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**Simulation of charged particle interaction with
oriented crystals using Geant4**

Dr. Alexei Sytov

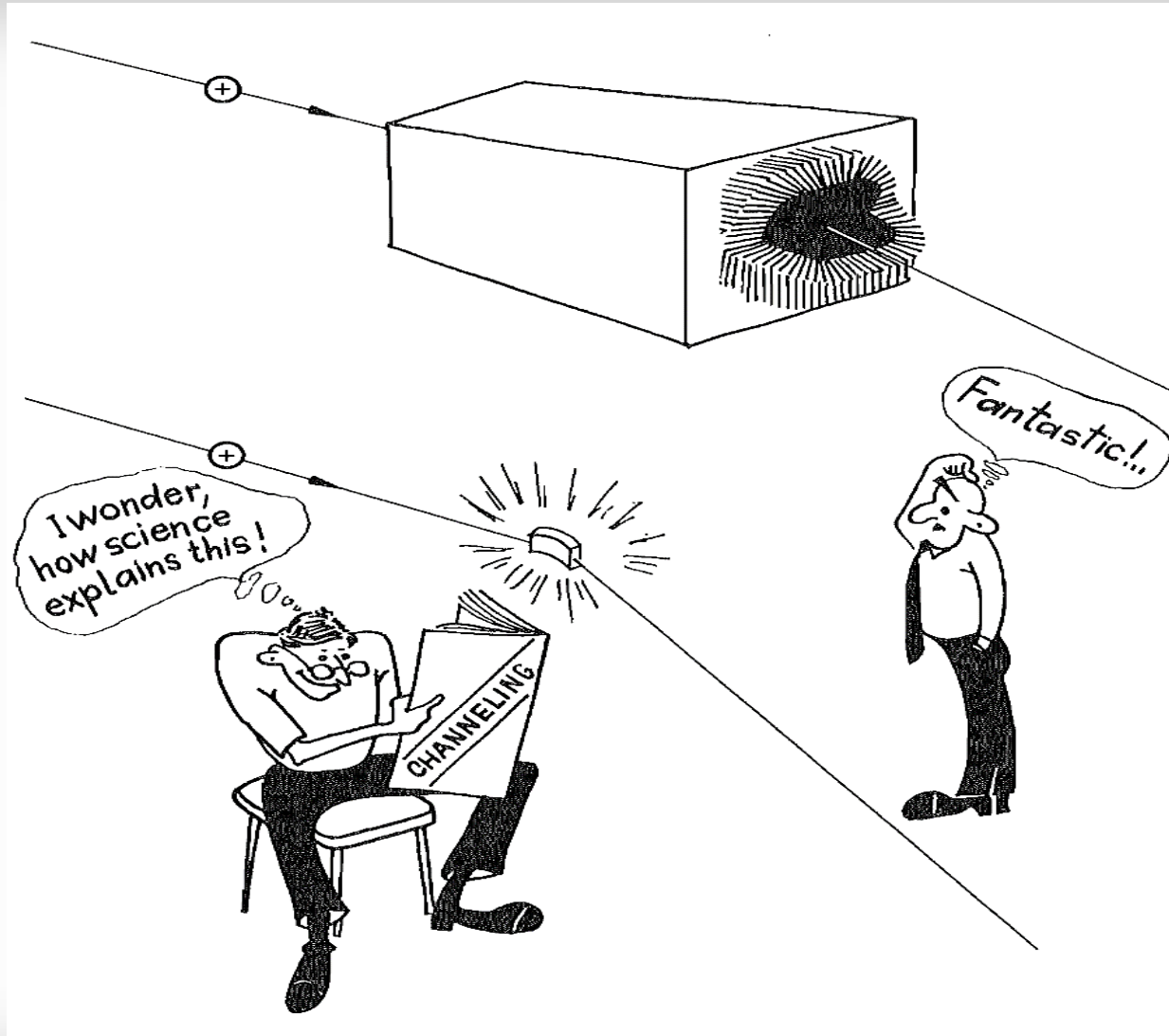
High1 Workshop on Particle, String and Cosmology

High1 Resort, 23/01/30

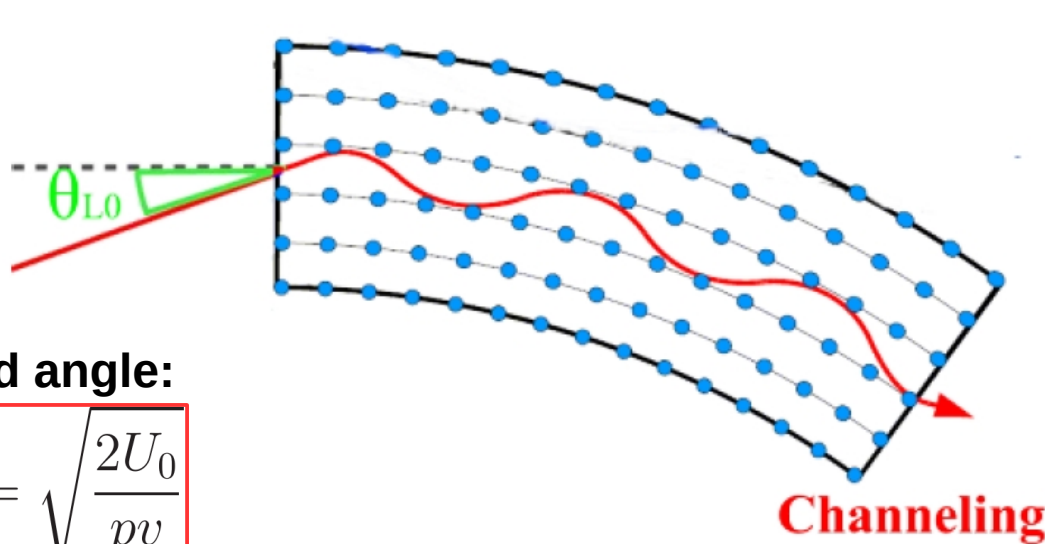
Outline

- **The world of channeling effect**
 - Channeling, Radiation and pair production
 - Electromagnetic shower acceleration
 - Main applications
- Implementation of the new physics into Geant4
 - Main conception: **FastSim** interface
 - What has been done by now?

