On the influence of the PWO crystal structure on the CMS ECAL performance

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Motivation

Crystals are widely used in the high energy physics, e.g. the electromagnetic calorimeter ECAL of Compact Muon Solenoid at LHC is made of PWO crystals.

In spite of this, the influence of the crystal structure on the process of electron, positron and gamma-quanta energy measurement was neither analyzed, nor taken into consideration in the determination of both the measured energy value and resolution.

It was predicted and observed [1-6] that both electron-positron pair production by gamma-quanta and gamma-quanta emission by electrons and positrons are strongly enhanced at the energies exceeding tens of GeV ***in oriented crystals.***

1. V.G. Baryshevsky, V.V. Tikhomirov, Sov. J. Nucl. Phys. **36** (1982) 153; Sov. Phys. JETP **58** (1983) 135.
2. V.V. Tikhomirov, Vestn. Belorussk. Univ. Ser. 1, **3** (1983) 27 [in Russian].
3. V.G. Baryshevsky, V.V. Tikhomirov, Sov. Phys. Uspekhi **32** (1989) 1013.
4. J.C. Kimball, N. Cue, Phys. Rep. **69** (1985) 125.
5. V.N. Baier, V.M. Katkov, V.M. Strakhovenko, Electromagnetic Processes at High Energies in Oriented Single Crystals (World Scientific, Singapore), 1998, 568 p.
6. A.I. Akhiezer, N.F. Shulga, High-Energy Electrodynamics in Matter (Gordon & Breach, New York), 1996, 400 p.

Crystal structure of PWO

The main challenge in supplying CMS ECAL at LHC by the several tens thousands crystal elements was not so much to grow crystals of the right dimensions, but to guarantee a good radial and longitudinal homogeneity within the boules and to ensure a high reproducibility from ingot to ingot.

Quality monitoring was performed by measuring key ***optical and scintillation*** parameters using dedicated automated spectrometer ACCOS developed by INP-Minsk. **PWO crystal structure did not checked during mass production.**

Structural characterization of PWO single crystal by x-ray diffraction showed

scheelite type structure (tetragonal, space group $I4_1/a$, a=5.456, c=12.020 Å).

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Journal of Alloys and Compounds 238 (1996) 46–48

Journal of ALLOYS AND COMPOUNDS

Structural characterization of $PbWO_4$ and related new phase $Pb_7W_8O_{(32-x)}$

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Journal of Alloys and Compounds 284 (1999) 104–107

Journal of ALLOYS AND COMPOUNDS

A new structural model for Pb-deficient $PbWO_4$

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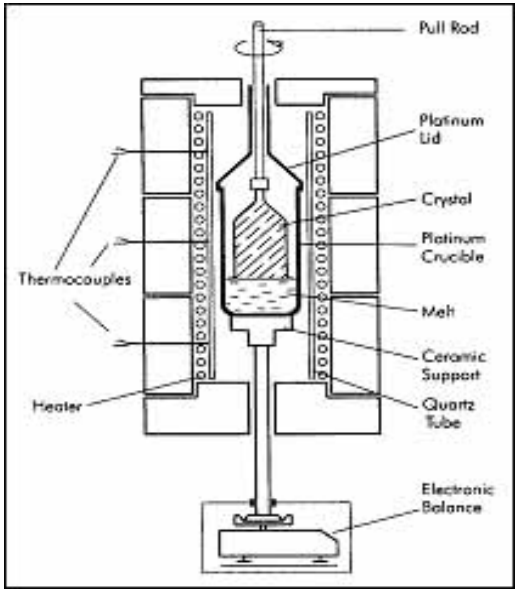
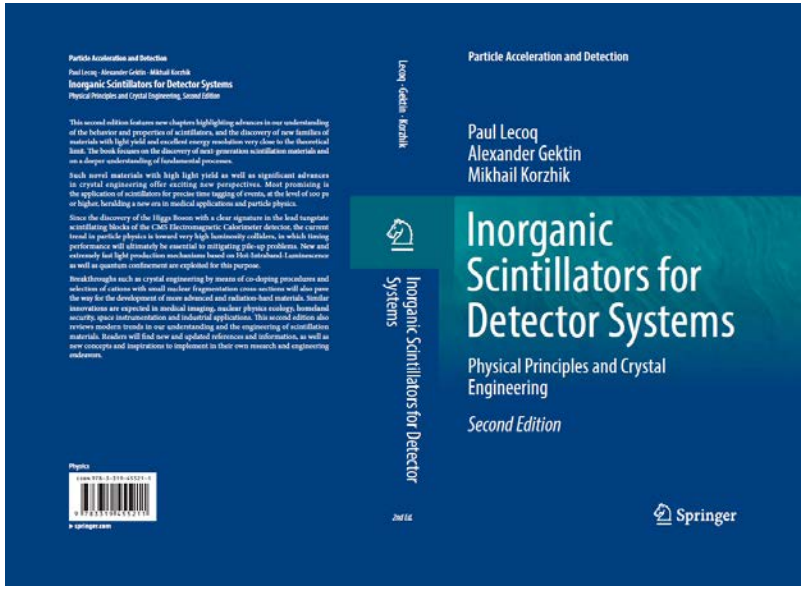
PWO technology and production

