Improvements of the crystal routine for collimation studies

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Abstract
A routine has been implemented to simulate interactions of protons with bent crystals in the collimation version of SixTrack. This routine is optimized in view of producing high-statistics tracking simulations of collimation cleaning assisted by bent crystals. Fine tuning and comparisons with experimental data of coherent effects which a particle can experience in a bent crystal have been carried out. The data taken with 400 GeV beams at the CERN-SPS North Area in the framework of the UA9 experiment are used to benchmark the routine. Further checks on low probability interactions have been made, leading to significant improvements in the description of interactions with crystals. Comparisons with other simulations tools are used to increase our confidence in the scaling to higher energies.

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IMPROVEMENTS OF THE CRYSTAL ROUTINE FOR COLLIMATION STUDIES

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Abstract

A routine has been implemented to simulate interactions of protons with bent crystals in the collimation version of SixTrack. This routine is optimized in view of producing high-statistics tracking simulations of collimation cleaning assisted by bent crystals. Fine tuning and comparisons with experimental data of coherent effects which a particle can experience in a bent crystal have been carried out. The data taken with 400 GeV at the CERN-SPS North Area in the framework of the UA9 experiment are used to benchmark the routine. Further checks on low probability interactions have been made, leading to significant improvements in the description of interactions with crystals. Comparisons with other simulations tools are used to increase our confidence in the scaling to higher energies.

INTRODUCTION

Various routines to describe the interaction between charged particles and bent crystals have been developed in past years. Different simulation approaches might be adopted: from analytical calculation of the equation of motion of charged particles in the crystalline potential [1], to the implementation of crystal geometry in wide-range simulation tools, such as FLUKA and GEANT4, where their standard Monte Carlo routines are used, but rescaled on the impact parameters and considerations on coherent effects in bent crystals [2, 3]. However, for the CERN Large Hadron Collider (LHC) collimation studies these two approaches would be too demanding in terms of computing time, because of the very high statistics needed and the coupling with other simulation tools required to predict the beam loss pattern expected along the whole accelerator. Thus, a pure Monte Carlo approach was adopted for the crystal routine implemented in SixTrack [4, 5], which is the main tool used at CERN by the Collimation Team for these studies.

The crystal routine implemented in SixTrack was developed as a stand-alone routine, and tuned to reproduce the experimental data taken on the extraction line of the CERN Super Proton Synchrotron (SPS), with protons of 400 GeV in the framework of the UA9 Experiment [6]. It was then inserted in SixTrack keeping its stand-alone feature, and is based on random extraction of the interaction experienced depending by probability distributions rescaled with respect to the impact parameters [7]. The routine is mainly composed of a part that treats the coherent interactions in bent crystals and a scattering subroutine that describes the interactions with amorphous materials. Regarding coherent interactions, the main selection is based on the impinging angle of the protons. If this angle is below the critical channeling angle ($\theta_c$) the possibility to experience either Channeling (CH), Dechanneling (DC), or Volume Reflection$^1$ (VR) are calculated. If the impacting angle is above $\theta_c$, the proton can undergo either VR, Volume Capture (VC), DC after VC, or the crystal is seen as amorphous material (AM). The amorphous interactions subroutine takes into account the possibility to experience: Single Diffractive, Nucleus-Proton elastic, Proton-Proton elastic, Rutherford Scattering$^2$ and Deep Inelastic events. This subroutine is called each time a proton is not undergoing to coherent interactions. The angular deflection given by Multiple Coulomb Scattering and the Ionization energy loss are applied to any impinging protons, depending on its impact parameters.

An overview of the main improvements, benchmark, and energy scaling in this crystal routine is given.

AMORPHOUS INTERACTION

In the LHC the main source of losses that leak out of the collimation system, limiting its cleaning performance, is due to Single Diffractive events, experienced by halo particles when repeatedly intercepted by the collimators. Thus, a good modelization of these events, as well as of all the nuclear point-like interactions, is needed. Particular attention was devoted to the description of energy loss by ionization.

Scattering routine

The crystal routine used a scattering model independent from the one in the SixTrack collimation module. Detailed comparison with experimental data and other scattering routines showed that the initial implementation, well suited for the modelling of coherent interactions, features some simplistic approximations mainly of the topology and energy scaling of Single Diffractive events, and Nuclear Elastic interactions. Thus, a new scattering routine has been implemented, introduced above and based on the models used in SixTrack to describe the interactions of protons with standard collimator jaws [8]. Main gains with respect to the previous treatment are: correlation between kick and energy loss in Single Diffractive events, improved cross sections of nuclear events and relative energy scaling, better parametrization of Nuclear Elastic events, and implementation of Rutherford Scattering.

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$^1$ It is flagged as VR, but involves a model to describe the transition from amorphous to VR.

$^2$ Single Coulomb scattering at big angle.
All the key parameters useful for Collimation studies are now in agreement with data and other simulation tools, i.e. within the experimental resolution and known errors due to different approximations in the codes. The continued effort to improve collimation simulation predictions is also discussed in a companion paper [9].

