



INTEGRATION OF ORIENTATIONAL COHERENT EFFECTS OF ORDERED STRUCTURES IN GEANT4

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Motivation

- "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."
- In October 2012 the first Geant4 release with support for crystal structures was released.
- Processes of solid state physics can be implemented to obtain more realistic simulation of current experiments which use crystals in their experimental apparatus.
- Coherent effects can strongly affect physical process of particles in crystals.

Motivation

- Stand-alone software to simulate coherent effects do not allow to consider all the processes already implemented into Geant4.
- Geant4 is continuously updated and physics models have been extensively validated (no need to reinvent the wheel).
- Implementation of coherent effects into Geant4 lead to:
 - evaluation of their influence on current simulation made with Geant4
 - addition of the Geant4 toolkit advantages to the simulation of current and new experiments based on them

Summary

- Orientational effects of charged particles in crystals
- ✓ Geant4 General Introduction
- ✓ Geant4 Channeling in Bent Crystals With Geant4
- ✓ExExCh extended example
- Comparison with published experimental data
- Future perspectives
- √Summary

ORIENTATIONAL EFFECTS OF CHARGED PARTICLES IN CRYSTALS

Particle interaction with aligned crystals



Condition for coherent effects: particle direction of motion nearly aligned with crystal planes or axes.

Crystal

 Ordered pattern of atoms.



Ki-Bum Kim, SPIE Newsroom, DOI: 10.1117/2.1200812.1396

Crystal

- Ordered pattern of atoms.
- Aligned atoms can be seen as planes or axes.



Ki-Bum Kim, SPIE Newsroom, DOI: 10.1117/2.1200812.1396

Charged Particle Interaction



Amorphous



Crystal

- Ordered pattern of atoms.
- Aligned atoms can be seen as planes or axes.
- Strong electromagnetic field between planes and between axes (GeV/cm).



ECHARM - E. Bagli, V. Guidi, V. A. Maisheev, PRE 81, 026708 (2010)

Crystal

- Ordered pattern of atoms.
- Aligned atoms can be seen as planes or axes.
- Strong electromagnetic field between planes and between axes (GeV/cm).
- Particle direction aligned with planes or axes



DYNECHARM++ - E. Bagli, V. Guidi, NIMB 309, 124 (2013)

Interplanar potential

 The aligned atom can be seen as a single axis or plane by a particle moving aligned with them (continuum approximation by Lindhard).





Straight crystal

 Particle whose direction of motion is aligned with crystal planes are captured under channeling.



Straight crystal





Channeling & Dechanneling



Positive vs. negative particles



Positive particles oscillate between atomic planes; negative particles repeatedly cross them.



Dechanneling of positive and negative particles



Channeled negative particles are dechanneled faster than positive ones due to higher probability to suffer nucler incoherent scattering;

Ultra thin bent crystals are required for efficient deflection of negative particles

N.B. L_d decrease with energy, being some tens of microns for 1 GeV p10) electrons in Si [1].

[1] W. Lauth, H. Backe, P. Kunz, A. Rueda, Int. Journal of Modern Physics A, 25, 1 136-143 (2010)

Dechanneling of positive particles



Two mechanisms of dechanneling for positive particles:

Electronic dechanneling

Exponential approximation for the dechanneling processes:

$$N_{ch}(z) \approx N_u e^{-z/L_n} + N_s e^{-z/L_e}$$

For 400 GeV/c proton channeled in the Si (110) at 273 K [1,2]

Nu = 19.5 % Ns = 80.5 %

[1] W. Scandale, et al., Physics Letters B 680, 129 (2009). [2] V. Biryukov, Y. Chesnekov, and V. Kotov, Crystal Channeling and Its Applications at High-Energy Accelerators (Springer, 1996).

Dechanneling of negative particles



Bent crystal

- Channeled particles follows the crystal curvature and are deflected (1.).
- Particle whose trajectories is tangent to crystalline planes are "reflected" by the potential barrier (3.)



Bent crystal





Orientational phenomena in bent crystals



Bent crystal

Varying the crystal orientation with respect to the beam direction orientational effects are observed:

- 1. No effect
- 2. Channeling
- 3. Dechanneling
- 4. Volume reflection
- 5. Volume capture
- 6. No effect



Bent crystal

Varying the crystal orientation with respect to the beam direction orientational effects are observed:

- 1. No effect
- 2. Channeling
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- 6. No effect





W. Scandale et al., PRL 98, 154801 (2007)

Collimation with bent crystals

- Crystal can be used as a primary collimator to deflect particles of the halo toward a secondary collimator.
- Main advantage is the possibility to deflect the beam out and reduce the beam losses.
- a) standard collimation system
- b) crystal collimation system



Beam loss reduction

Measurement of the ratio of the beam loss in the CERN SPS ring with 120 GeV/c protons and Si (110) crystal varying the crystal orientation with respect to beam direction.





