Simulation of orientational coherent effects via Geant4

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Abstract. Simulation of orientational coherent effects via Geant4 beam manipulation of high- and very-high-energy particle beams is a hot topic in accelerator physics. Coherent effects of ultra-relativistic particles in bent crystals allow the steering of particle trajectories thanks to the strong electrical field generated between atomic planes. Recently, a collimation experiment with bent crystals was carried out at the CERN-LHC, paving the way to the usage of such technology in current and future accelerators. Geant4 is a widely used object-oriented tool-kit for the Monte Carlo simulation of the interaction of particles with matter in high-energy physics. Moreover, its areas of application include also nuclear and accelerator physics, as well as studies in medical and space science. We present the first Geant4 extension for the simulation of orientational effects in straight and bent crystals for high energy charged particles. The model allows the manipulation of particle trajectories by means of straight and bent crystals and the scaling of the cross sections of hadronic and electromagnetic processes for channeled particles. Based on such a model, an extension of the Geant4 toolkit has been developed. The code and the model have been validated by comparison with published experimental data regarding the deflection efficiency via channeling and the variation of the rate of inelastic nuclear interactions.

1. Introduction

The interaction of either charged or neutral particles with crystals is an area of science under development. Coherent effects of ultra-relativistic particles in crystals allow the manipulation of particle trajectories thanks to the strong electric field generated between crystal planes and axes [1, 2]. Important examples of the interaction of neutral particles in crystals include production of electron-positron pairs and birefringence of high energy gamma quanta [3]. Radiation emission due to curved trajectories of charged particles in bent crystals has been seen to enhance photon production through bremsstrahlung, channeling radiation, PXR, undulators [4].

Various applications of orientational phenomena with crystals have been proposed and investigated such as

- beam steering [5]
- extraction and collimation in circular accelerators [6]
- splitting and focusing of external beams [7].

Indeed, the reduction of the nuclear interaction rate for channeled positive particles in bent crystals [8] has been proven to lower beam losses throughout the SPS synchrotron [9].
In addition, crystals have been proven to work in the same way for Pb ions [10]. Beam extraction with bent crystals obviates the need for electric current and cooling (especially if a superconductor) and its associated maintenance costs to deflect a particle beam, especially at high energy.

Understanding coherent effects for the interaction of particles with aligned structures have always exploited opportunities furnished by the most advanced computers and computational methods of the current period. In 1963 Oen and Robinson [11] investigated particle behavior in crystal lattices using an IBM 7090 and noticed that particles moving near planes and axes had anomalously long ranges. Their Monte Carlo code was based on a binary collision model and was capable of predicting the experimental results observed in 1963 [12]. The binary collision model allows the determination of the trajectory of a low-energy particle in a crystal with high precision, but it is computationally expensive due to the need to solve the equation of motion of a particle with an integration step smaller than the cell distance between two neighboring atoms, which is typically less than 1 Å.

In 1965 Lindhard [13] showed that the motion of relativistic charged particles under channeling is approximated well by classical physics equations and, as a consequence, also the potential and its related quantities. In particular, Lindhard proposed the idea of approximating the interaction of swift particles with aligned atoms by the interaction with a single string of atoms, i.e. the so-called continuous potential approximation. The same idea holds for interactions with a crystalline plane. By adopting the continuous approximation, the equation of motion can be solved in one dimension for planar channeling with an integration step of up to 1 μm for GeV particles [14, 15, 16, 17], but with a high computational cost for each particle due to the necessity of integrating over the full particle trajectory. As an example of the capability of such a method, in 1987 Vorobiev and Taratin predicted the volume reflection phenomenon in bent crystals [18] which was first observed in 2006 by the H8RD22 collaboration [19].

In the last few years experiments at CERN external beam lines [20, 21, 22] have made available a large amount of high-resolution data thanks to the ability to track trajectories of ultra-relativistic particles with μrad resolution [23]. Such improvements in the experimental knowledge of orientational effects have led to the development of Monte Carlo simulations based on the experimental cross sections of orientational phenomena [24, 25].