The world of the channeling effect

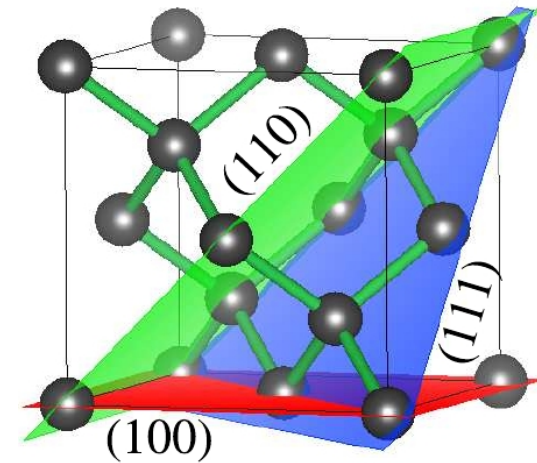


Channeling effect*



Lindhard angle:

$$\theta < \theta_L = \sqrt{\frac{2U_0}{pv}}$$



Channeling* is the effect of the penetration of charged particles through a monocrystal quasi parallel to its atomic axes or planes. In dependence on the crystal alignment along either planes or atomic strings channeling can be divided into

- **Planar channeling**
- **Axial channeling**

Planar/Axial field $10^9/10^{11}$ V/cm

*J. Stark, Zs. Phys. 13, 973–977 (1912)

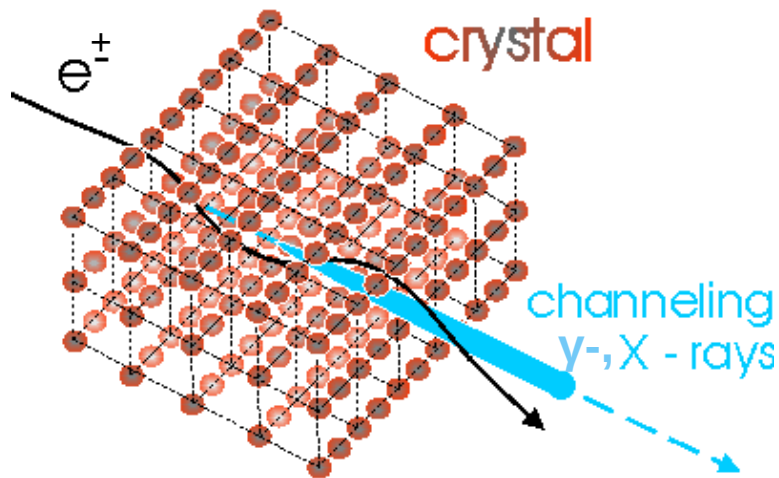
J. A. Davies, J. Friesen, J. D. McIntyre, Can J. Chem. 38, 1526–1534 (1960)

M. T. Robinson, O. S. Oen, Appl. Phys. Lett. 2, 30–32 (1963)

J. Lindhard, Kgl. Dan. Vid. Selsk. Mat.-Fys. Medd. 34 No 4, 2821–2836 (1965)

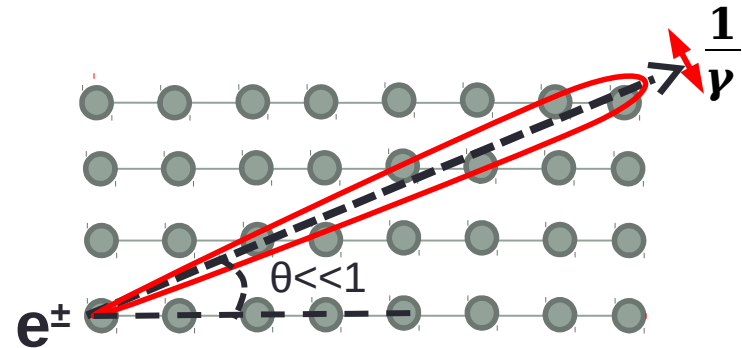
Coherent effects in a crystal

Channeling radiation*

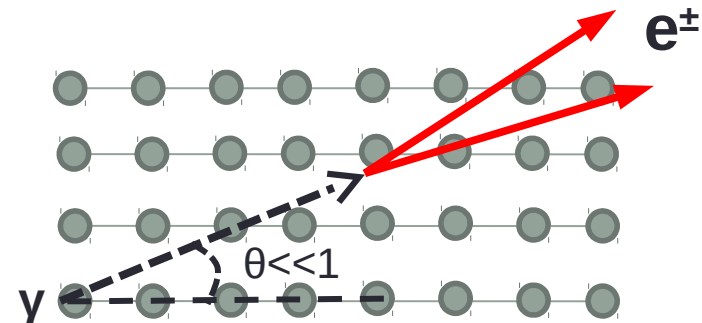


Coherent effects preserve
up to few mrad of particle
direction vs the crystal axis

Coherent bremsstrahlung**



Coherent pair production***



*M.A. Kumakhov, Phys. Lett. A 57(1), 17–18 (1976)

**B. Ferretti, Nuovo Cimento 7, 118 (1950).

***M. Ter-Mikaelian, Sov. Phys. JETP 25, 296 (1953).

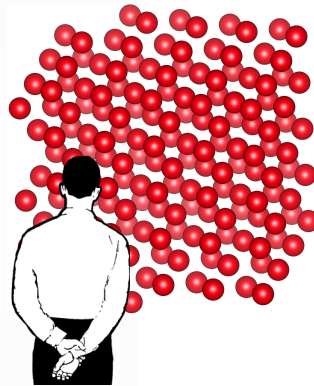
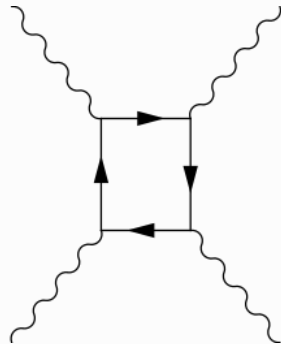
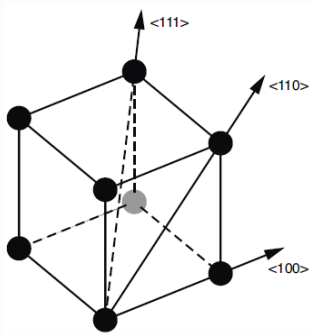
*** H. Überall, Phys. Rev. 103, 1055 (1956).

Electromagnetic shower acceleration

Axial field
 10^{11} V/cm

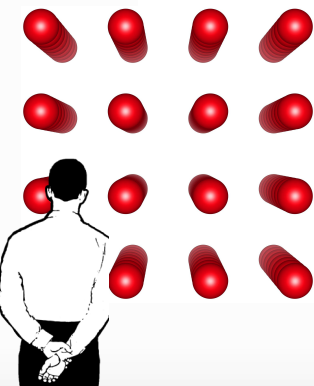
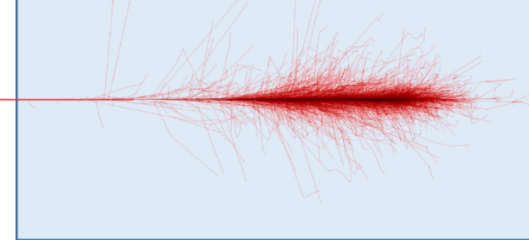


Approaching the
Schwinger limit
starting from few
GeV for **e⁺/e⁻**



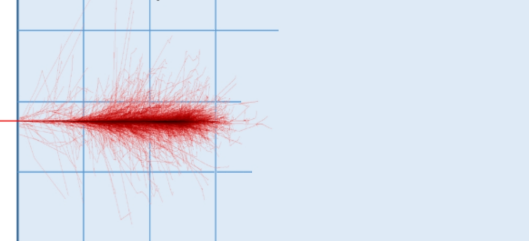
Particle

Amorphous or randomly oriented crystal



Particle

Oriented crystal



The **radiation** intensity and
the **pair production** cross-
section **drastically increase**
in **oriented crystals!**

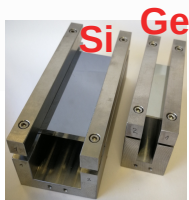
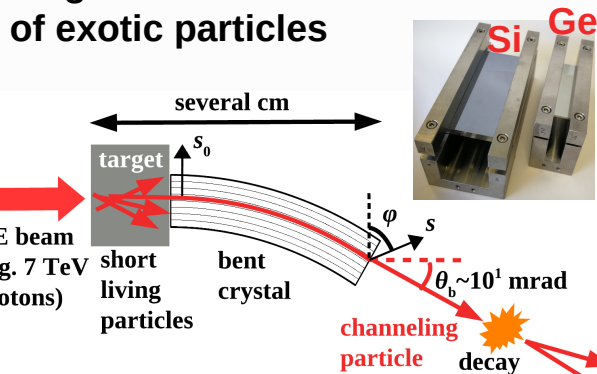
Shower development in the
field of axes is **accelerated**.
The radiation length is
considerably reduced*.