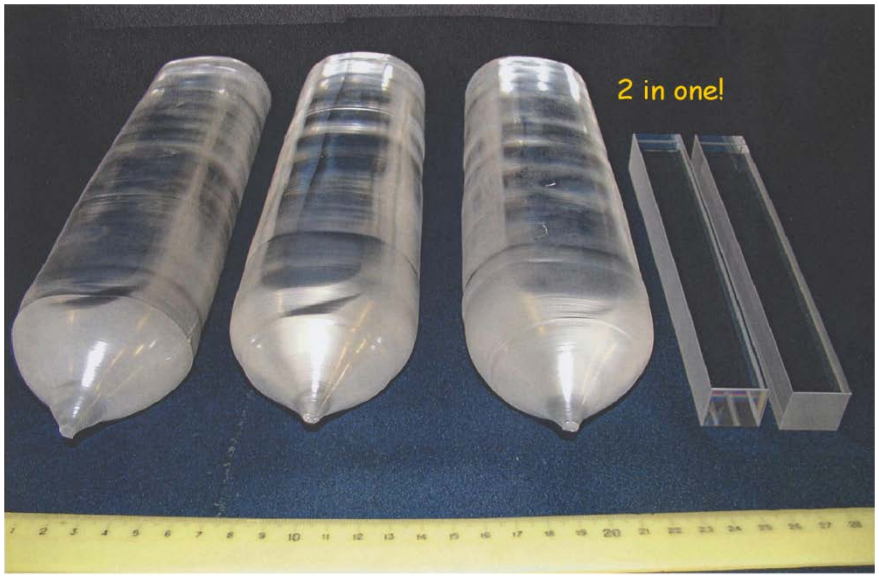


Low gradient Czochralski technique

Crystal growth puller Crystal-3M, 1,165 deg C melt



Book coming soon



PWO crystals in boules and CMS ECAL cells

PWO growth peculiarities

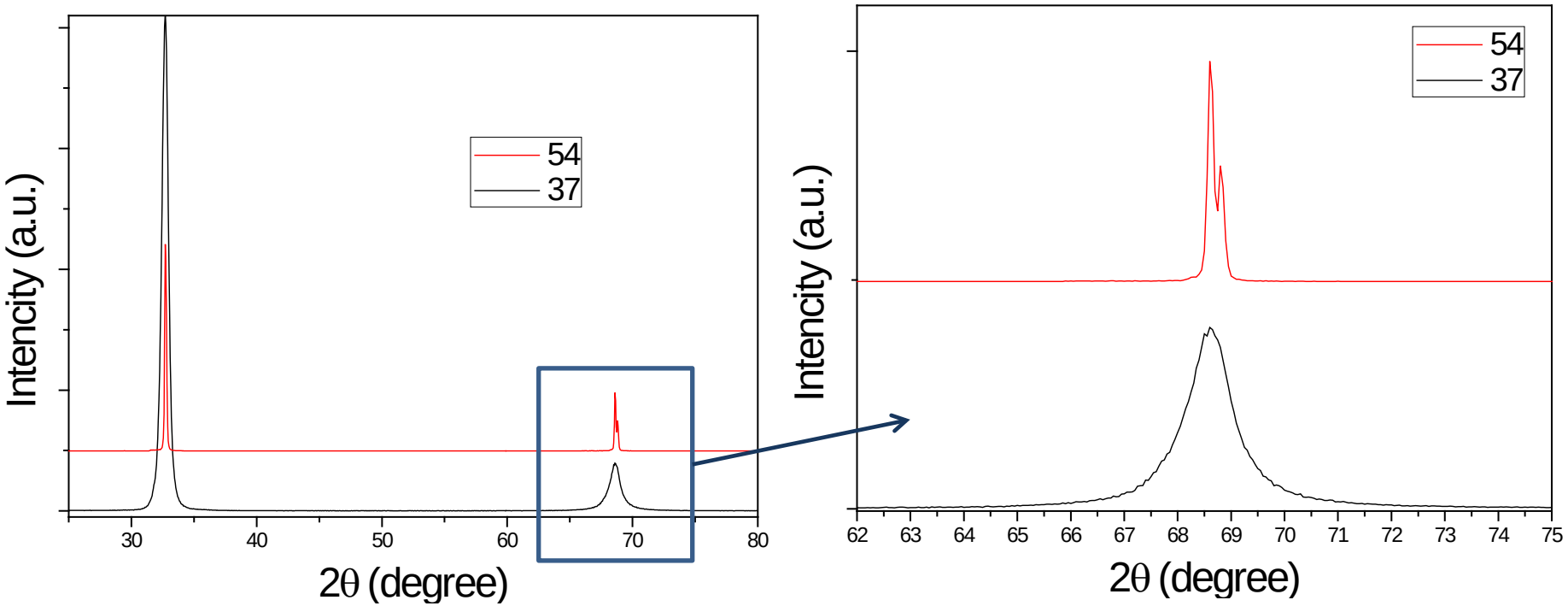
To increase the efficiency of raw material conversion into the crystalline mass, it is necessary to proceed to several sequential crystallizations from one crucible by means of raw material refilling after each growth process.