LHC crystal-based collimation



2 bent Si crystals were mounted on the LHC on February 2014 to be tested as primary collimators under planar channeling condition

GEANT4

General introduction

The Monte Carlo method

- It is a mathematical approach using a sequence of random numbers to solve a problem
- Particles are tracked one-by-one, step-by-step and, after a reasonable number, the correct information can be extracted



The Monte Carlo method

 MC is the most efficient way of estimate quantity in 3D when compared to first-order deterministic method



Monte Carlo vs deterministic/analytic methods

Complexity of problem (geometry)

Monte Carlo codes

On the market

- MCNP
 - neutrons mainly
- Penelope
 - e- and gamma
- PETRA
 - protons
- EGSnrc
 - e- and gammas
- PHIT
 - protons/ions
- FLUKA
 - any particle

Geant4

- GEometry ANd Tracking
- References
 - Geant4 a simulation toolkit Nucl. Inst. and Methods Phys. Res. A, 506 250-303
 - Geant4 developments and applications
 Transaction on Nuclear
 Science 53, 270-278
 - http://geant4.cern.ch

Geant4

General Info

- Developed by an International Collaboration:
 - Established 1998
 - ~100 members globally
- C++ language
- Open source
- Two releases per year

Advantages

- Because C++ & Open Source:
 - No black box
 - Easily extendable and customizable
- Can handle complex geometries
- Regular development, updates, bug fixes and validation
- Many physics processes and particles already implemented.

User case: LHC @ CERN



- All four big LHC experiments have a Geant4 simulation
 - M of volumes

MS

Physics at the TeV scale

- Benchmark with testbeam data
- Key role for the Higgs searches

User case: Satellites

- Typical telescope:
 - Tracker
 - Calorimeter
 - Anticoincidence





User case: Treatment planning

Therapy beam line



Geant4 Simulation

- Treatment planning for hadrontherapy and proton-therapy systems
 - Goal: deliver dose to the tumor while sparing the healthy tissues
 - Alternative to less-precise (and commercial) TP software
- Medical imaging
- Radiation fields from medical accelerators and devices
User case: Treatment planning

Therapy beam line



Geant4 Simulation



User case: Dark matter

CDMS experiment

- Measurement of the recoil energy imparted to a nucleus due to collisions with WIMPs
- Employment of detectors highly sensitive to the ionization and phonon signals that results from a WIMP-nucleus collision.
- Geant4 simulation of the detector response with phonon and electrons propagation in Ge crystal.

Detectors



GEANT4

Channeling & Volume Reflection in Bent Crystals

Simulations Of Channeling

- Simulations of the orientational phenomena in crystals can be worked out via different methods:
 - By solving the equation of motion, many approaches can be used, depending on the particle kinetic energy.
 - < eV : quantum mechanics</p>
 - > eV & < KeV : molecular dynamics
 - > KeV : binary collisions
 - > MeV : continuous potential
 - "Emulation" method, by using cross-section of the processes available through experimental data and analytical equation
 - Implemented into Geant4 coherent interactions between charged particles and crystals at high-energy (> MeV)

Continuum potential approximation

- Particle impinge on a crystal close to atomic planes or axes.
- Particle "sees" aligned atoms as a unique axis.
- Aligned axes form planes.
- Particle interaction with atoms can be approximated through interaction with atomic planes or axes [1].



J. Lindhard, Danske Vid. Selsk. Mat. Fys. Medd. 34, 14 (1965)

Continuum potential calculation

ECHARM

 Calculation method based on the expansion of the electrical characteristics of crystals in Fourier series.

$$\varphi(\mathbf{r}) = \frac{4\pi e}{\Delta} \sum_{g \neq 0} \sum_{l=1}^{N} Z_l S(Z_l, \mathbf{g}) \frac{[1 - F(Z_l, g)]}{g^2} e^{-i\mathbf{g} \cdot \mathbf{r}}$$

- Electrical characteristics are averaged over planes and axes.
- Different approximation for atomic form factor.
- Approximation for any planes or axes for cubic structure.