Applications*

Crystal-based collimation or beam extraction from an accelerator

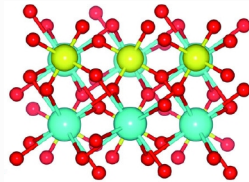


Measurement of dipole magnetic and electric moments of exotic particles

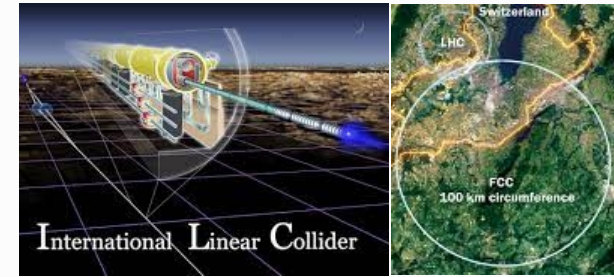
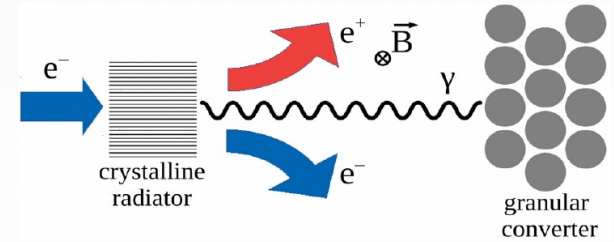


Gamma-ray Space Telescope

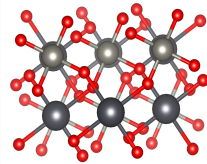
Ultrashort crystalline calorimeter



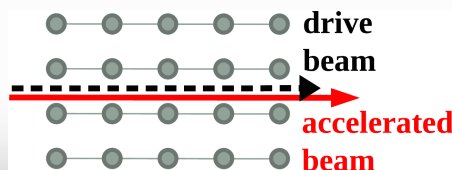
Positron source for future e⁺/e⁻ and muon colliders



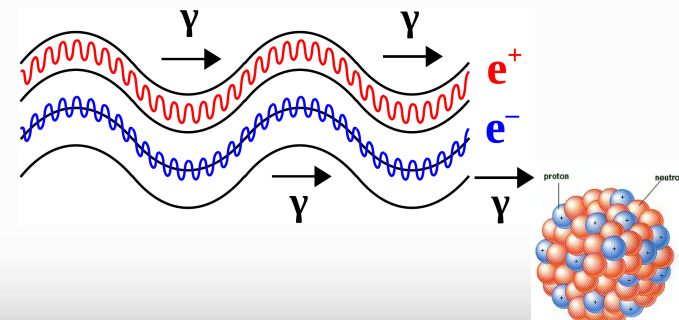
Oriented crystals



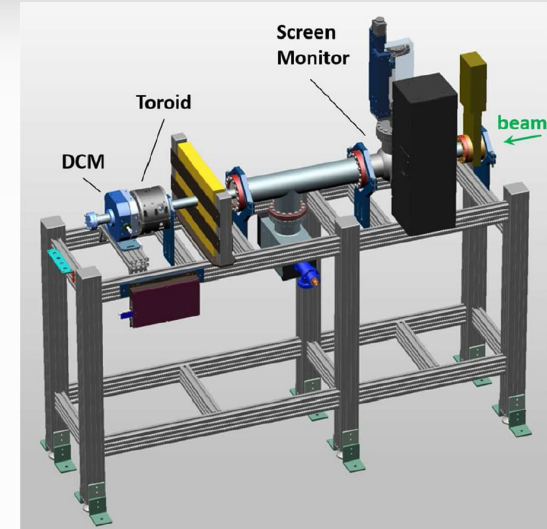
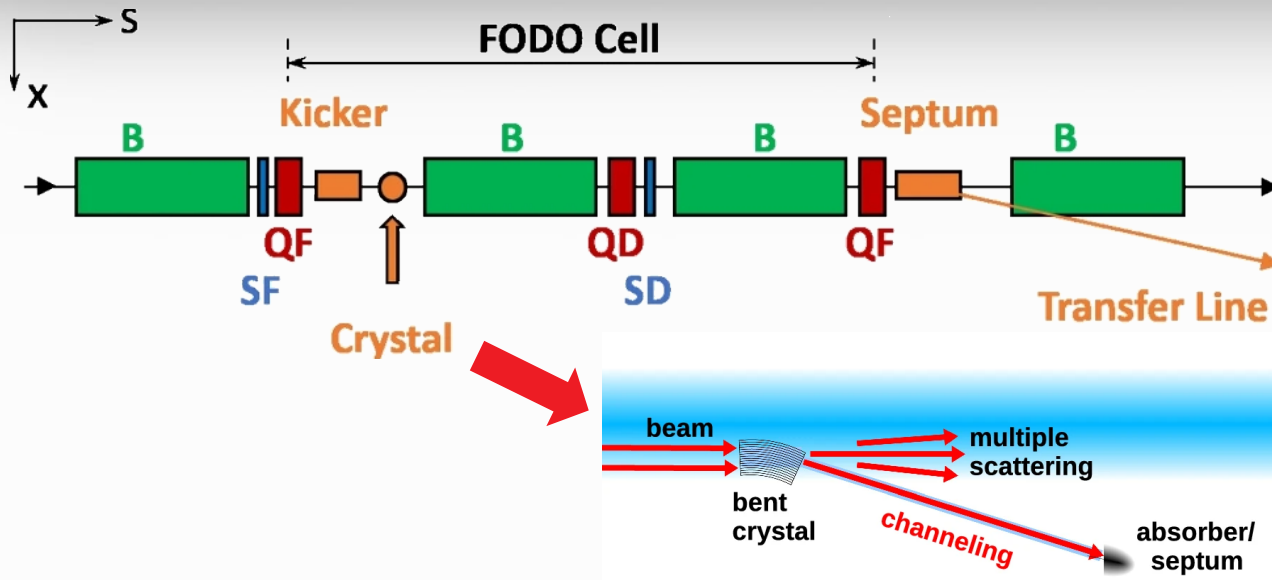
Plasma acceleration



X and γ -ray source for nuclear and medical physics



Crystal-based extraction: possible setup at DESY-II



Crystal-based beam extraction: applied only for protons,
never applied for electrons

Advantages:

- Extraction of **primary** low-emittance and very **intense electron beam** in a **parasitic mode**.
- The **extraction line** including septum magnets already **exists** => **ideal for prove-of-principle**
- Few GeV electron beam, **typical for electron synchrotrons** existing in the world.