The possibility to reprocess rejected crystals as well as waste from mechanical processing is also an important aspect of the economy of the production. Such an approach allows to bring the coefficient of raw material effective use up to 85%. **However, the increasing number of crystallization in crystals results in a progressive increase of defect concentration.**

It has been demonstrated that up to 15 successive crystallizations can be made with crystals of 40 mm diameter with a good reproducibility of their optical parameters if a proper tuning of the stoichiometric composition is made at each refill.

PWO structure at mass production

Two samples (1st and 13th crystallisations) from the PWO mass production batch have been investigated through the parallel X-ray beam diffraction of the λ_{Cu}=0.154179 nm line on the Ultima IV diffractometer. Both of them clearly demonstrate the **presence of the crystalline structure**; however the quality of them differs.



Theoretical approaches

Strong Field Quantum Electrodynamics effects can be observed *in crystals* at accessible energies

V.G. Baryshevsky Channeling, radiation and reactions in crystals at high energies. 1982. (in Russian)

V.G. Baryshevsky, V.V. Tikhomirov // Phys. Lett. A90 (1982) 153 *and* A96 (1983) 215

Creation of transversely polarized high-energy electrons and positrons in crystals

V. B. Baryshevskiĭ and V. V. Tikhomirov

Belorussian State University

(Submitted 21 October 1982)
Zh. Eksp. Teor. Fiz. **85**, 232–242 (July 1983)

Synchrotron-type radiation processes in crystals and polarization phenomena accompanying them

V. G. Baryshevskiĭ and V. V. Tikhomirov

Institute of Nuclear Problems, V. I. Lenin Belorussian State University, Minsk

Usp. Fiz. Nauk **159**, 529–565 (November 1989)

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New Crystal-Assisted Pair-Creation Process

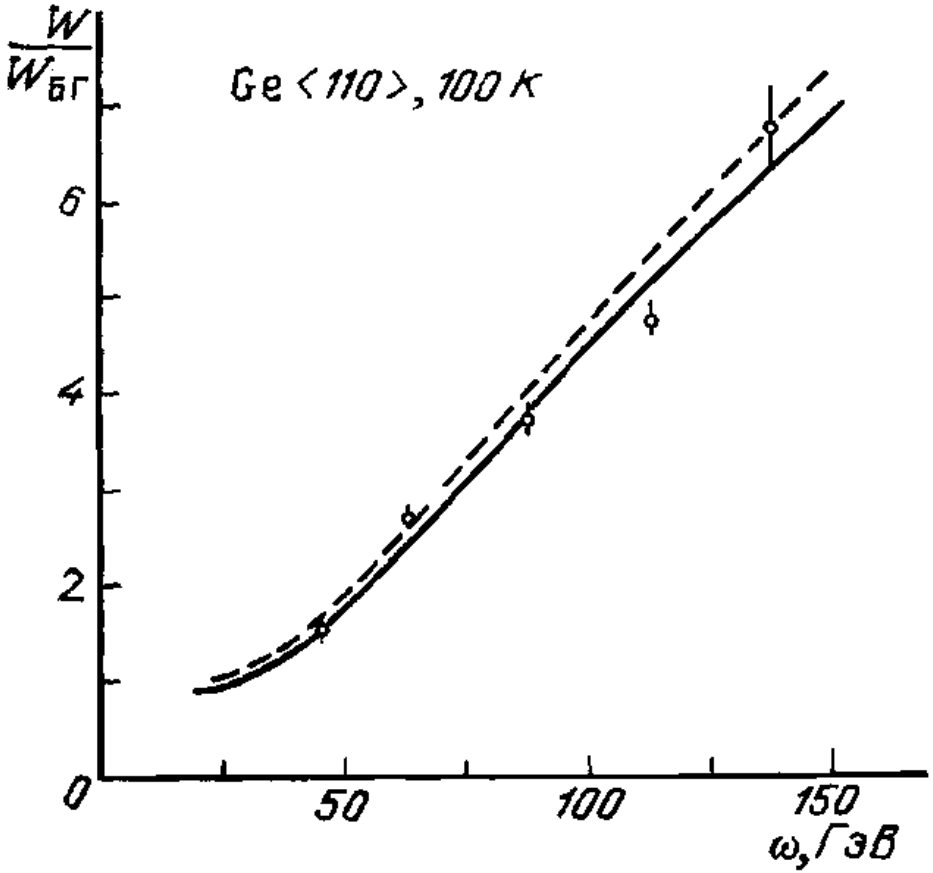
J. C. Kimball, N. Cue, L. M. Roth, and B. B. Marsh
Department of Physics, State University of New York at Albany, Albany, New York 12222

(Received 24 January 1983)

