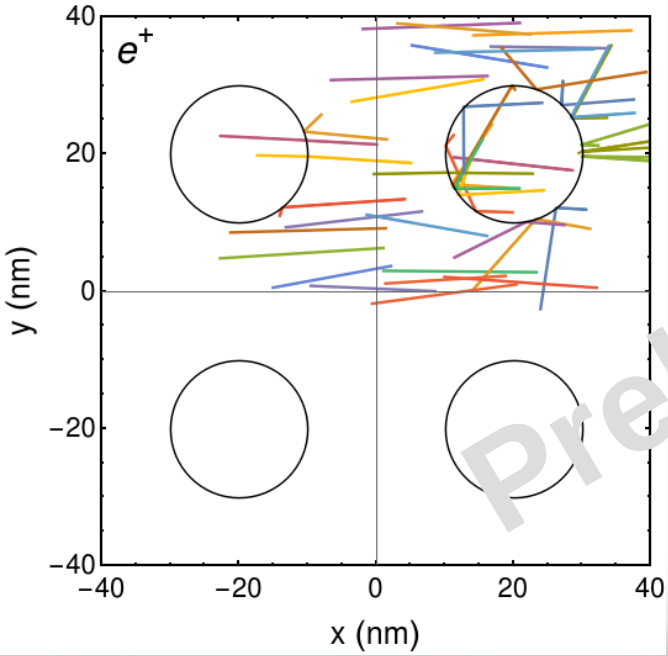
* F. Sarasini et al. Composites Part B 243 (2022) 110136

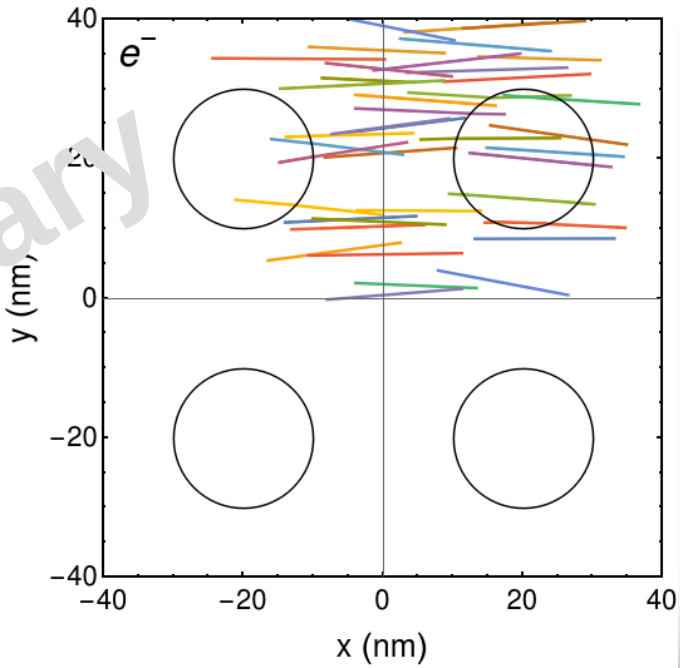
# Channeling simulations in CNT: trajectories, ideal case