In 2013 a model for the simulation of planar channeling of positive particles in bent crystals was proposed [26] for Fluka [27]. The model relies on the continuous potential approximation. Channeling particles follow the bend of the crystal until they either exit the crystal or are dechanneled. Single scattering is treated via a microscopic approach and its effects on transverse energy are cumulative. The number of events caused by nuclear interactions is modified for channeled particles due to the variation of the relevant cross sections.

Nowadays Monte Carlo simulations of the interaction of particles with matter are usually done with toolkits such as Geant4 [28] and Fluka [27]. Such Monte Carlo codes are continuously expanded and improved thanks to the collaborative effort of scientists from around the world. Geant4, an object-oriented toolkit, has seen a large expansion of its user community in recent years. As an example, applications simulated by Geant4 range from particle transportation in the ATLAS detector [29] to calculations of dose distribution curves for a typical proton therapy beam line [30], and from radiation analysis for space instruments [31] to early biological damage induced by ionizing radiation at the DNA scale [32].

In November 2012 a version of Geant4 with the first implementation of a physical process in a crystal was released. In fact, an extension was developed to manage properties of periodic structures in Geant4. The process of phonon propagation within Ge crystals was added to the toolkit [33], but no orientational effects for charged particles were developed at that time. All physical processes implemented in Geant4 require the interaction length of the process to be calculated. Thus, the cross section of the process must be known or computed in order for
the process to be added to the toolkit. In addition, the concurrent presence of many physical processes requires the use of an integration step greater than a \( \mu \)m to limit the computational time. As a result, the full solution of the equation of motion is not suitable. An alternative approach would be to simulate orientational effects using a parametrization of experimental data, but such data (channeling of negative particles in bent crystals, for example) do not currently exist.

In this paper we present a general model for the simulation of orientational effects in straight and bent crystals for high energy charged particles. The model is based on the continuous potential approximation but does not rely on the full integration of particle motion. The model has been implemented in Geant4 version 10.3, and validated against experimental data.

2. Geant4 implementation

The Geant4 toolkit allows new physical processes to be added to the standard ones it already provides. The new process must provide its mean interaction length and how particle properties are affected by the interaction. The model proposed in this paper has been implemented by a class describing the orientational process, and two wrapper classes that modify the material density in existing processes. In addition, classes for the fast calculation of crystal characteristics have been developed to allow the simulation of orientational processes with no need for external software.

Full details on the model can be found in [34].

2.1. Geant4 process for channeling

The ProcessChanneling class used for the implementation of orientational processes inherits from the G4VDiscreteProcess virtual class. The channeling process is valid only in a volume with a crystal lattice. A crystal lattice is present if a XVPhysicalLattice class is attached to the physical volume. The XVPhysicalLattice class collects all the crystal data, such as unit cell and lattice type.

When a particle crosses the boundary between two geometrical volumes, one with and one without a crystal lattice, the channeling process limits the step of the particle and checks if the particle is subject to orientational effects. A uniformly distributed random number is generated to determine the impact position of the particle on the crystal channel, \( x_{in} \), and thus compute the initial potential energy \( U_0 \). The particle momentum is projected on the channeling plane to evaluate the transverse momentum. If the particle satisfies the channeling condition, \( E_{x_{in}} \theta_{in} < U_0 \), the channeling process proposes to the Geant4 kernel an alignment of the particle momentum with the direction of the channeling plane. The condition for channeling is recomputed until the particle exits the volume with the crystal lattice.

2.2. Crystal

The XVPhysicalLattice class was introduced into Geant4 to attach a crystal lattice to a physical volume. This class was extended to collect all the crystal data, such as unit cell and lattice type. Specifically, two classes, XLogicalBase and XUnitCell, were added. The first contains the type and arrangement of the atoms.

