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On the influence of crystal structure on the electromagnetic shower development in the lead tungstate crystals

V.G. Baryshevsky [a], V.V. Haurylavets [a], M.V. Korjik [a], A.S. Lobko [a,*], V.A. Mechinsky [a], A.I. Sytov [a,b,c], V.V. Tikhomirov [a,b], V.V. Uglov [b,d]

[a] Institute for Nuclear Problems, Belarusian State University, Minsk, Belarus
[b] Belarusian State University, Minsk, Belarus
[c] University of Ferrara, Ferrara, Italy
[d] National Research Nuclear University MEPhI, Moscow, Russia

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ABSTRACT

The development of high-energy electromagnetic showers in long oriented lead tungstate crystals, accelerated by the effects induced by the strong field of atomic strings, is simulated for the first time. For that the characteristics of pair production and gamma-radiation by electrons or positrons were first simulated by the direct application of Baier-Katkov formulae in a thin PWO crystal to derive the scaling coefficients of the corresponding Bethe-Heitler cross sections to be incorporated into GEANT4 for the simulation of the electromagnetic shower development in a long crystal. Simulation results demonstrate the significant influence of the crystal structure on the $e^{\pm}$ and gamma-quanta registration processes in the existing homogeneous electromagnetic calorimeters and gamma-telescopes as well as wide possibilities of improving their performance in future developments.

1. Introduction

Many homogeneous electromagnetic calorimeters (e.g. BELLE, BaBar, CMS ECAL, KTeV, PANDA, etc.) and some gamma-telescopes use crystal scintillators for high-energy electron (positron) and gamma-quantum total energy measurements. The structure of scintillator crystals clearly has to influence on the performance of the existing devises as well as can open up the ways to widen the possibilities of the ones which can be built in future. However the experimental study of the electromagnetic shower acceleration in thick crystals at high energies [1–4] was not accompanied by the development of simulation methods which could be used to enlighten the role of scintillator crystal structure. The simulation tools, commonly used in high energy physics, such as GEANT4, FLUKA and EGS4, are also incapable to take into consideration the crystal structure influence of both radiation and pair production. To demonstrate the influence of the latter on the CMS ECAL performance, on the Higgs boson mass measurement in particular, in this paper we simulate for the first time the profile of energy deposition by electromagnetic showers induced by detected $e^{\pm}$, γ in the 23 cm long ECAL lead tungstate (PWO) crystals combining the power of radiation and pair production probability evaluation by Baier-Katkov formulae with that of the extended electromagnetic shower simulation by GEANT4.

2. Strong field effects in crystals at high energies

A possibility of increase of both the intensity of gamma-quantum radiation by electrons (positrons) and the rate of $e^{\pm}$ pair production (PP) by gamma-quanta, induced by the coherent particle interaction with coordinated atoms in crystals, was predicted in 50-th [5–8] and widely explored experimentally [7,9]. However, the Coherent *Bremsstrahlung* theory [5–8] was founded on Born approximation, describing the particles in terms of plane waves, completely neglecting the crystal field influence on particle motion, the channeling effect in particular. As a consequence, the theory [5–8] incorrectly predicted both unphysical growth of the probabilities of radiation and PP with energy and complete suppression of both of the latter at zero angle of particle incidence with respect to crystal planes and axes.

An essential modification of both the energy and orientational dependencies of the coherent processes in crystals at high energies was predicted by the theory [10–12], based on the consistent consideration of particle interaction with the averaged field of atomic planes and strings [10], instead of plane wave approximation used

* Corresponding author.
E-mail address: alexander.lobko@cern.ch (A.S. Lobko).

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in [5–8]. In particular, it was demonstrated in [11] and, later, in [13–15] that, starting from the particle energies from several to tens and hundreds of GeV, depending on the crystal, axis or plane choice, both radiation and PP processes shift to the smallest particle incidence angles, becoming more and more similar to that in the uniform electromagnetic field, justifying the name of synchrotron-type radiation and PP processes [12]. Neither Coherent *Bremsstrahlung* theory [5–8] no simulation method [16] based on the latter are able to describe this essential modification of radiation and PP.

The orientational dependence of the synchrotron-type processes, the probabilities of which reach their maxima at zero incidence angle, is characterizes by the typical angle V_0/m, where V_0 is the axial potential amplitude and m is electron mass, first introduced in [11]. Since $V_0 \sim 0.5$ keV for both Pb and W atomic strings of the PWO crystal, one has $V_0/m \sim 1$ mrad in the latter. Accordingly, the increase of radiation and pair production probabilities has to reach its maximum at sub-milliradian angles of incidence with respect to PWO main crystal axes, preserving considerable value up to the one degree. Since the value V_0/m exceeds much the channeling angle θ_{ch} and since the multiple scattering angle does not reach $V_0/m \sim 1$ mrad at the $e^{\pm}$ energies of about 10 GeV and higher, the evaluation of the PP probability and radiation intensity increase in crystals can be considerably simplified by reducing consideration to the incidence angle region $\psi \sim V_0/m$ of the maximum radiation intensity and pair production rate.

Another salient feature of the synchrotron-type processes in crystals are their saturation, reached after one-two order amplification in the TeV-energy region at the smallest particle incidence angles, as well as the large number of accompanying polarization and spin effects [10–12]. Some of the predicted features of the synchrotron-type processes in crystals have been already observed in the large number of experiments [13–15,17], the most pronounced results of which were the 7–8 time increase of PP probability at zero incidence angle as well as a sudden observation [17] and immediate explanation [18,19] of the radiative cooling effect. The latter proved to be the first demonstration of the radiative energy loss ability to influence the channeling particle dynamics stronger, than the ubiquitous Coulomb multiple scattering process.