Can be applied at:

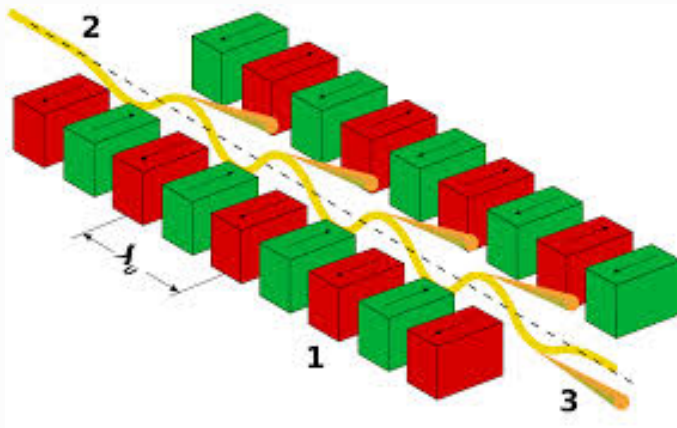
- DESY-II and any e-/e+ synchrotron or a **synchrotron light source**

Have been already applied at:

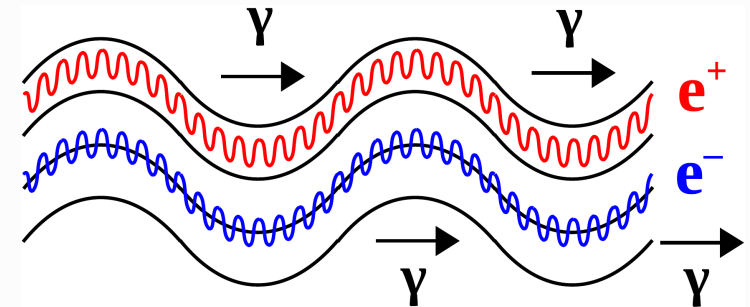
- **LHC, Tevatron, SPS, RHIC, U-70**

Channeling radiation in a bent crystal: Crystalline undulator

Classical scheme: magnetic undulator in a free electron laser
laser **soft X-rays** $\lambda_u \sim \text{cm}$



Innovative scheme: Crystalline undulator*
-> **Hard X-rays and gamma rays** $\lambda_u < \text{mm}$



Advantage:

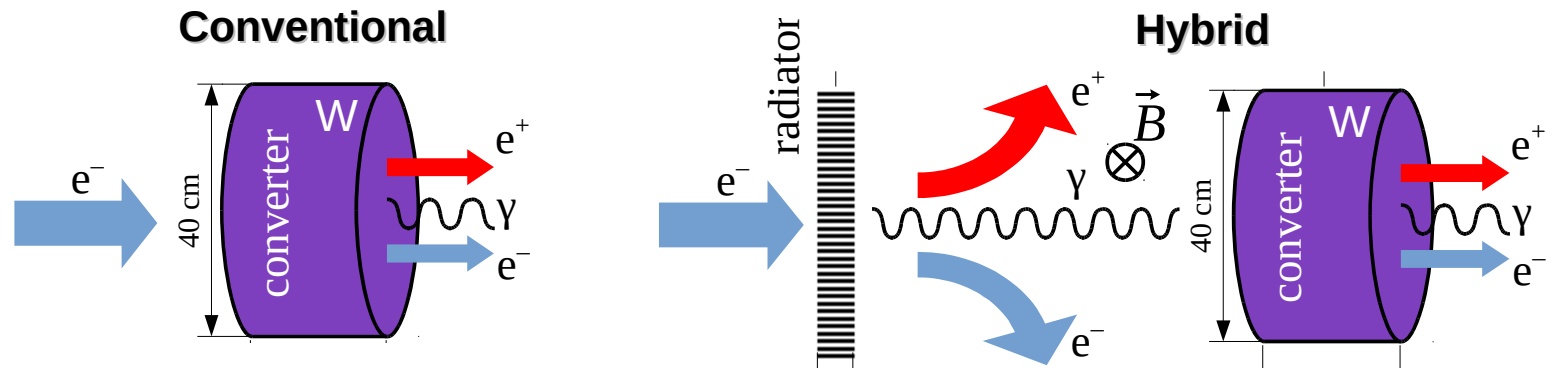
- Intense X- and gamma-rays produced in a crystal, in a compact piece of material

Crystalline X and gamma-ray source **can be applied** in:

- **Nuclear physics**
- **Medical physics**

 EU project MSCA RISE N-LIGHT G. A. 872196
Coordinator MBN RESEARCH CENTER (Germany)

Crystal-based hybrid positron source*



Coherent effects in a crystal accelerate electromagnetic shower development

Coherent effects of e.m. shower in a crystal:

- Channeling radiation/coherent bremsstrahlung
- Coherent pair production

Advantages of the hybrid positron source:

- **Higher** positron yield
- Considerably lower peak deposited energy inside the target => **higher beam intensities, longer target lifetime**

Hybrid positron source can be applied at:

- FCC-ee
- ILC
- Muon collider

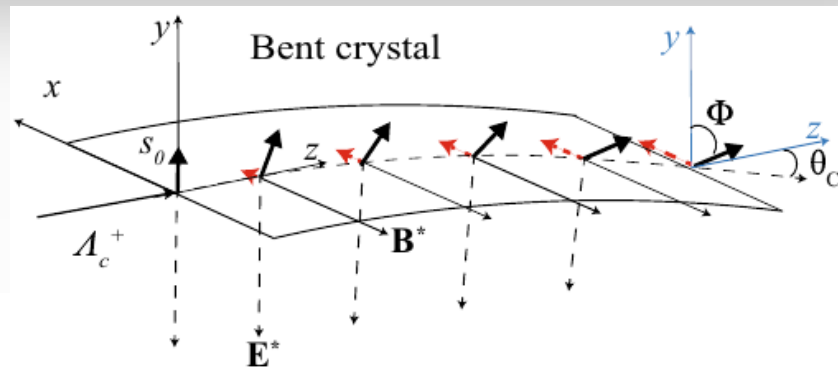


Simulation model can be also applied for ultrashort crystalline calorimeter

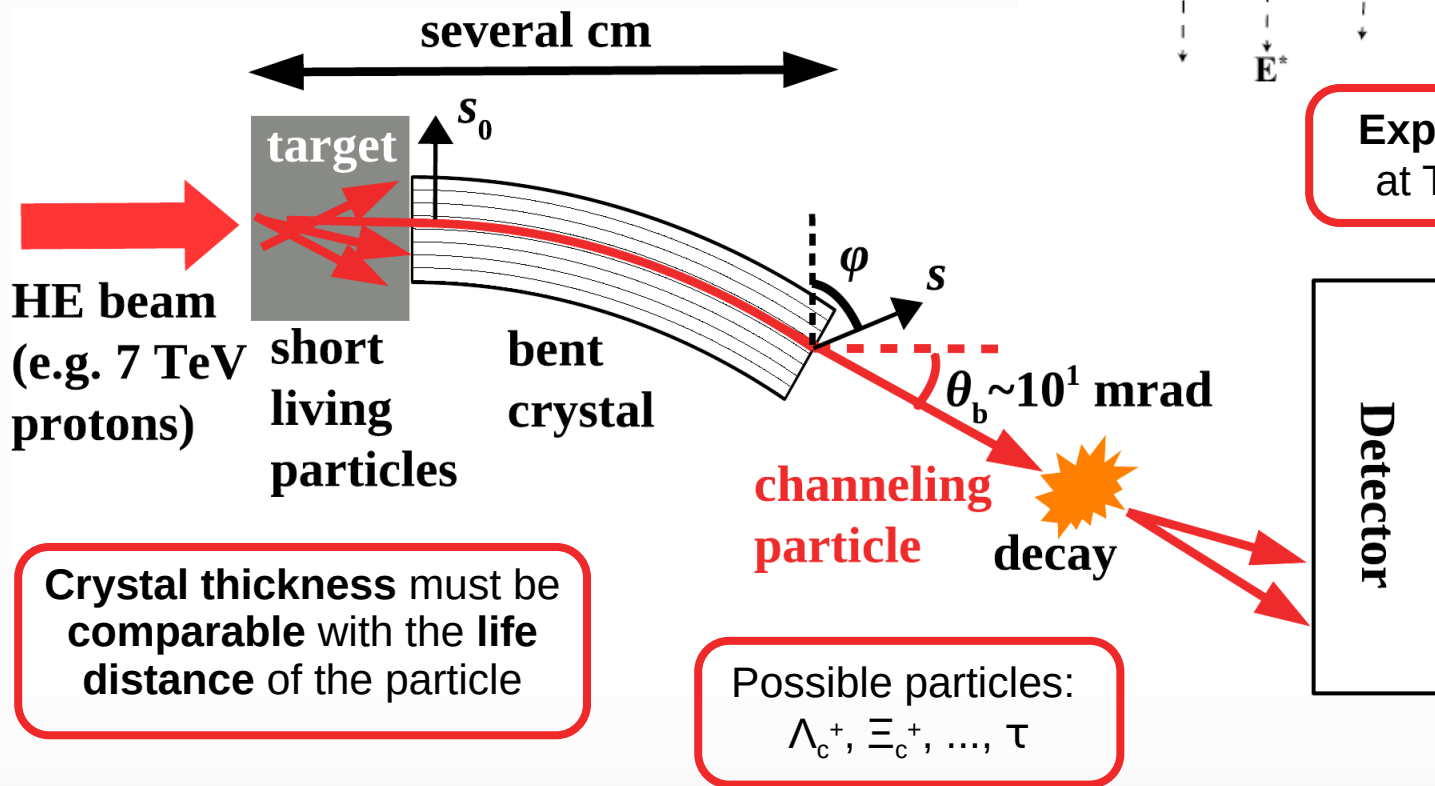
Search of MDM&EDM of short living particles using the effect of spin rotation in oriented crystals*

What we want:

● To measure **MDM** and **EDM** of exotic baryons



Experimental proof at Tevatron for Σ^{+**}



Crystal thickness must be comparable with the life distance of the particle

Possible particles:
 $\Lambda_c^+, \Xi_c^+, \dots, \tau$

* V. G. Baryshevskii, Pis'ma Zh. Tekh. Fiz. 5, 182 (1979)

**D. Chen et al. (E761 Collaboration) Phys. Rev. Lett. 69, 23 (1992)

Plasma wake-field acceleration in oriented crystals*

$$E[\text{GV/m}] = m_e \omega_p c / e \approx 100 \sqrt{n_0 [10^{18} \text{cm}^{-3}]}$$

**Acceleration
gradient:**

1-10 TeV/m

Considerably **higher electron density** in a **solid state** than in a gaseous plasma

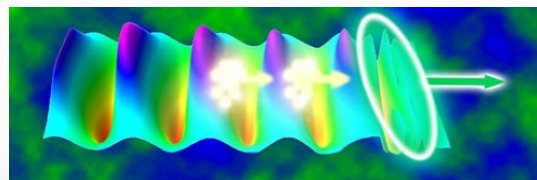
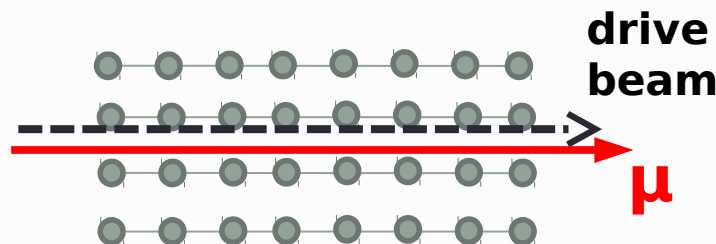
Channeling makes crystal almost **transparent** both to accelerated and to drive beam

Possible drive beam:

- X-rays
- electrons
- heavy high-Z beams

Possible accelerated beam:

- **muons**
- e+/e-
- protons



Compact muon collider?

* R. Ariniello, ..., and T. Tajima, **Snowmass**'2021 AF6: Advanced Acceleration Concepts, arXiv: 2203.07459

T.Tajima, M.Cavenago, Crystal X-ray accelerator, Phys. Rev. Lett., 59(13), 1440 (1987).

Marie Skłodowska-Curie Action Global Individual Fellowships by A. Sytov in 2021-2024, 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)

Progress of channeling physics implementation into Geant4



GEANT4
A SIMULATION TOOLKIT

Geant4 is a toolkit for the simulation of the **passage** of particles **through matter**. Its areas of application include **high energy, nuclear** and **accelerator physics**, as well as studies in **medical** and **space science**.

Solution: Geant4 FastSim interface

A. Sytov thanks **Prof. Vladimir Ivanchenko (CERN)** for this solution and the group of **Prof. Pablo Cirrone (INFN LNS)**, in particular **Dr. Luciano Pandola** as well as **Prof. Kihyeon Cho** and **Dr. Kyungho Kim (KISTI)**, **Prof. Susanna Guatelli** and **Prof. Anatoly Rosenfeld (University of Wollongong)** for fruitful discussions!