The second groups the unit cell information, i.e., the sizes and the angles of the cell, and holds a vector of pointers to as many XLogicalBase objects as needed. In the XVPhysicalLattice class a pointer to an XUnitCell object is stored. The information stored in a XUnitCell object may be used to compute electrical characteristics under the continuous approximation of the channeling processes. Thus, the XVCrystalCharacteristic class was developed.
2.3. Wrappers
At each step in a crystal, the particle momentum can be modified by any of the Geant4 processes. Such modifications vary the transverse energy of a particle and may cause dechanneling, that is, the overcoming of the potential well maximum. The average densities of nuclei and electrons change as a function of the transverse energy of the particle. Thus, these densities should be recomputed at each step and used to modify the cross-section of the physics processes which depend on the traversed quantity of matter.

In order to modify the cross-section of existing processes and to preserve code reusability for future releases of Geant4, wrapper classes for the G4VDDiscreteProcess and G4VEnergyLoss classes were developed. For both these classes, the interaction length of discrete processes is resized proportionally to the modified material density. For the continuous energy loss of the G4VEnergyLoss processes, the traversed length is resized proportionally to the modified average density. For each wrapped process a wrapper object must be instantiated. The wrappers need only the average density to recompute the process cross-section. Thus, in principle, it may work independently of the ProcessChanneling class.

3. Example of application: Si(110) strip
In order to give an insight into the capability of the code to manage crystalline structures at different conditions, we have studied the most adopted crystal for collimation experiments, i.e., a Si strip crystal with (110) bent atomic planes and a thickness of 2 mm.

By considering a proton beam of 400 GeV/c momentum interacting with such a crystal, the channeling efficiency depends mainly on the interplanar potential and the rate of incoherent interaction with nuclei and electrons. The rate of incoherent interaction is determined by the average density of nuclei and electrons seen by the particle under the channeling condition. Thus, it depends on the potential and the density model used for the calculation. In this paper we focus on the dependence of the channeling efficiency from the curvature radius and the thermal vibration amplitude of the atoms in the crystal lattice.

For a bent crystal, the potential well in the co-moving reference frame of the particle is lowered by the contribution of the centrifugal force acting on the particle and the interplanar spacing suitable for channeling is reduced (see Figure 1). Thus, the channeling efficiency is spoiled at \( \sim (1 - R_c/R)^2 \) [35].

The second parameter which affects the channeling efficiency is the temperature of the crystal. Indeed, the higher is the temperature, the wider is the vibration amplitude of the atoms in the lattice. Therefore, also in this case, the potential well is lowered and the interplanar space available for channeling is shortened as shown in Figure 2. The model for the calculation of the potential modifies the shape of the well, causing a different result of the calculation especially for small bending radii, i.e. near the critical bending radius (0.7 m for 400 GeV/c protons [37]. Thus, this important parameter should be carefully considered in order to evaluate the efficiency of a particular strip, e.g., the strip used for the extraction from a circular accelerator because of the need for a high deflection angle.

3.1. Bending radius
Ref. [37] represents a systematic work on the experimental study of the dependence of the channeling efficiency as a function of the bending radius. The 400 GeV/c proton beam of the CERN-SPS H8 external line interacts with a 2 mm long Si (110) crystal bent with different radii. Figure 3 shows the deflection efficiency for channeling vs. radius of curvature [38].

The results from the Geant4 code are in general agreement with the experimental data. However, approaching \( R = R_c \), the discrepancy between experimental data and simulation increases. Such behavior is expected because of the lack of knowledge of the exact density distribution between atomic planes. Indeed, it was shown that the variation of the model for
the calculation of the potential affects mainly the channeling efficiency at small bending radii [37].

3.2. Thermal Vibration Amplitude

The dependence of the channeling efficiency from the thermal vibration amplitude of the atoms in a crystal lattice for a short bent crystal, i.e. for a crystal with length along the beam direction comparable to the nuclear dechanneling length (1.5 mm for 400 GeV/c protons) [39], has not been experimentally investigated yet. Thus, the comparison of the code with the experimental data can not be worked out.