E. Bagli, V. Guidi, V. Maisheev, Phys. Rev. E 81, 026708 (2010)

Si (111) Planar Potential



"Emulation"

- Analytical approximations [1,2] and experimental data [3,4] to calculate the cross section of the phenomena.
- Less computational time than integration of the equation of motion.
- Theoretical knowledge of orientational planar phenomena has been largely verified through results to be treated via a macroscopic approach.
- It can be used to simulate known crystal effects, but can not be used to predict strange or new phenomena

[1] V.M. Biryukov, Y.A. Chesnokov and V.I. Kotov, *Crystal channeling and its application at high-energy accelerators*, Springer-Verlag, Berlin Germany (1997).
[2] V.A. Maisheev, *Phys. Rev. ST Accel. Beams* 10 (2007) 084701 [physics/ 0607009].

[3] Y.M. Ivanov et al., *Phys. Rev. Lett.* 97 (2006) 144801.

[4] W. Scandale et al., *Phys. Rev. Lett.* 101 (2008) 234801.

Multistrip for multi volume reflection



Emulation results

Horizontal Deflection Angle [µrad] 0 00-100 0 00-100 0 00-100 10² 10 10 -100 🛉 -400 (a) 5 -500<mark>-600</mark> -400 -200 0 200 400 600 Horizontal Incoming Angle [µrad] Normalized Counts Not aligned 0.06 6 **Multiple Volume Reflection** 0.05 0.04 0.03 0.02 0.01 0 100 200 Horizontal Deflection Angle [µrad] -100 -200 0

Experiment



Emulation

Numerical integration

- Integration of the equation of particle motion through Velocity-Verlet numerical method [1].
- Electric field experienced by particles in the interaction with the oriented crystal is evaluated through continuum potential approximation [2].
- Transverse energy variation due to interaction with electrons and nuclei is taken into consideration through Kitagawa and Ohtsuki approximation [3] applied to multiple scattering approximation [4].
- Possibility to add crystal defects, undulating structures and radiation computation, etc... to the simulation.

[1] L. Verlet, Phys. Rev. 159, 98 (1967); Phys. Rev. 165, 201 (1967)
[2] J. Lindhard, Danske Vid. Selsk. Mat. Fys. Medd. 34, 14 (1965)
[3] M. Kitagawa and Y. H. Ohtsuki, Phys. Rev. B 8, 3117–3123 (1973)
[4] J. Beringer *et al.* (Particle Data Group), Phys. Rev. D86, 010001 (2012)

Geant4 Approach

In order to exploit the Geant4 features a new approach is needed:

- Integration of the equation of motion is computational too expensive because step has to be smaller than oscillation period (~60 µm for 400 GeV/c protons channeling in (110) Si).
- "Emulation" approach requires the knowledge of analytic equation and do not allow the estimation of the variation of nuclei density seen by a channeled particle

Geant4 Approach - Steps

- 1. The particle initial transverse energy is computed at the entrance of the crystal. This is the only information stored.
- 2. At each step, which can be limited by the other Geant4 processes, the variation of transverse energy is computed.
- 3. If the particle is still under channeling, the momentum of the particle is aligned with the crystal planes, otherwise the particle leaves the channeling state and the momentum direction varies.
- 4. Under channeling, a modified value of nuclei and electron density is passed to the Geant4 processes via the biasing technique.

Geant4 processes modification

By modifying the trajectory of the particle and the density of the material "seen" by the particle the orientational effects in a crystal affect all the Geant4 physical process.

The trajectories of channeled particles are "forced" to be tangent to crystal curvature.

The density of materials seen by the channeled particles depends on transverse energy of the particles.



Crystal

The crystal object is built adding to the standard Physical Volume the Crystal Structure in which the Unit Cell and the Lattice are defined.



Crystal

The crystal object is built adding to the standard Physical Volume the Crystal Structure in which the Unit Cell and the Lattice are defined.



Geant4 – Channeling only

- The initial transverse energy is evaluated at the crystal entrance.
- If the particle is under channeling and no other Geant4 processes are activated, the particle remains under channeling until the end.



Geant4 – Channeling + Other Processes

 If other Geant4 processes are activated, they modify the transverse energy and can let the particle dechannel, e.g. single scattering on nuclei.



Condition for channeling



Dechanneling & Volume Reflection





- Before the simulation starts, the table of the average density ratio vs. the transverse energy is computed or loaded.
- The path is integrated over one oscillation period.