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 //.....ooo00000ooo.....ooo00000ooo.....ooo00000ooo.....ooo00000ooo.....
82
83 G4bool TestModel::ModelTrigger(const G4FastTrack& fastTrack)
84 {
102 }
103
104 //.....ooo00000ooo.....ooo00000ooo.....ooo00000ooo.....ooo00000ooo.....
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

Baseline simulation code: CRYSTALRAD

Main conception – tracking of charged particles in a crystal in averaged atomic potential

Program modes:

- **1D** model – particle motion in an interplanar potential
- **2D** model – particle motion in an interaxial potential

Simulation of the different physical processes:

- Multiple and single **Coulomb scattering** on nuclei and electrons.
- **Nuclear scattering**
- **Ionization energy losses**
- **Crystal geometry**

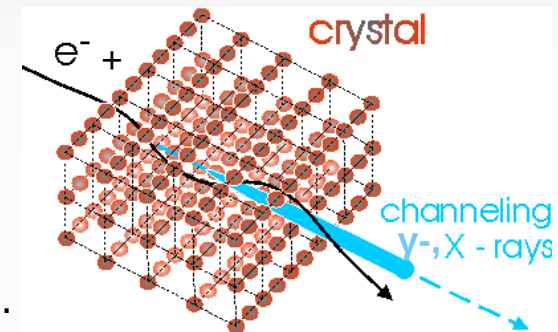
Baier-Katkov formula:

integration is made over the classical trajectory

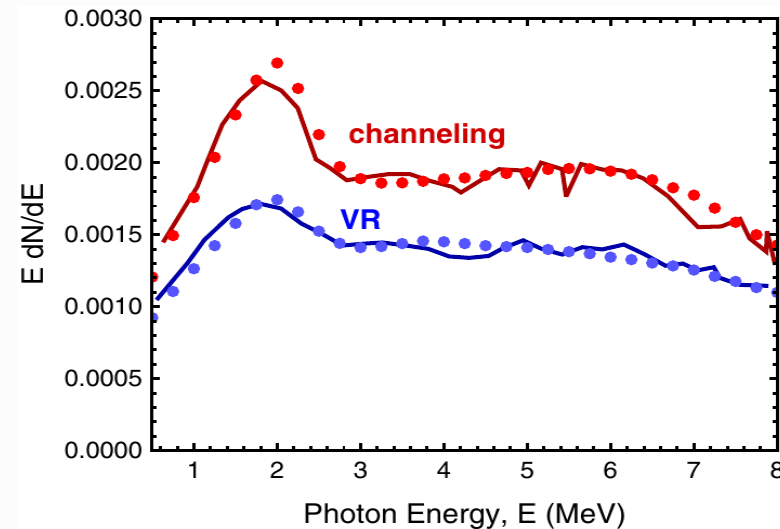
$$\frac{dE}{d^3k} = \omega \frac{dN}{d^3k} \frac{\alpha}{4\pi^2} \iint dt_1 dt_2 \frac{[(E^2 + E'^2)(v_1 v_2 - 1) + \omega^2 / \gamma^2]}{2E'^2} e^{-ik'(x_1 - x_2)}$$

Advantages:

- High calculation speed
- **MPI** parallelization for high performance computing



CRYSTALRAD vs experiment



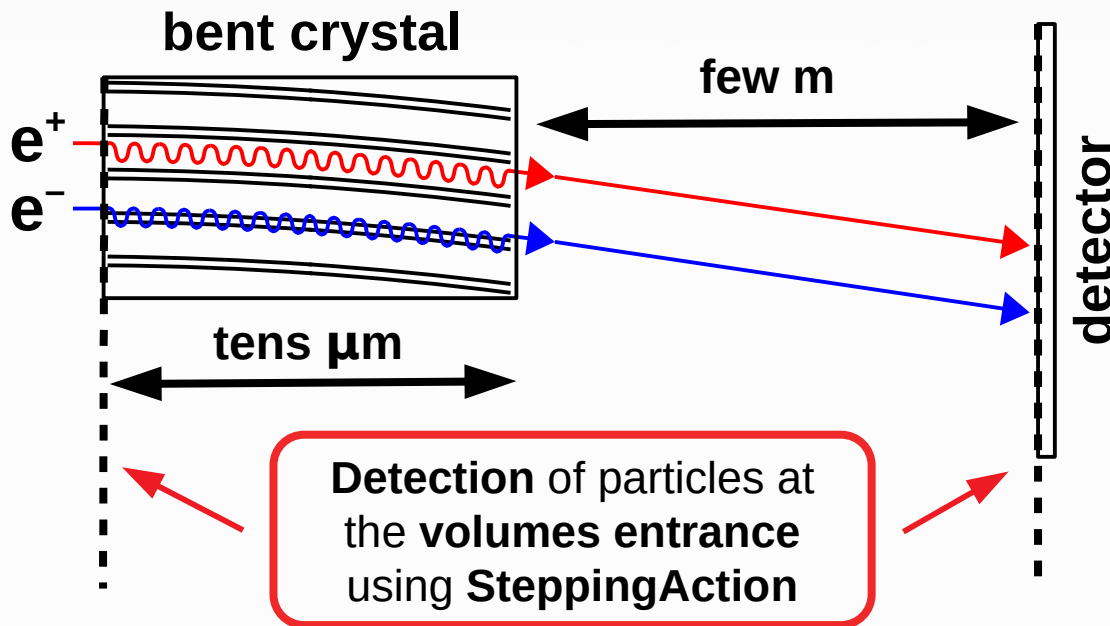
A.I. Sytov, V.V. Tikhomirov. NIM B 355 (2015) 383–386.

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

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

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



Beam setup in **run.mac** using **GPS** commands; all the **geometry** in **DetectorConstruction**

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

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



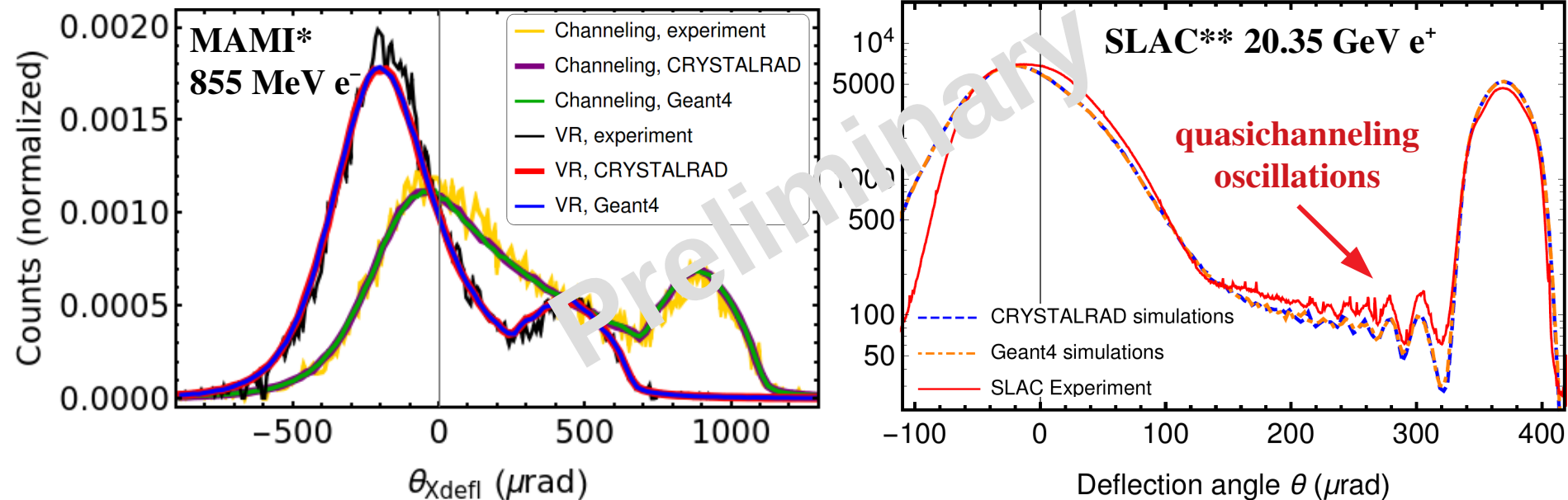
*A. Mazzolari et al. Phys. Rev. Lett. 112, 135503 (2014)