**Ionization energy loss**

Energy losses are particularly important for the stability of particle trajectory in a synchrotron machine. Thus, special attention was also devoted to energy losses by ionization. A fixed value of $\frac{dE}{dx}$ given by the Bethe-Bloch formula at 400 GeV was used. A new subroutine to calculate the energy losses by ionization for each impinging particle has been implemented. Moreover, because of the ultra-relativistic $\beta\gamma$ regime in which crystals will work in the LHC, the probability of ionization losses in the long tail of the Landau distribution is taken into account as well. However, the energy loss by ionization in the short crystals foreseen for the LHC (4 mm of Silicon for the first implementation, see [10]) is very small compared to energies that play a key role in the particle loss around the ring. At 7 TeV the mean energy loss by ionization is of a few MeV, i.e. it gives a $\delta p/p \sim 10^{-6}$ which is well within the arc acceptance of $\delta p/p < 10^{-2}$. This means that too many passages through the crystal would be needed to lose a proton in the arc due to ionization energy loss, without the occurrence of any nuclear event. This shows that energy loss by ionization has not a crucial role in our studies, however it has been included in the most realistic and efficient way for our simulative purpose.

**COHERENT INTERACTIONS**

The models used to describe all the coherent interactions in bent crystals were probed as well. The main benchmark and improvements are reported in this Section.

**Benchmark and tuning**

One of the key parameters is of course the single pass channeling efficiency measured on the SPS extraction line. Its benchmark is made with respect to experimental results reported in [11]. A pencil beam impacting on a bent crystal was simulated, with key parameters (i.e. angular divergence, length and bending of the beam and the crystal, respectively) set to reproduce the same conditions of the experimental test. Then, the same data analysis is applied. The result is shown in Fig. 1. An agreement within 2% and 5% was found, with respect to our reference code\(^3\) [11] and experimental data, respectively.

The same set of data was used to update the free parameters used to describe the Nuclear Dechanneling length. The agreement with respect to experimental data has been improved significantly. The Nuclear Dechanneling length measured in [11] is of ~ 1.5 mm, while the simulated one was of ~ 0.9 mm. After the fine tuning of such free parameters a value of ~ 1.35 mm is obtained, increasing the agreement with the measured one from ~ 60% up to ~ 90%. A feeling of how this influences the kicks acquired by the impinging protons is given in Fig. 2, where the entries are normalized to the mean of the Channeling peak.

**Nuclear interaction rate**

An important upgrade has been the implementation of nuclear interactions for Channeled particles. In the previous version of the code, particles could experience nuclear interactions only if out of any coherent regime in bent crystals. The need of this improvement became evident when comparing simulation results with respect to experimental data reported in [12]. What was achieved with the previous version of the code and after this implementation is shown in Fig. 3. When protons are considered trapped between crystalline planes, the occurrence of nuclear interactions is now taken into account by using cross sections rescaled by the average nuclear density seen. What reported in Fig. 3

\(^3\) Extensively tested in the UA9 Collaboration, and already established to be predictive.
must be compared with Fig. 6 in [12], and gives a good agreement with respect to our reference code [1], and experimental data. However, two small discrepancies are present between Fig. 3 and what reported in [12], which are related to the nuclear interaction rate for either crystal in amorphous orientation, and big impacting angle\(^4\) with crystal in channeling orientation. Regarding the case of crystal in amorphous orientation, this is due to the theoretical approximation made. The expected probability of having an inelastic interaction is given by \( P = \sigma \cdot \rho \cdot l \), where \( \sigma \), \( \rho \) and \( l \) are the total inelastic cross section, atomic density, and path in the material, respectively. In the crystal routine of SixTrack the total inelastic cross section is calculated from approximation in the Particle Data Group, while using the Glauber's approximation a better agreement is seen. About protons impacting with big angles when the crystal is in channeling orientation, the discrepancy is due to the approximations made for the calculation of the average nuclear density seen by the channeled protons\(^5\), on which the cross sections are rescaled. It is too strong for large oscillating particles, but it does not involve numerical calculation of complex integrals, keeping the routine fast enough for our purpose. However, the expected angular distribution of the impacting halo on crystal used as primary collimator is \(< 1 \mu\text{rad}\). This means that all impinging protons will be very close in angle to each other and almost parallel with respect to the beginning of the bent crystalline planes, and such a situation is well described by the approximation used.

**Energy scaling**

Another key parameter for predictions on the expected performance of crystal-assisted collimation in the LHC, is the scaling with energy of coherent effects in bent crystals. Comparisons with respect the code described in [1] are reported. The single pass Channeling and Volume Reflection efficiency were compared. What achieved in the comparison between the Monte Carlo routine in SixTrack and the analytical one is shown in Fig. 4. An agreement within 2% is found.

**CONCLUSION**

Recent improvements of the crystal routine implemented in the collimation version of SixTrack were described. This simulation setup provides to date the only way to simulate loss maps around the ring of complex machines like the SPS and the LHC, taking into account proton-crystal interactions, complete collimation layouts, aperture models and accurate 6D particle tracking. Recent code development was focused on improving aspects relevant for the LHC case and addressed in particular the single pass channeling efficiency, dechanneling model, and topology, energy loss, rate of nuclear point-like interactions with very low probability, including the scaling with energy of any interaction implemented. The benchmark with available experimental data at energies up to 400 GeV and with state-of-the-art crystal simulation tools for higher energies make us confident that this tool is adequate for predicting crystal collimation performance of the 7 TeV LHC. Accurate modeling of proton crystal interactions is available in a simulation setup that provides high-statistic loss maps simulations.

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\(^4\) i.e. comparable with the critical channeling angle.

\(^5\) The bigger is the impacting angle, the larger is the oscillation between crystalline planes.
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