Straight crystal



Density Ratio



Depending on the transverse energy of the particle, the density "seen" is different

- Nuclei and electron density tables are stored for positive and negative particles.
- This approach can be used for crystal with dimension parallel to the beam much longer than the channeling oscillation period.



Geant4 processes

Discrete processes

The mean free path of the discrete processes is recomputed at each step using the modified density because it is directly proportional to the density (ρ) of the material.

Continuous processes

Material density (ρ) for the calculation of continuous energy loss (dE/dx) is modified at each step (dx=pdz) to enable the reduction or the enhancement of the energy loss due to channeling.



 For negative particles the ratio is always higher than unity. Thus, the particles interact more frequently with nuclei and electrons in a crystal under coherent effects than in an amorphous media with the same average atomic density.



GEANT4

ExExCh extended example

Channeling Example in Geant4



Experimental Setup

- The example simulates the channeling of 400 GeV/c protons in bent Si crystal.
- The example provides the physical model for planar channeling and volume reflection in bent crystals.
- Physical model published in:
 - <u>E. Bagli</u>, M. Asai, D. Brandt, A. Dotti, V. Guidi, D. H. Wright, "A model for the interaction of high-energy particles in straight and bent crystals implemented in Geant4", European Physics Journal C 74, 2996 (2014)

Deflection Angle Distribution



10²

10

1

Deflection Angle Distribution



Temperature Dependence (G4)



COMPARISON WITH PUBLISHED EXPERIMENTAL DATA

Model validation

- Simulation of experiments in which the crystal role is predominant
- Experiment with single-pass beam instead of multi-turn beam to reduce the complexity of the simulation.
- Three measurements selected:
 - Nuclear dechanneling and channeling efficiency for protons
 - Inelastic interaction rates under channeling for protons
 - Dechanneling length for π^{-}

Nuclear dechanneling and channeling efficiency for protons

Physics Letters B 680 (2009) 129-132



Observation of nuclear dechanneling for high-energy protons in crystals

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ARTICLE INFO

ABSTRACT

Article history: Received 10 June 2009 Received in revised form 22 June 2009 Accepted 25 August 2009 Available online 27 August 2009 Editor: M. Doser Channeling in a short bent silicon crystal was investigated at the CERN SPS using 400-GeV/c protons with an angular spread much narrower than the critical channeling angle. Particle dechanneling due to multiple scattering on the atomic nuclei of the crystal was observed and its dechanneling length was measured to be about 1.5 mm. For a crystal with length comparable to such dechanneling length, an efficiency of 83.4% was recorded, which is close to the maximum value expected for a parallel beam and exceeds the previously known limitation of deflection efficiency for long crystals.

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The experiment goal was to measure the nuclear dechanneling length for positive particles.

During the measurement, a record deflection efficiency was observed.

Because the measurement regards the dechanneled particle fraction, the elastic scattering is fundamental.

PACS:

Experimental setup



Nuclear dechanneling length



Channeling efficiency vs. incoming angle



Experimental measurements (a) UA9 collaboration simulations (a) Geant4 Simulations (b)

W. Scandale et al., Phys. Lett. B 680 (2009) 129
Inelastic interaction rates under channeling for protons Nuclear Instruments and Methods in Physics Research B 268 (2010) 2655-2659



Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B





Probability of inelastic nuclear interactions of high-energy protons in a bent crystal

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ABSTRACT

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Keywords: Crystal Channeling Volume reflection Nuclear interactions Probability of inelastic nuclear interactions in a short bent silicon crystal for its orientations optimal for channeling and volume reflection was investigated using 400 GeV/c protons of the CERN SPS. The contribution of nuclear interactions from channeled protons was observed to be about 3–4% of the probability for the amorphous orientation. For the crystal orientation optimal for volume reflection the nuclear interaction probability of protons was a few percents larger than in the amorphous case. It was shown that in the limiting case of a quasi parallel beam realizing for the collider beam halo the inelastic nuclear losses should decrease by more than five times, which is an additional advantage of a crystal as a primary collimator for the LHC collimation system.

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The experiment goal was to measure the nuclear interaction rate of positive particles with a crystal oriented at different angles with respect to channeling position.

Thus, the modification of the average density experienced by a particle becomes fundamental for the simulation of this experiment.