A. Sytov et al. Eur. Phys. J. C 77, 901 (2017)

First simulations with Geant4 channeling model: beam deflection by a bent crystal



Geant simulations vs experiment and CRYSTALRAD simulations



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

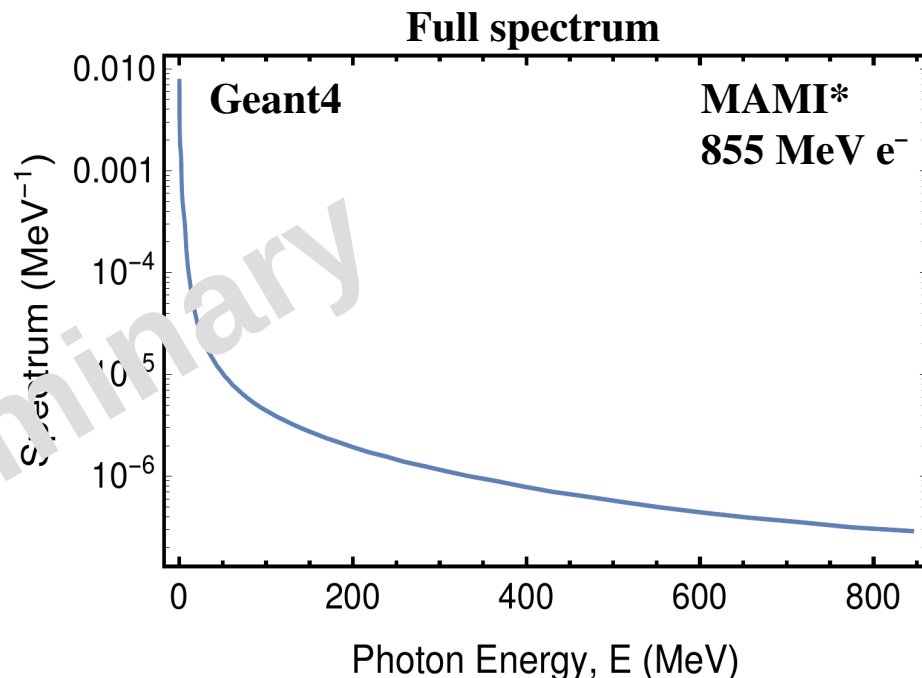
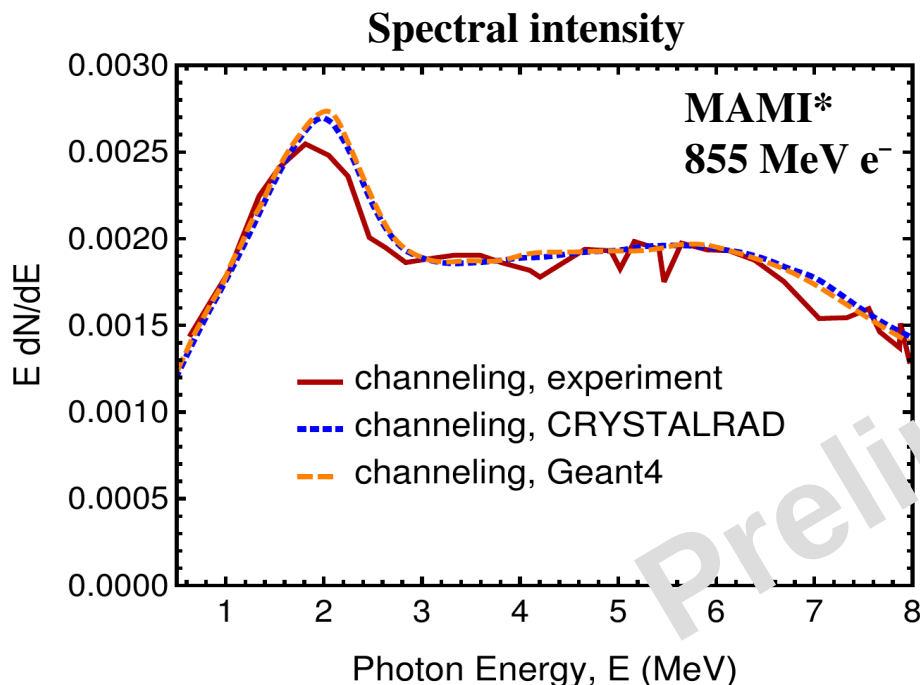
**T. N. Wistisen, ..., and A. Sytov. Phys. Rev. Lett. 119, 024801 (2017)

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

G4BaierKatkov:

- **Physics list independent**
- Activated in the **DetectorConstruction** and used in **ChannelingFastSimModel**
- Can be used **outside channeling model** (e.g. in **SteppingAction**)
- Provides **radiation spectrum** for single-photon radiation mode
- Provides generation of **secondary photons**

Geant simulations vs experiment and CRYSTALRAD simulations



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.);
G4LogicalVolume* crystalLogic = new G4LogicalVolume(crystalSolid,Silicon,"Crystal");
CrystalN1 = 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
    ChannelingFastSimModel* ChannelingModel = new ChannelingFastSimModel("ChannelingModel",RegionCh);
    //set the type of crystal planes
    G4String lattice = "(111)";
    //activate the channeling model
    ChannelingModel->Input(CrystalN1,lattice);
    //setting bending angle of the crystal planes (default is 0)
    BendingAngle = 0.905*mrاد;
    ChannelingModel->GetCrystalData()->SetBendingAngle(BendingAngle);