The simple formulae of the radiation and PP processes in a uniform field, even after a considerable improvement, can be applied at the smallest incidence angles only. Since the quantum features of particle motion in the averaged crystal field become negligible at such $e^{\pm}$ energies and since the radiated photon energy becomes comparable with that of emitting $e^{\pm}$, Baier-Katkov semi-classical method proves to be quite the most suitable tool for both synchrotron-type radiation and PP process treatment [14]. The latter gives the possibility to evaluate the characteristics of the synchrotron-like radiation and pair production at the large interval $\psi \sim V_0/m$ of incidence angles, at which both these processes are most intensive and practically interesting. A direct numerical integration of Baier-Katkov formulae, which was both practically implemented and compared with experiment in [19–22], will be also the most solid way to provide below the first quantitative predictions for the radiation and PP processes in crystal scintillators which cannot be taken into consideration by Coherent *Bremsstrahlung* theory [5–8,16].

The strongly enhanced coherent processes of radiation and pair production in crystals are inevitably accompanied by the incoherent ones, which closely remind that in the field of isolated atoms and electrons. While the coherent scattering process is well described by the classical relativistic mechanics at the high energies considered, the nature of the incoherent one by individual atomic cores remains quantum at any energy [23]. A joint description of both the particle classical motion in the averaged field and quantum incoherent scattering by Wigner function demonstrates [24] that when the latter is accompanied by the relatively large transverse momentum transfers $\Delta p_{\perp} \gg \hbar/u_1$, it can be described by slightly modified Rutherford (Mott) cross section, applied at the local nuclear density on the particle trajectory. Here u_1 is the root-mean-square amplitude of atom thermal vibrations, p is particle momentum and Δp its transverse component. However, in the opposite case of the smallest transverse momentum transfers $\Delta p_{\perp} \leqslant \hbar/u_1$, the Wigner function of the transverse particle motion attains negative values. Though the latter makes it impossible to interpret the Wigner function in terms of scattering cross section, it allows one to introduce a positive average square of the angle of the multiple small-angle scattering of classically moving particle. Thus, the consistent approach to the incoherent scattering process on each step of a classical particle trajectory has to include the sampling of both the single scattering by the "large" angles $\vartheta \geq \vartheta_2 = \xi\hbar/u_1 p$, where $\xi = 3 \div 5$ is a numerical coefficient, described by the Mott cross section, and the multiple one by the "small" angles $\vartheta < \vartheta_2$, characterized by the squared scattering angle, evaluated with the assistance of the Wigner function. However, at the high above-barrier motion of particles along z direction, constituting sub-milliradian angles with a crystal axis, the latter can be described by its average over the coordinate plane normal to the crystal axis or plane [25]

$$\begin{aligned}\langle d\vartheta_s^2(z)/dz\rangle &= n\int_0^{\vartheta_2}\int_0^{2\pi}\vartheta^2\frac{d\sigma}{d\Omega}[1-\exp(-p^2\vartheta^2u_1^2)]d\varphi\vartheta d\vartheta\\ &= 4\pi\frac{Z^2\alpha^2 n}{\varepsilon^2}\{\ln(1+a)+[1-\exp(-ab)]/(1+a)\\ &\quad +(1+b)\exp(b)[E_1(b+ab)-E_1(b)]\},\end{aligned}$$

where ε is particle energy, n is crystal atomic density and

$$E_1(x)=\int_x^{\infty}e^{-t}dt/t,\quad a=\vartheta_2^2/\vartheta_1^2,\quad b=p^2\vartheta_1^2u_1^2,$$

which preserves the effect of incoherent scattering suppression by collision correlation, introduces into the theory of radiation and PP in [6,26,27].

3. The simulation approach

Structural characterization of PWO single crystal by X-ray diffraction revealed the scheelite-type tetragonal structure with a = 5.456 Å, c = 12.020 Å with an imposed superstructure with a = 7.7208 Å, c = 12.0417 Å, induced by the Pb deficiency in the melt composition [28]. As these results were obtained at the early stage of the PWO investigation with laboratory samples, additional checking measurements were performed during the current effort. Two samples randomly extracted from the PWO mass production batch have been investigated through the diffraction of a parallel X-ray beam of the $\lambda_{Cu} = 0.154179$ nm line on Ultima IV diffractometer. Both of the samples clearly proved the presence of the crystalline structure, demonstrating the intensive (200) and (400) diffraction peaks (which correspond to the crystal lattice parameter a = 5.479 Å), despite the considerable variation of the X-ray reflex width, connected with the technology of the crystal growth at the factory, when a number of consecutive crystallizations are made from the single crucible load. In total, we consider the results of our structural measurements generally consistent with the previous studies.

The first realistic simulations [19] of electron radiation in 185 μm Ge crystal, though being conducted on a supercomputer, yielded quite a modest statistics. Present simulations of radiation in 1–2 mm crystals [20–22] still remain time consuming. This makes it evident that the simulations of electromagnetic shower development in much thicker 23 cm PWO crystals of ECAL CMS is impossible without drastic simplifications. In order both to estimate the possible effect of crystal structure influence on