Simulations with **CRYSTALRAD** simulation code*

**Simulation parameters**:
Beam: $e^-/e^+$
Divergence: 10 μrad
CNT diameter: 20 nm
CNT length: 0.2 mm



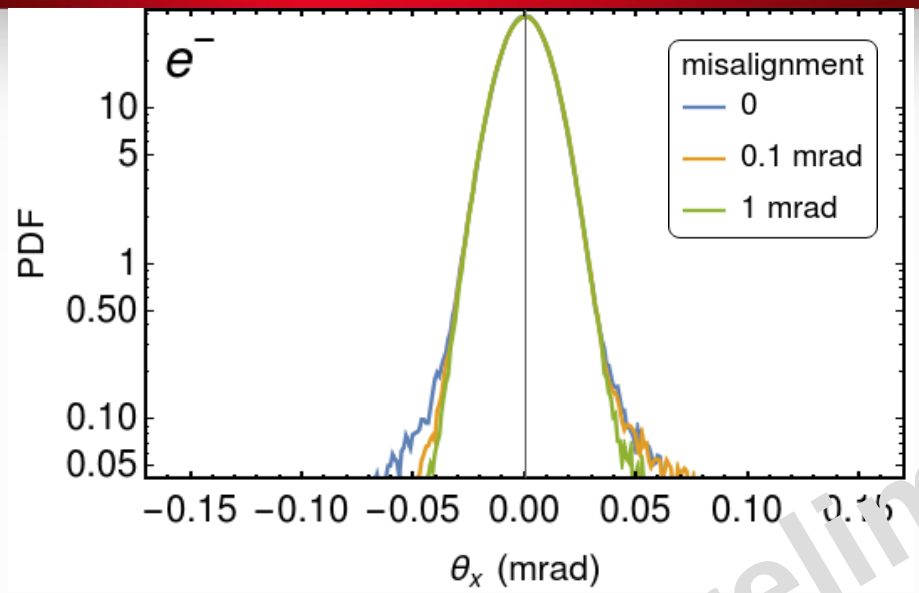



