Reply to Comment on ‘Radiation from multi-GeV electrons and positrons in periodically bent silicon crystal’

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Received 30 April 2018
Accepted for publication 19 June 2018
Published 23 July 2018

Abstract
A reply to the criticism raised in the Comment by Kostyu (Comment on ‘Radiation from multi-GeV electrons and positrons in periodically bent silicon crystal’) is provided.

The Comment [1] on our paper [2] addresses three major issues:

(i) the undulator oscillations of the projectiles in a small-amplitude short-period (SASP) periodically bent crystal (PBC),
(ii) the accuracy of a ‘snap-shot’ model (we use the terminology introduced in [3]) of the projectile scattering in a crystalline medium,
(iii) phase relations of the projectile oscillations and the SASP profile shown in figure 1 of our paper.

A response to these issues is provided below.

(i) The original publication [4] on the SASP PBC contained a conclusion that it is practically impossible to see the undulator oscillations in the simulated trajectories. Though the main concern of our studies [2] was the radiation produced in SASP PBC by multi-GeV electrons and positrons, we found it relevant to also visualize the simulated trajectories for the same bending profile and the same projectile energy 855 MeV as in [4] and to check whether the trajectories display the SASP oscillations. We have indeed revealed that the oscillations are well distinguishable and pointed this out. In the current Comment, the author presents the new results of simulations for the same set of parameters, where the undulator oscillations are also well distinguishable. Thus, there is an agreement between the new simulations and our results on this issue. In terms of physics, we find it concise that the simulations do show the undulator oscillations in the trajectories which are responsible for the radiation spectra produced in SASP PBC.

(ii) The results of our studies [2] were obtained from numerical simulations of the channeling with the MBN Explorer package [5, 6]. The relevant theoretical and computational background has been discussed elsewhere [3] referred in [2]. In MBN Explorer, the trajectories of projectiles are computed by numerical integration of the classical relativistic equation of motion accounting for the interaction of a projectile with all atoms of the crystalline environment simulated in a large dynamically-simulated interaction box. In this respect, the interaction is described on a full-atomic level which is more advanced than other approaches employed by now.

The simulations presented in [4] and in the Comment are obtained employing a ‘snap-shot’ model for the interaction of the projectile with the crystalline constituents. This model, initially introduced in [7], is based on the assumption that due to a high speed the projectile interacts with a crystal atom within a time interval short enough to substitute the atom with its ‘snap-shot’ image: instead of a continuously distributed electron cloud the atomic electrons are treated as point-like charges placed at fixed positions around the nucleus. Next, the model implies that the interaction of an ultra-relativistic
projectile with each atomic constituent, electrons included, can be reduced to the classical Rutherford scattering from a static, infinitely massive point charge. The acts of scattering result in change of the projectile momentum at the instants corresponding to minimal distances between the projectile and the scattering centers, whereas between the scattering events the momentum determines a transnational motion of the projectile. As a result, the projectile trajectory is approximated by a piecewise linear curve the vertices of which correspond to the scattering events.

Though the ’snap-shot’ model is attractive as it saves numerical efforts in simulating the trajectories, it allows for unrealistic hard collisions of the projectiles and electrons at the latter are considered as recoilless charges. Apart from this, there is another conceptual inconsistency of the model. An ultra-relativistic projectile, indeed, ‘sees’ atomic electrons at some fixed positions. However, by no means can they be considered as static charges. In accordance with the fundamentals of quantum mechanics, atomic electrons are subject to the probability distribution in the momentum space and, thus, each atomic electron has a momentum at the instant when a projectile passes nearby. Within the framework of the ’snap-shot’ model one cannot consistently account for the electron momenta in the collision process with the projectile. Hence, intrinsically, the model introduces a non-controllable uncertainty in the scattering angle in each individual scattering event.

We agree that appropriate statistical distribution of many such centers around crystalline atoms properly models the atomic potentials acting on the projectiles, in particular the Moliere potentials [3, 7]. However, in practical simulations, non-zero statistical weight of hard collisions of the projectiles with spatially fixed electrons overestimates the increase of the root-mean square scattering angle with increasing the propagation distance. As a result, the ‘snap-shot’ model over-counts de-channeling events resulting from the hard collisions. This issue was discussed in supplementary material in [3] and in appendix E in [8].

(iii) It is noticed in the Comment that the phases of the short-period oscillations in trajectories presented in figure 1 in [2] are not consistent with the SASP bending profiles shown. In fact, as the figure caption implies, shown are the 12 μm long segments of the trajectories related to different parts of the PBC (where the phases are by all means consistent with the periodicity of the force field). We admit that a more transparent reflecting this in the caption would avoid the question about phase synchronization of the short-period oscillations between the samples in the figure.

To illustrate the consistency in the phases as well as to react to the concern expressed in the Comment on the accuracy of the procedures implemented in MBN Explorer, we provide figure 1 which shows the simulated trajectory of a 855 MeV electron propagating in the SASP periodically bent Si(110) crystal. The amplitude and period of the bending are 0.4 Å and 400 nm, respectively. The cosine profile of the periodically bent (110) plane is shown by the dashed curve. The thick curve represents the projection of the 3D-trajectory on the (yz) plane where z axis is directed along the (110) crystallographic plane (dashed straight line). More details on the trajectories simulation one finds in [9].

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References

[1] Kostyuk A 2018 Comment on ‘Radiation from multi-GeV electrons and positrons in periodically bent silicon crystal’ J. Phys. B 51 168001
[2] Bezchastnov V G, Korol A V and Solov'yov I A 2014 Radiation from Multi-GeV electrons and positrons in periodically bent silicon crystal J. Phys. B 47 195401
[3] Sushko G B, Bezchastnov V G, Solov'yov I A, Korol A V, Greiner W and Solov'yov A V 2013 Simulation of ultra-relativistic electrons and positrons channeling in crystals with MBN explorer J. Comput. Phys. 252 404–18
[4] Kostyuk A 2013 Crystalline undulator with a small amplitude and a short period Phys. Rev. Lett. 110 115503
[5] MBN 2018 http://mbnxexplorer.com/
[6] Solov'yov I A, Korol A V and Solov'yov A V 2017 Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer (Berlin: Springer) p 447
[7] Kostyuk A, Korol A V, Solov’yov A V and Greiner W 2011 Planar channeling of 855 MeV electrons in silicon: Monte Carlo simulations J. Phys. B: At. Mol. Opt. Phys. 44 075208
[8] Korol A V, Solov’yov A V and Greiner W 2014 Channeling and Radiation in Periodically Bent Crystals 2nd edn (Berlin: Springer)
[9] Korol A V, Bezchastnov V G, Sushko G B and Solov’yov A V 2016 Simulation of channeling and radiation of 855 MeV electrons and positrons in a small-amplitude short-period bent crystal Nucl. Instrum. Methods Phys. Res. B 387 41–53