Synchrotron-like pair production in crystals

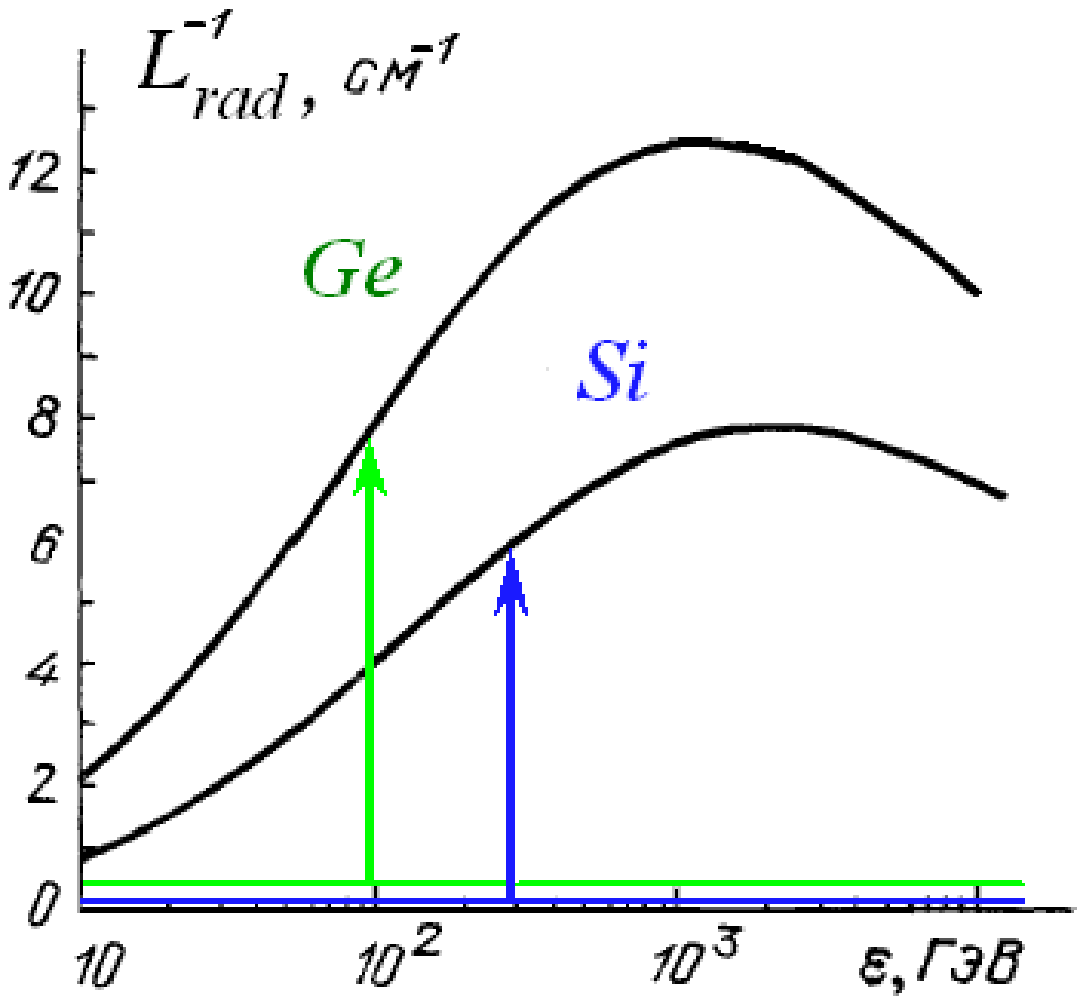
Prediction: *V.G. Baryshevsky, V.V. Tikhomirov* // Phys. Lett. A90 (1982) 153, A96 (1983) 215

Observation: *Bak J. F. et al.* // Phys. Lett. 1988. Vol. B202. P. 615.



Pair production probability vs gamma-quantum energy
for <110> Ge 100K axis in Bethe-Heitler PP probability units.

Synchrotron-like radiation processes effectively reduce radiation length up to several times



V.N. Baier, V.M. Katkov, V.M. Strakhovenko. Sov. Phys. Usp. 1989

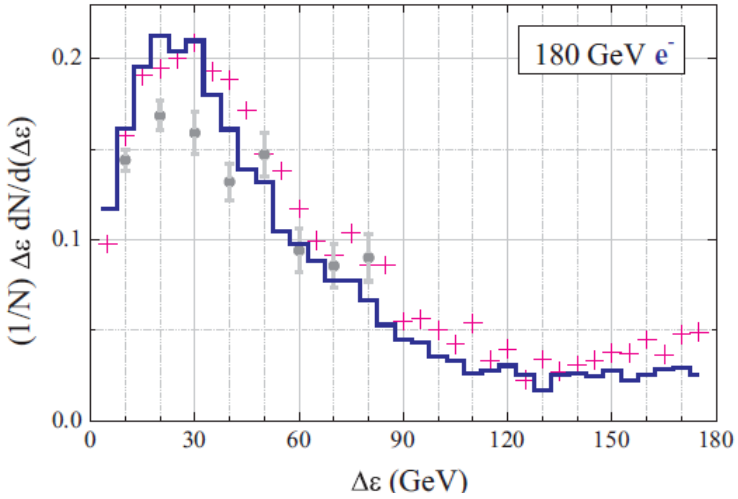
Recent development and verification of ***simulation methods***