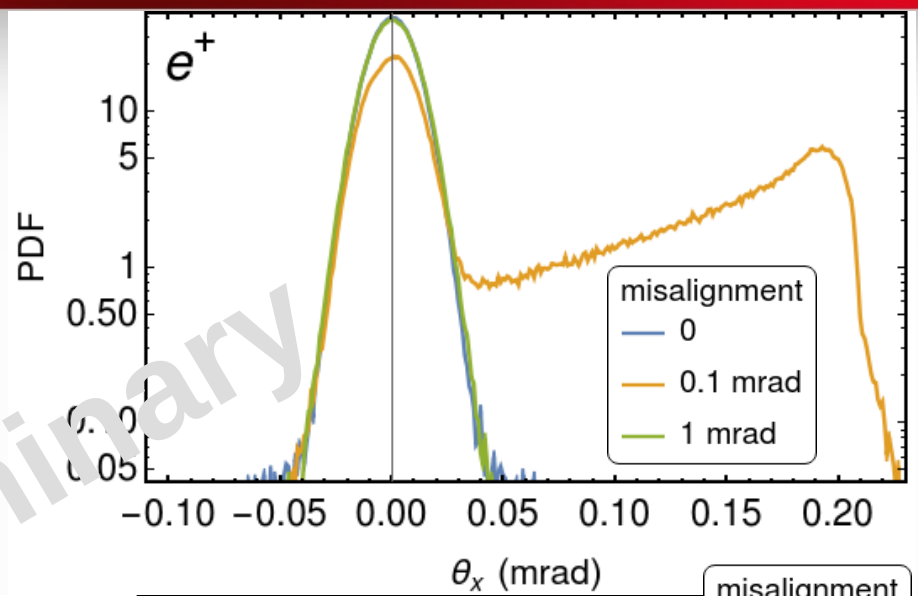



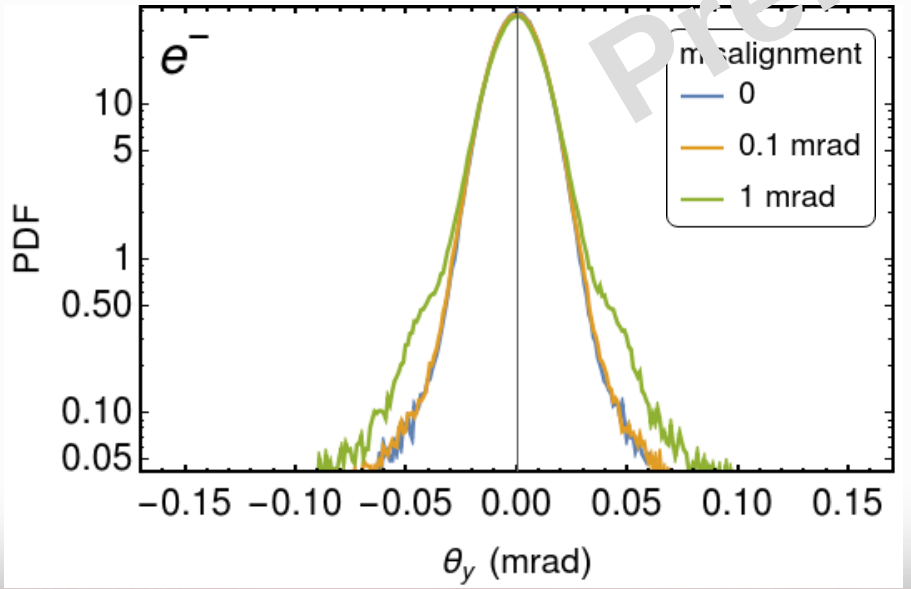

Preliminary

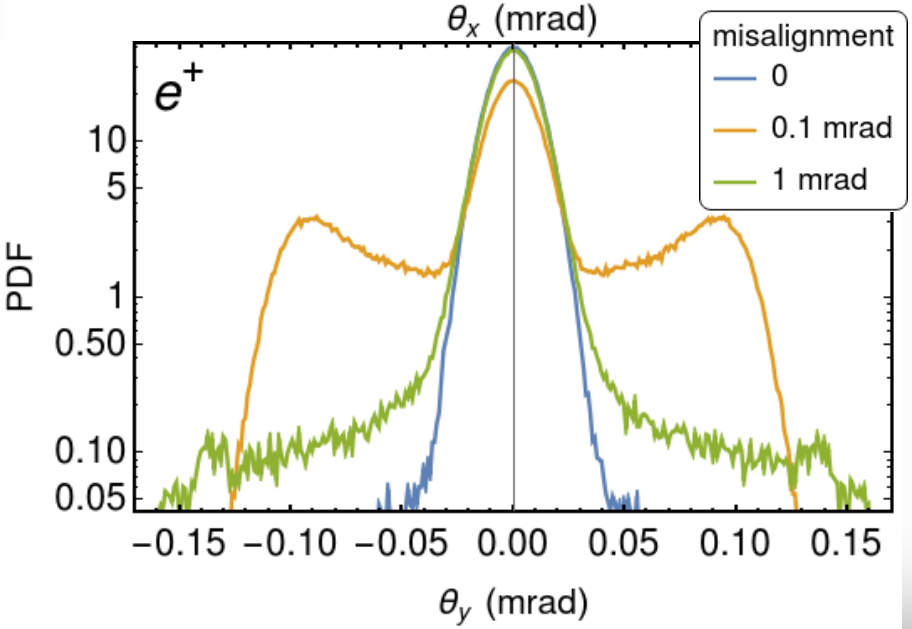
*A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. PRAB 22, 064601 (2019)