    //activate radiation model (do it only when you want to take into account
    //radiation production in an oriented crystal; it takes a lot of computational power)
    ChannelingModel->RadiationModelActivate();
}
```

Get crystal region

Channeling FastSim
model declaration

Physical volume

Model activation

Additional options

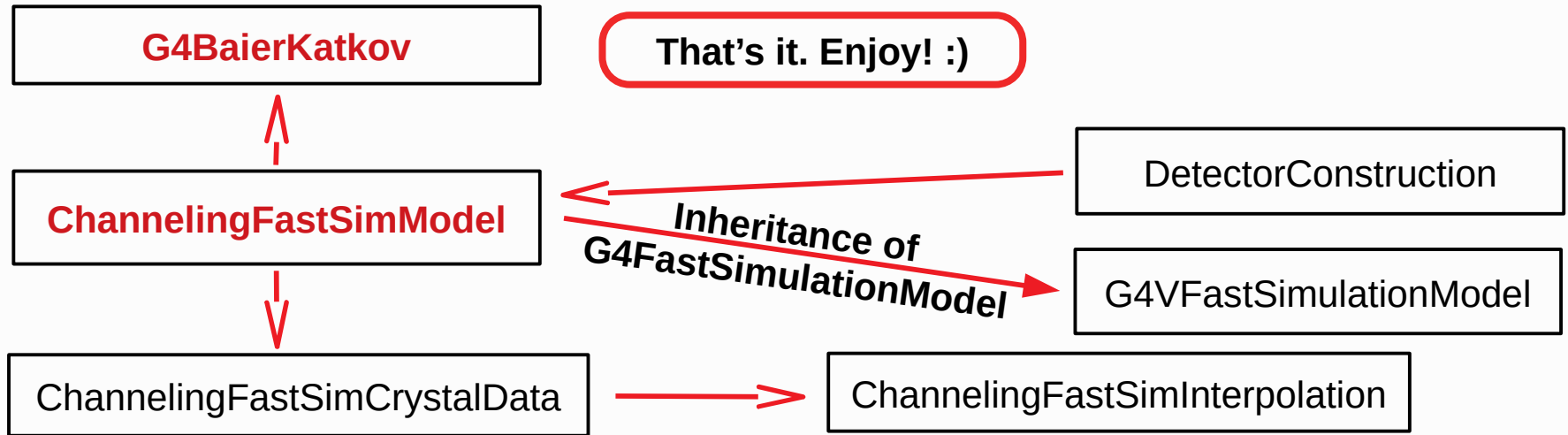
Radiation model
activation

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 );
```

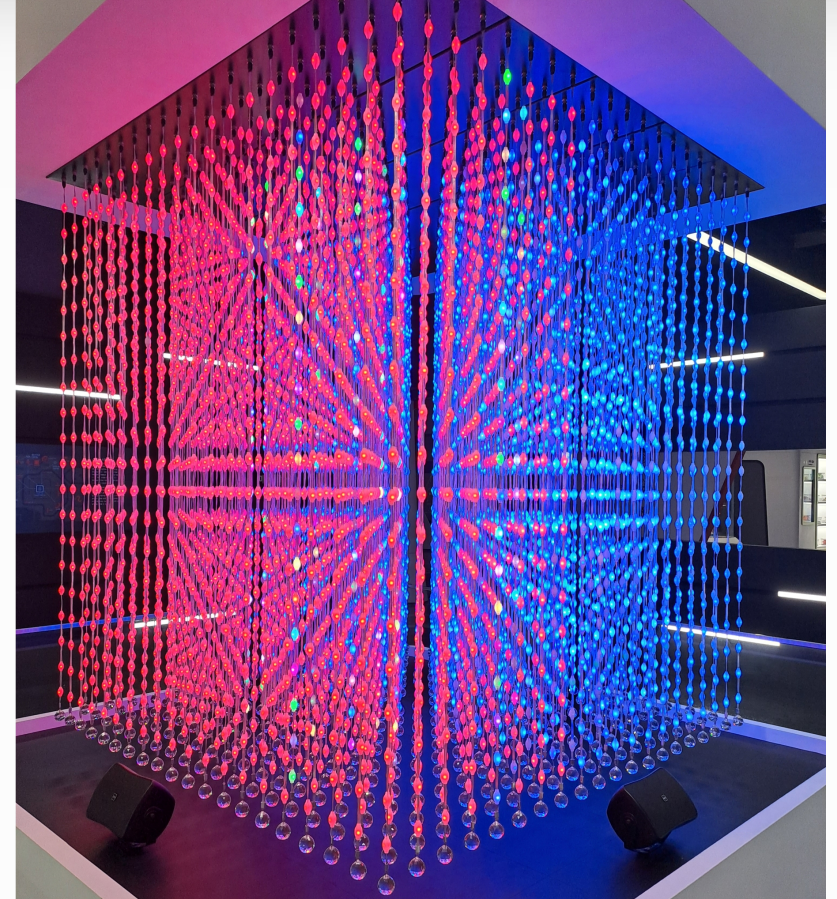
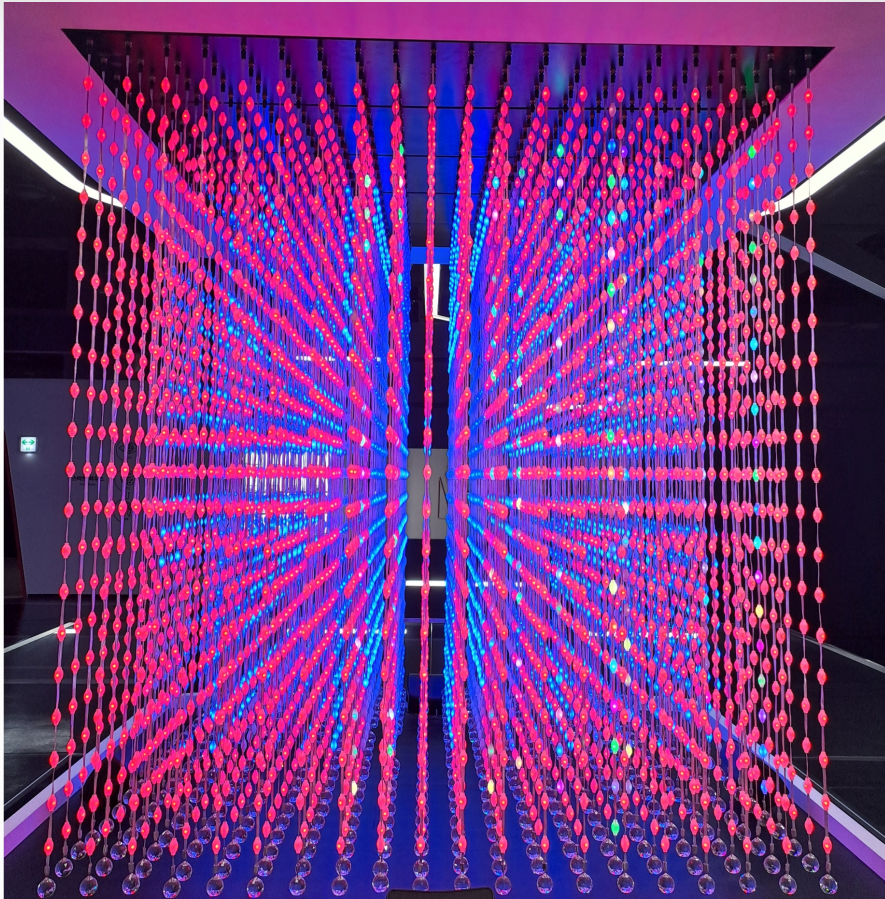


Physics list independent

Conclusions

- The goal is to implement **electromagnetic processes in oriented crystals** into **Geant4** which will bring to a large scientific and industrial community most of possible applications of a crystal.
- The Geant4 examples that will be developed can be **applied** in **nuclear** and **medical physics** (radiation source), at e-/e+ colliders – **ILC**, **FCC-ee** and **muon collider** (positron source) and at all **e-/e+ synchrotrons** existing in the world (crystal-based beam extraction).
- Additional applications are ultrashort crystalline **calorimeter**, exotic particles **MDM** and **EDM measurement**, and **plasma wakefield acceleration**.

Crystal lattice model in the National Science Museum (Daejeon)



Thank you for attention!