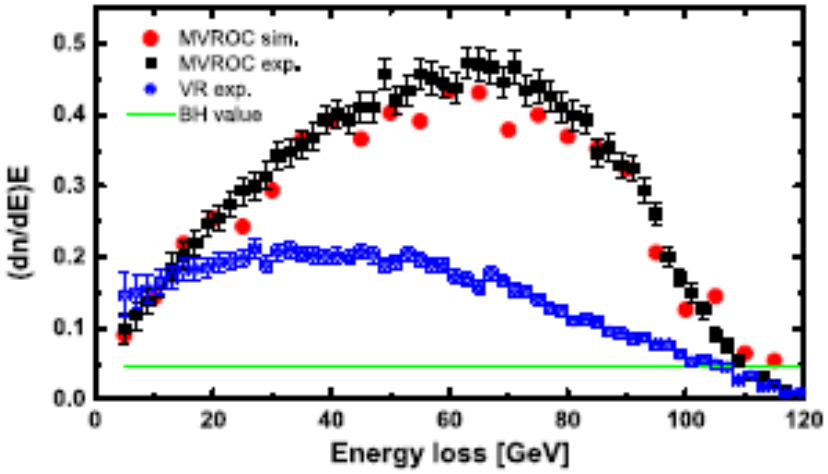
V. Guidi, L. Bandiera, V.V. Tikhomirov, Phys. Rev. A. 86 (2012) 042903

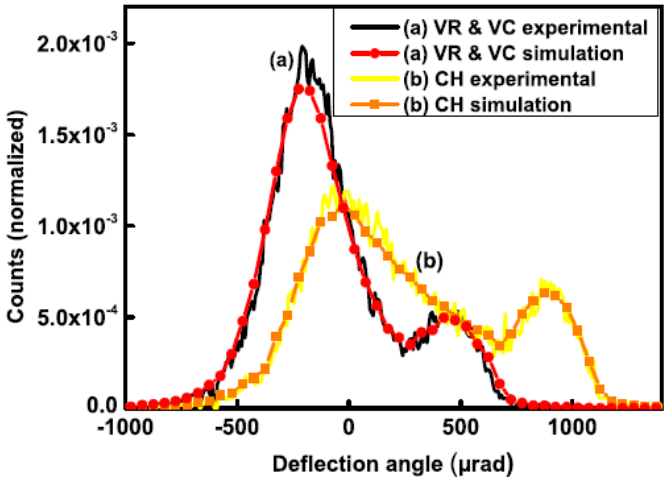
L. Bandiera ... V. Guidi,.. V.V. Tikhomirov , Phys. Rev. Lett. 111 (2013) 255502 .

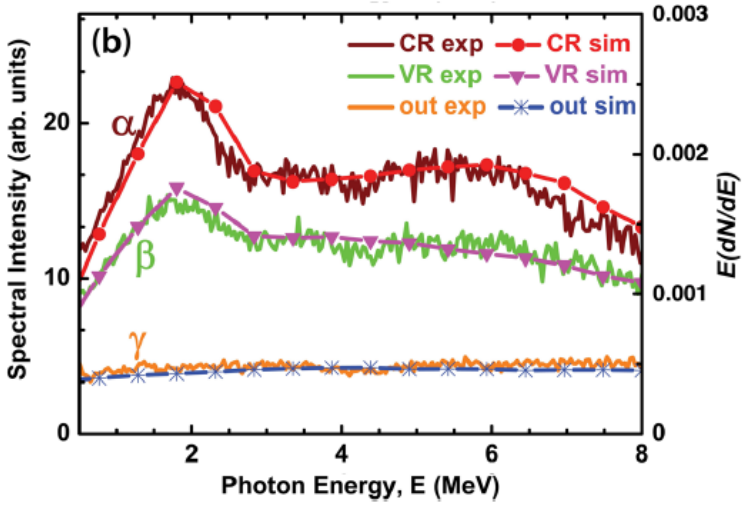
A. Mazzolari ... V. Guidi, ..V.V. Tikhomirov , Phys. Rev. Lett. 112 (2014) 135503.

L. Bandiera ... V. Guidi,.. V.V. Tikhomirov , Phys. Rev. Lett. 115 (2015) 025504.









Methodology

To estimate the PWO crystal structure influence on the energy deposition, the GEANT4 simulation of electromagnetic shower development in a structureless PWO standard sample routinely implemented in GEANT4 was used as a ***benchmark***.

First, the characteristics of both pair production and gamma-quantum emission in the PWO crystal have been evaluated by the method developed earlier for various gamma-quantum and electron (positron) energies.

The obtained pair production probabilities and electron (positron) energy loss lengths, increased due to the influence of the PWO crystal structure, have been introduced into the GEANT4 simulations through the increase of the corresponding values for the **structureless** PWO.

Procedure in more detail

To estimate the maximum possible effect of crystal structure, incident particle momenta were directed along one of <100> or equivalent <010> PWO crystal axes. First, electron (positron) trajectories in the crystal field of oriented PWO were simulated. For that both the particle motion in the averaged potential of the PWO crystal atomic string was evaluated and its incoherent scattering was continuously sampled along the trajectories.

The obtained realistic electron and positron trajectories were used to simulate by the Baier-Katkov method both the radiation intensity and pair production rate. These values, obtained through an integration by final particle states, were divided by the same values for the amorphous PWO, yielding the energy-dependent coefficients of radiation and pair production enhancement in the PWO crystal.