# Channeling simulations in CNT: angular distributions of deflected beam, ideal case



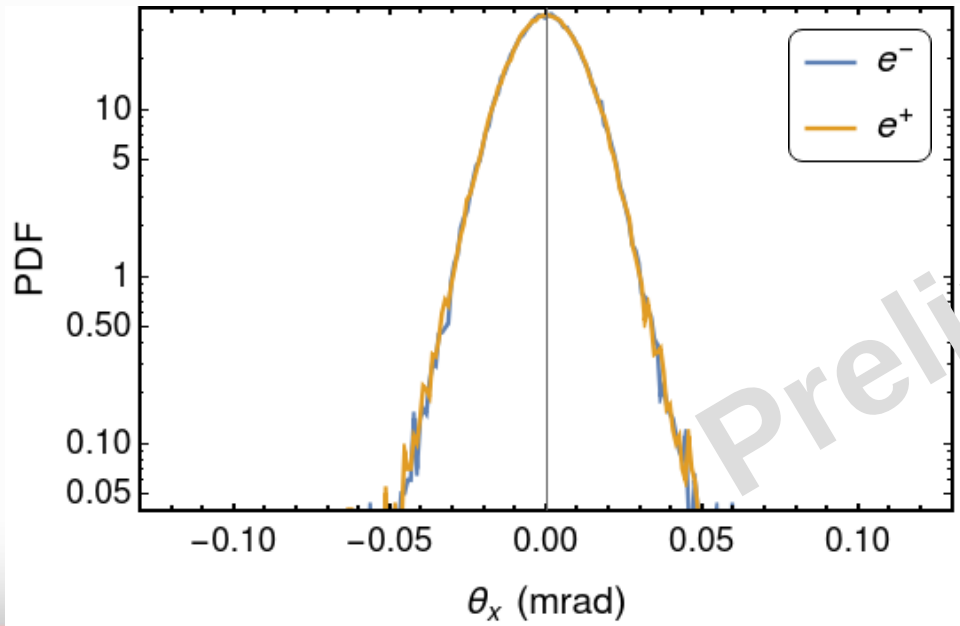

Preliminary

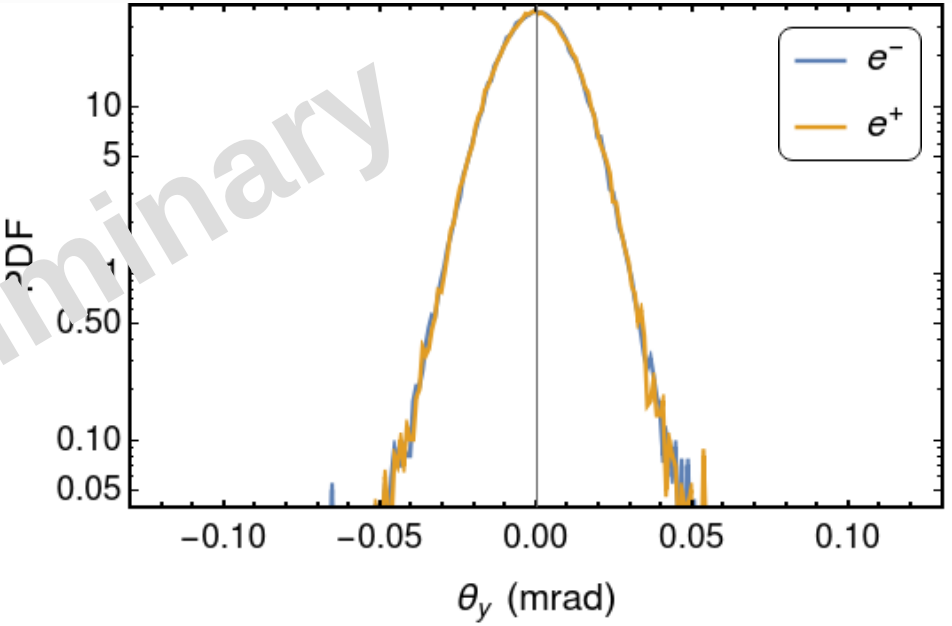
# Channeling simulations in CNT: angular distributions of deflected beam, more realistic case

**Simulation parameters**:
"Random forest" of nanotubes with the angular misalignment 1 mrad/100 nm along the nanotube.

**Desirable** for plasma acceleration but still **not realistic.**
**Real misalignment is degrees/100 nm**

**No** traces of **coherent effects**
but
r.m.s angle = 10.9 μrad
(compare with 10 μrad of initial angular divergence)
**Multiple scattering** increased.




Preliminary

# Acknowledgments

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- **GEANT4INFN** project (INFN Geant4 group);
- **INFN OREO, PRIN E+BOOST, INFN GALORE, RD-MUCOL, RD-FCC,**
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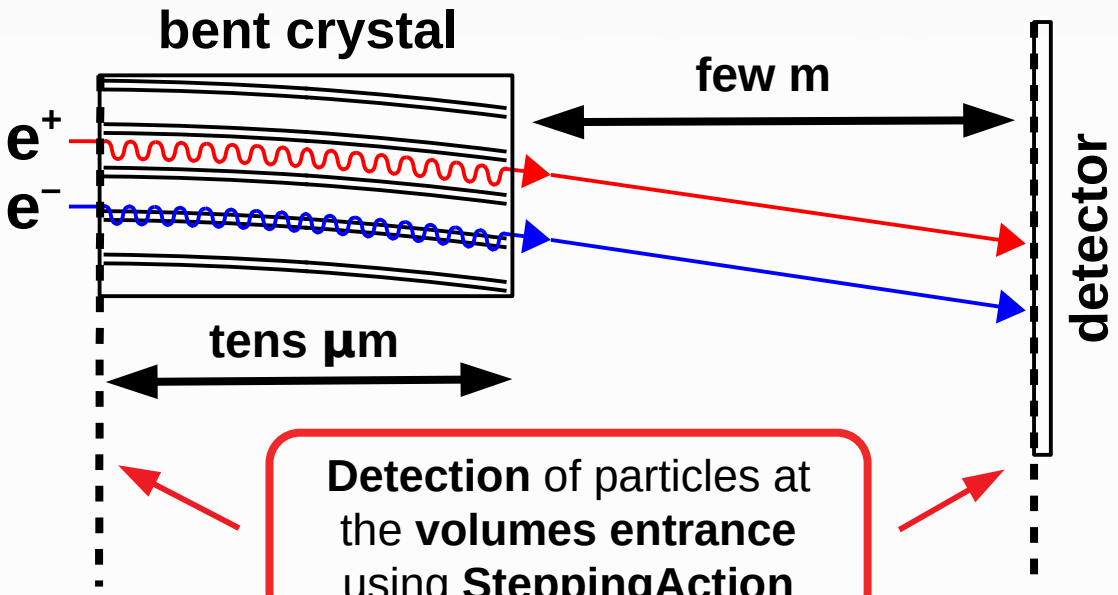
감사합니다 !