For the simulation, the case of a 400 GeV/c proton beam with a 10.68 µrad divergence interacting with a Si (110) 2 mm long strip with a 13.91 m bending radius is considered. The range of the studied thermal vibration amplitudes lays between the limits ~ 0.5 – 2.0 Å, corresponding to the 0 K and the Thomas-Fermi radius, respectively [40]. The model used for the evaluation of the potential is based on the Moliere potential averaged over thermal vibration amplitude which is part of the Geant4 code. Figure 4 shows the results of the simulation. The spoiling of the deflection efficiency as a function of the thermal vibration amplitude increase is observed. The efficiency is calculated for a fraction of particles which enter with an angle lower than 5 µrad and 10 µrad with respect to the channeling plane orientation. An interesting feature is the different slope of the efficiency variation for the two cases. Indeed, the wider cut on the angular beam divergent seems to be more sensitive to the variation of the potential well. This is expected because the particles that enter at a higher angle have a reduced portion of the potential well which can offer them a good channeling condition. On the contrary, the particles which enter with an angle lower than 5 µrad are captured with a lower transverse energy, resulting in a high efficiency also at larger thermal vibration amplitudes.

4. Conclusions

The dependence of the channeling efficiency as a function of the curvature radius and the thermal vibration amplitude for the Geant4 channeling code is studied. The most adopted Si strip for
channeling experiments in circular accelerators was simulated. The Geant4 code is capable of estimating the variation of the efficiency and to take into consideration the different behavior of the channeling efficiency as a function of the portion of the beam divergence considered.

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References
[1] Tsyganov E 1976 Some aspects of the mechanism of a charge particle penetration through a monocrystal Tech. rep. Fermilab preprint TM-682
[2] Tsyganov E 1976 Estimates of cooling and bending processes for charged particle penetration through a mono crystal Tech. rep. Fermilab preprint TM-684
[3] Okazaki Y, Andreyashkin M, Chouffani K, Endo I, Hamatsu R, Inuma M, Kojima H, Kunashenko Y P, Masuyama M, Ohnishi T, Okuno H, Pivovarov Y L, Takahashi T and Takashima Y 2000 Physics Letters A 271 110 – 114 ISSN 0375-9601 URL http://www.sciencedirect.com/science/article/B6TVM-40MT5SH-W/2/482bc36defc38072423f66458244178d
[4] Ter-Mikaelian M L 1972 High-energy Electromagnetic Processes in Condensed Media (New York: Wiley)
[5] A F Elishev et al 1979 Phys. Lett. B 88 387 – 391 ISSN 0370-2693 URL http://www.sciencedirect.com/science/article/pii/0370269379904921
[6] W Scandale et al 2010 Nucl. Instrum. Methods Phys. Res., Sect. B 268 78 – 82 ISSN 0168-583X URL http://www.sciencedirect.com/science/article/pii/S0168583X1000635X
[7] Robinson M T and Oen O S 1963 Phys. Rev. 132(6) 2385–2398 URL http://link.aps.org/doi/10.1103/PhysRev.132.2385
[8] Lindhard J 1965 Danske Vid. Selsk. Mat. Fys. Medd. 34 14
[9] Smulders P and Boerma D 1987 Nucl. Instrum. Methods Phys. Res., Sect. B 29 471
[15] Taratin A 1998 Physics of Particles and Nuclei 29 437 – 462

[16] Biryukov V M 1995 Phys. Rev. E 51(4) 3522–3528 URL http://link.aps.org/doi/10.1103/PhysRevE.51.3522

[17] E Bagli and V Guidi 2013 Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 309 124 – 129 ISSN 0168-583X URL http://www.sciencedirect.com/science/article/pii/S0168583X1300308X

[18] Taratin A and Vorobiev S 1987 Phys. Lett. A 119 425 – 428 ISSN 0375-9601 URL http://www.sciencedirect.com/science/article/pii/0375960187905871

[19] Yu M Ivanov et al 2006 Phys. Rev. Lett. 97(14) 144801 URL http://link.aps.org/doi/10.1103/PhysRevLett.97.144801

[20] W Scandale et al 2007 Phys. Rev. Lett. 98(15) 154801 URL http://link.aps.org/doi/10.1103/PhysRevLett.98.154801