Experimental setup



Interaction rates vs. integration angle



W. Scandale et al., NIMB 268 (2010) 2655

- Beam loss after collimation is directly proportional to the rate of inelastic interaction.
- By using the crystal in channeling mode the inelastic interaction rate is strongly reduced.
- In the experiment:
 - 1. Crystal not in channeling
 - 2. Crystal in channeling
 - 3. No crystal

Nuclear interactions rate variation



Dechanneling length for π-

Physics Letters B 719 (2013) 70-73



Measurement of the dechanneling length for high-energy negative pions

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ABSTRACT

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Keywords: Crystal Channeling Beam manipulation We studied the dechanneling length of 150 GeV/c π^- interacting with a short bent silicon crystal. Dechanneling length measures the rate and the strength of incoherent interactions of channeled particles in a crystal. The mechanism of dechanneling of negatively charged particles has been elucidated through simulation and experiment. It was found that the dechanneling length for negative particles is comparable to the nuclear dechanneling length for positive charges. Indeed, dechanneling of negative particles occurs as a result of incoherent interactions with the nuclei because the trajectories of such particles always intersect atomic planes, explaining the lower channeling efficiency for such particles. Obtained results can be useful for the design of crystals for manipulating high-energy negative particle beams through channeling.

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The experiment goal was to measure the dechanneling length for negative particles.

The comparison with the simulation furnishes information about the capability of the model to treat negative particles.

Experimental setup



Dechanneling of negative particles



FUTURE PERSPECTIVES

Coherent radiation in crystal



Channeling radiation



- Channeled particle oscillate between or on atomic planes.
- The oscillatory motion lead the particle to emit radiation with a defined frequency.
- The incoherent interaction modify the trajectory and lead the particle to generate photon with different energies.

Coherent Bremsstrahlung

- The same happens for particles which traverse the crystal with a small angle to the planes, but not under channeling (over-barrier particles)
- Such particles are repeatedly attracted/ repelled by the planes, generating coherent radiation.



Orientational effect in "deformed" crystals



DYNECHARM++

E. Bagli and V. Guidi, NIMB 309, 124 (2013)

Dislocations



Mirror



W. Scandale et al., Phys. Lett. B 734, 1 (2014

DYNECHARM++

Radiation



L. Bandiera, E. Bagli, V. Guidi, V.V. Tikhomirov, "RADCHARM++", Channeling 2014

Undulator



E. Bagli et al., EPJC, under publication, (2014), http://arxiv.org/abs/1410.0251

Geant4 implementation



Features

- Only transverse energy variation tracked.
- No information on exact position and momentum.
- Longer step (Faster) than full numerical solution of equation of motion.

Geant4 implementation





Geant4 implementation

Possible features

- Maintain current implementation of:
 - Modification of Geant4 process cross-section.
 - Crystal classes.
 - Channeling process & condition.
- Between each step solve exact trajectory.
- Possibility to estimate:
 - Coherent radiation production.
 - Influence of defects.
 - Undulating structures.
 - Mirror effect.
 - ...
- Very slow.



SUMMARY

Geant4 Approach - Advantages

- Positive and negative particles can be treated with same algorithm. Since the potential well is different and the integrated density varies. The approach allows the estimation of different channeling probability for positive and negative particles.
- Modification of the cross section of the other phenomena is accounted thanks to the biasing techniques. Such technique is applicable to all the Geant4 physics list via a specific package (M. Verderi work).
- No limitation on crystal type. Only crystal information needed for the computation of potential and average density.
- Every particle generated in a Geant4 simulation may experience orientational processes. Thus, variation of shower is length for particle interacting with crystal can be simulated.
- No limitation in energy. Observed variation of Bragg peak for channeled particles in Si crystal with Geant4 simulation.

Geant4 Approach - Disadvantages

- Because of lack of information on the trajectory, some phenomena can not be simulated with current version, e.g., mirror effect and radiation production.
- Because of lack of information on the trajectory, outgoing angle is computed via analytical equation depending on particle transverse energy
- The mixed approach is compatible only with Geant4 Single Scattering models and not with Geant4 Multiple Scattering models. Thus, under channeling, the simulation is slower than standard Geant4 simulation.

Geant4 Approach – Future extension

- Simulation of full particle trajectory.
- The current classes can be updated in order to maintain
 - Implementation of crystal structures, which is independent from the channeling process
 - Modification of Geant4 processes cross-section via the biasing technique.
- Main consequences:
 - Terrible slowing down of the computation.
 - Possible to take into account all the orientational phenomena at high-energies.
 - Computation of the coherent radiation spectrum emitted by particles under coherent effects.
 - Modification of particle trajectory due to the presence of lattice variation, e.g., undulating structure, defects, etc...

THANK YOU FOR THE ATTENTION