# First Geant4 channeling example for electrons/positrons

- **Inspired by** our experiments* of **855 MeV electron** beam deflection by an ultrashort **bent crystal** at **Mainz Mikrotron MAMI**




**Detection** of particles at the **volumes entrance** using **SteppingAction**

**Multithreading** works!
Checked at the supercomputer
**Galileo100@CINECA** (Italy)
**NURION@KISTI** (Korea)

**Output** both in **root** (only primary particles) and in **textfile** (all the particles) format

***A. Mazzolari et al. Phys. Rev. Lett. 112, 135503 (2014)**

# Why the implementation of channeling and Baier-Katkov models into Geant4 is so challenging?

**Challenges of trajectory simulation**

- **Complicated geometry** of crystal planes/axes especially in a bent crystal;
- **Complicated spacial structure** of cristalline **electric fields** and **atomic density** depending on the material and alignment;
- Different types of **scattering dependent** on the charge particle **positions** vs crystal planes/axes;
- **Incompatibility** of channeling with **Geant4 standard physics lists**: especially with **multiple coulomb scattering** and **bremsstrahlung** process: impossible to modify **continuous-discrete Geant4** processes during execution.

**Challenges of Baier-Katkov**

- Need for **recording trajectory** in order to simulate the spectrum;
- Multidimensional integral => **low simulation speed**;
- Hard gamma radiation => need to **return** the particle **back to the radiation point**, which is **not allowed in Geant4** in a simple way.

# Old channeling model in Geant4

**Currently implemented***
**Channeling physics:**

- Only trajectories (**no radiation**)
- Only for hadrons
- Changing cross-sections using **Geant4 Biasing**

**To do:**

- To resolve the **problems** with modification of **continuous discrete processes**
- To add channeling of **e+/e-**
- To add channeling **radiation**
- To add coherent **pair production**

**Problem** with modification of the **electromagnetic physics list**:
class G4ChannelingOptrChangeCrossSection

```
93
94      switch (type) {
95          case fNotDefined:
96              fProcessToDensity[processName] = fDensityRatioNone;
97              break;
98          case fTransportation:
99              fProcessToDensity[processName] = fDensityRatioNone;
100             break;
101         case fElectromagnetic:
102             if(subType == fCoulombScattering ||
103                subType == fMultipleScattering){
104                fProcessToDensity[processName] = fCancelProcess;
105             }
106             if(subType == fIonisation ||
107                subType == fBremsstrahlung){
108                fProcessToDensity[processName] = fCancelProcess;
109             }
110             if(subType == fPairProdByCharged ||
111                subType == fAnnihilation ||
112                subType == fAnnihilationToMuMu ||
113                subType == fAnnihilationToHadrons){
```

It is not possible to turn off/to modify **continuous discrete processes** (multiple scattering, ionization losses) in this way but only **discrete processes**

**Crucial for e+/e-**
though not so important for high energy protons

*E. Bagli Eur. Phys. J. C 74, 2996 (2014)

# Manufacturing and characterization of bent silicon crystals @INFN Ferrara