Obtained coefficients were used to multiply the differential probabilities of radiation intensity and pair production probability used by GEANT4 regularly. GEANT4 simulation then was run to reveal the **maximum** crystal structure influence of the electromagnetic shower development in PWO.

GEANT4 modeling for PWO ECAL cell

CMS ECAL facts:

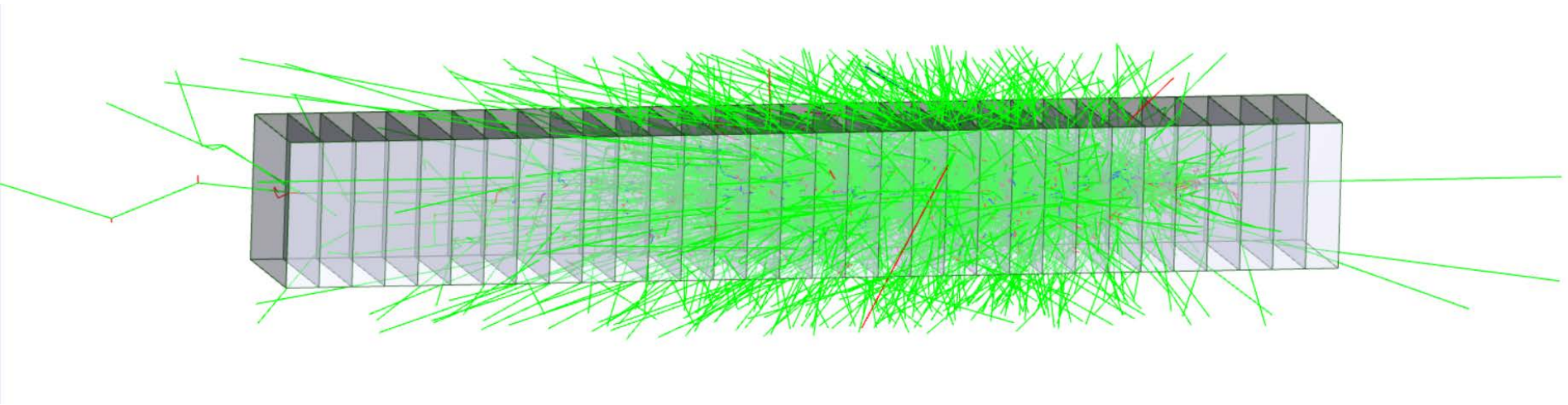
• Crystals shaped as truncated pyramids

• ECAL Barrel section:

- made of 61’200 cells

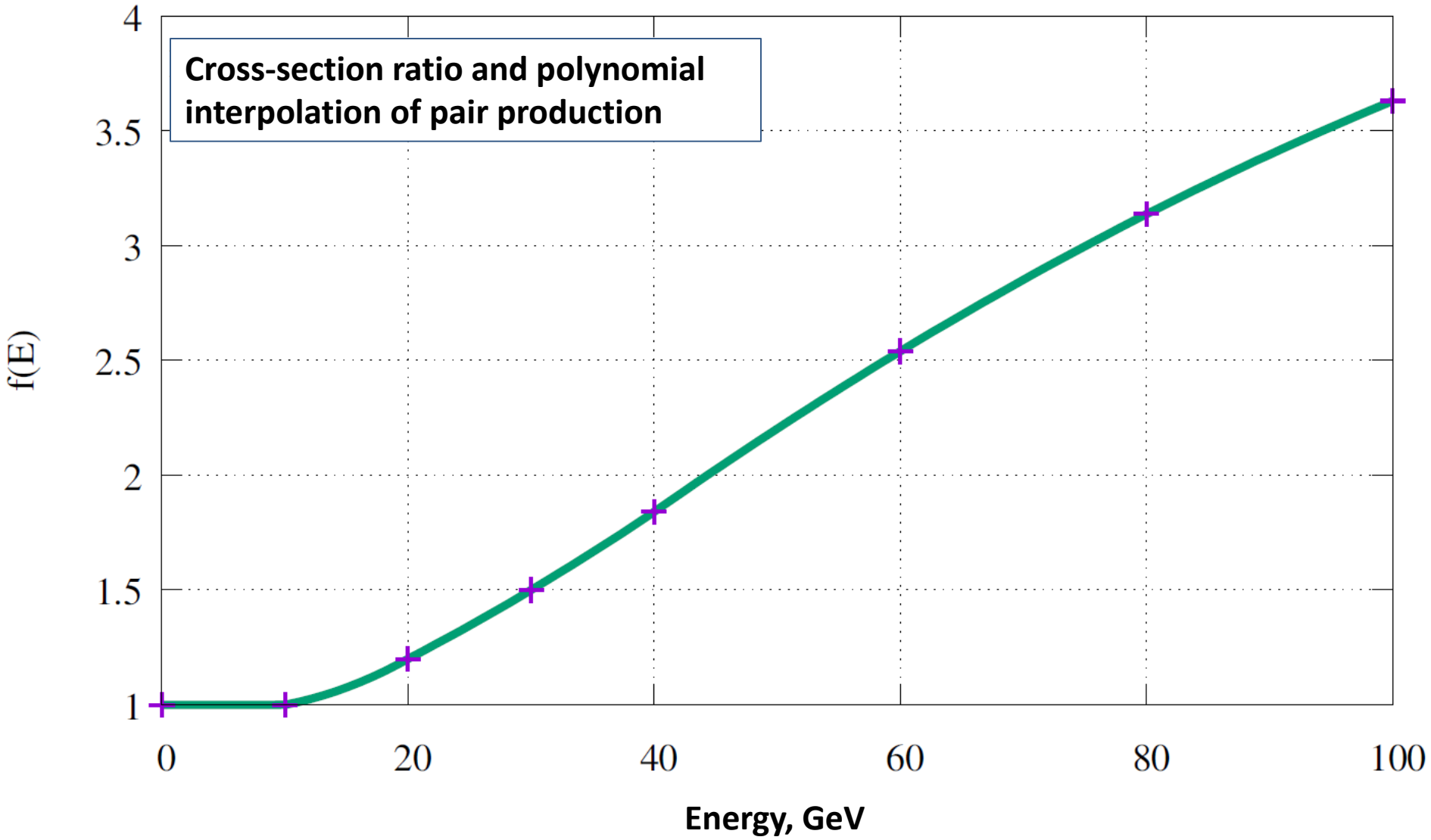
- front face 22x22 mm = 1x1 of Moliere radius