[21] W Scandale et al 2008 Phys. Rev. Lett. 101(23) 234801 URL http://link.aps.org/doi/10.1103/PhysRevLett.101.234801

[22] E Bagli et al 2013 Phys. Rev. Lett. 110(17) 175502 URL http://link.aps.org/doi/10.1103/PhysRevLett.110.175502

[23] L Celano et al 1996 Nucl. Instrum. Methods Phys. Res., Sect. A 381 124 – 129 ISSN 0168-583X URL http://www.sciencedirect.com/science/article/pii/S0168583X1300308X

[24] Hasan S 2010 Nucl. Instrum. Methods Phys. Res., Sect. A 617 449 – 452 ISSN 0168-9002 11th Pisa Meeting on Advanced Detectors - Proc. of the 11th Pisa Meeting on Advanced Detectors URL http://www.sciencedirect.com/science/article/pii/S0168900209019214

[25] E Bagli et al 2012 Journal of Instrumentation 7 P04002 URL http://stacks.iop.org/1748-0221/7/i=04/a=P04002

[26] Schoofs P, Cerutti F, Ferrari A and Smirnov G 2013 Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 309 115 – 119 ISSN 0168-583X URL http://www.sciencedirect.com/science/article/pii/S0168583X1300284X

[27] Ferrari A, Sala P R, Fassi A and Ranft J 2005 FLUKA: A multi-particle transport code (program version 2005) (Geneva: CERN)

[28] S Agostinelli et al 2003 Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 506 250 – 303 ISSN 0168-9002 URL http://www.sciencedirect.com/science/article/pii/S0168900203013688

[29] M Gallas et al 2005 Astroparticle, Particle and Space Physics, Detectors and Medical Physics Applications, Proceedings of the 9th Conference pp 551–555

[30] GGP Cirrone et al 2009 Nuclear Science Symposium Conference Record (NSS/MIC), 2009 IEEE pp 4186–4189 ISSN 1095-7863

[31] Santin G, Ivanchenko V, Evans H, Nieminen P and Daly E 2005 Nuclear Science, IEEE Transactions on 52 2294–2299 ISSN 0018-9499

[32] S Incerti et al 2010 International Journal of Modeling, Simulation, and Scientific Computing 01 157–178 (Preprint http://www.worldscientific.com doi/pdf/10.1142/S1793962310000122) URL http://www.worldscientific.com doi/abs/a/b/a/S1793962310000122

[33] D Brandt et al 2012 Journal of Low Temperature Physics 167 485–490 ISSN 0022-2291

[34] Bagli E, Asai M, Brandt D, Dotti A, Guidi V and Wright D H 2014 The European Physical Journal C 74 2996 ISSN 1434-6052 URL http://dx.doi.org/10.1140/epjc/s10052-014-2996-y

[35] Biryukov V M, Chesnekov Y A and Kotov V I 1996 Crystal Channeling and Its Applications at High-Energy Accelerators (Springer)

[36] Bagli E, Guidi V and Maisheev V A 2010 Phys. Rev. E 81(2) 026708 URL http://link.aps.org/doi/10.1103/PhysRevE.81.026708

[37] Bagli E, Bandiera L, Guidi V, Mazzolari A, Salvador D, Berra A, Lietti D, Prest M and Vallaza E 2014 The European Physical Journal C 74 1–7 ISSN 1434-6044 URL http://dx.doi.org/10.1140/epjc/s10052-014-2740-7

[38] Bagli, E., Asai, M., Brandt, D., Dotti, A., Guidi, V. and Wright, D. H 2014 Eur. Phys. J. C 74 2996 URL http://dx.doi.org/10.1140/epjc/s10052-014-2996-y

[39] W Scandale et al 2009 Phys. Lett. B 680 129 – 132 ISSN 0370-2693 URL http://www.sciencedirect.com/science/article/pii/S0370269309010089

[40] Gemmell D S 1974 Rev. Mod. Phys. 46(1) 129–227 URL http://link.aps.org/doi/10.1103/RevModPhys.46.129