- length 230 mm = 25.8 radiation lengths

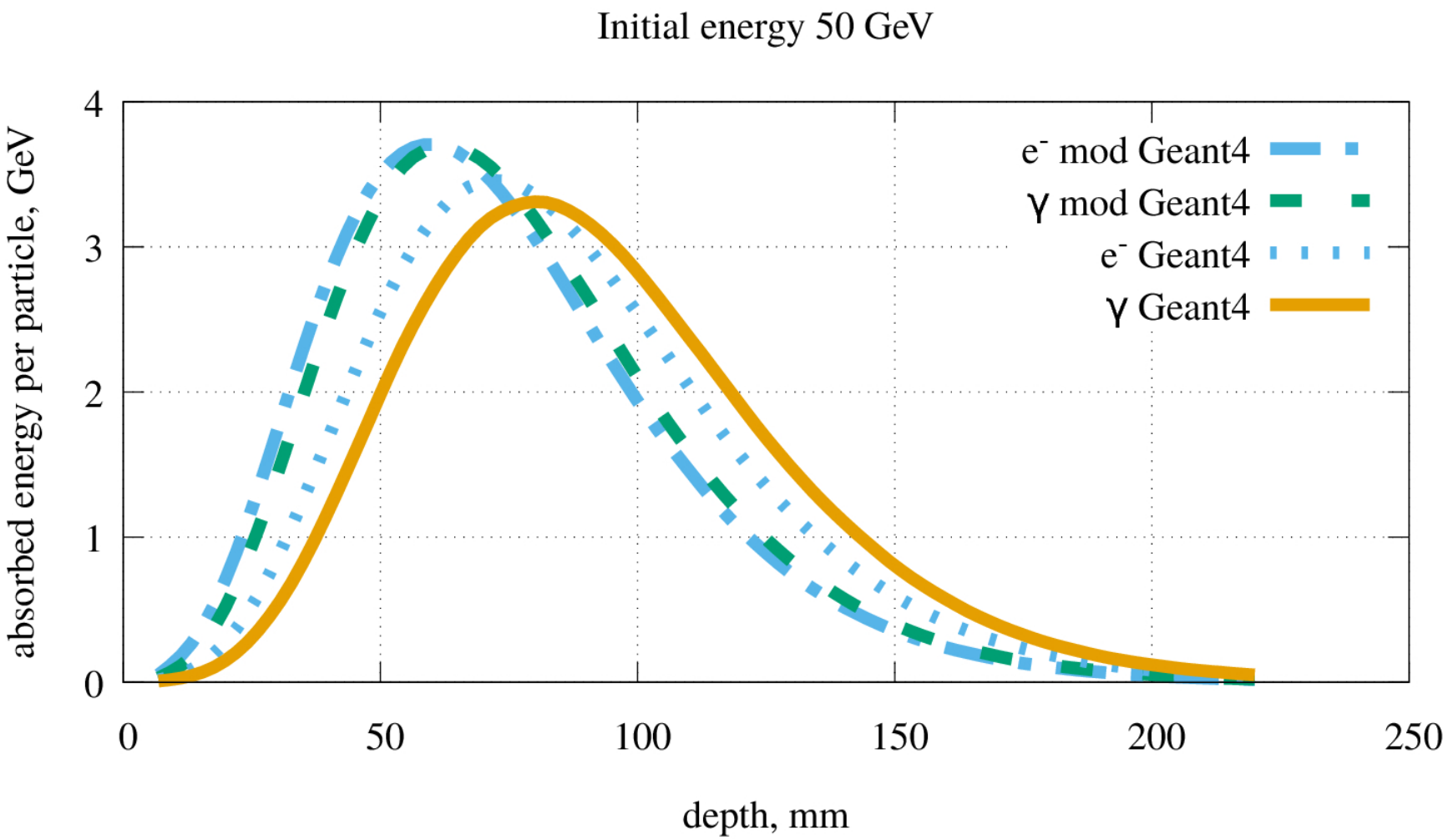


Shower visualization in GEANT4 simulation at single ECAL barrel cell

Example of correction coefficients and interpolation

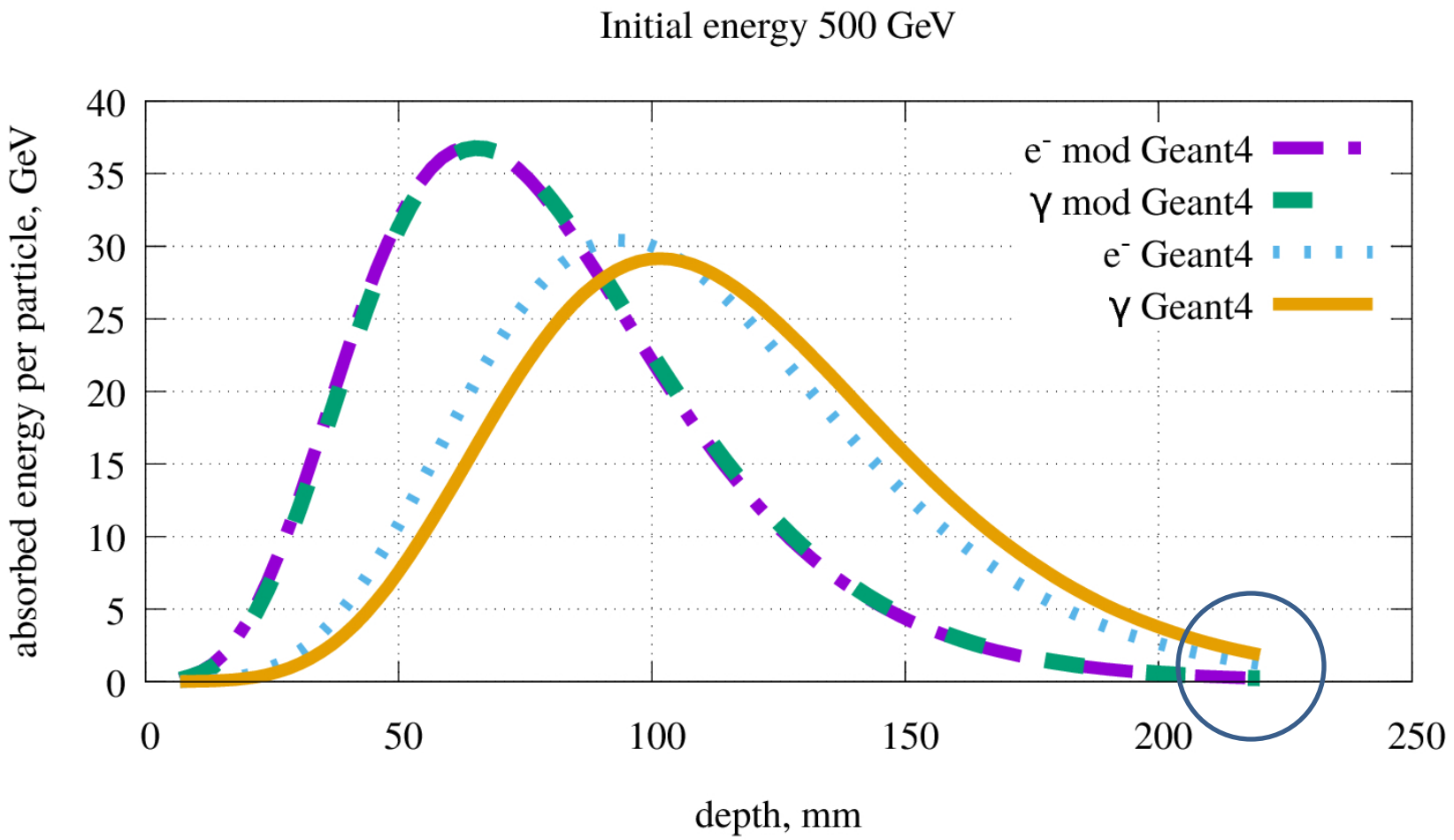


Results with modified GEANT4 functions



PWO radiation length is equal 0.89 cm, its Moliere radius=2.19 cm

Results with modified GEANT4 functions



Shower accelerated to approximately 4-5 radiation lengths, thus reducing rear leakage and constant term in the calorimeter energy resolution

Conclusions

Simulation *tool* and *first results* of simulations of the electromagnetic shower development accelerated by the crystal-assisted processes in the PWO crystals manufactured for the ECAL CMS are reported.

Message

- Obtained results *can be used* to refine the methods of a particle reconstruction by Compact Muon Solenoid at LHC (CERN);
- Obtained results *should be used* when performing detector study for Future Circular Colliders and other similar projects at energy frontier;
- Obtained results *should be used* for development of dedicated patches at relevant particle tracking computer toolkits, like GEANT4 and others.

Thank you for attention