Simulation of Beam Steering Phenomena in Bent Crystals

Valery M. Biryukov
IHEP Protvino, 142284 Moscow Region, Russia
E-mail: biryukov@mx.ihep.su
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Abstract

The simulation methods for the channeling phenomena in GeV/TeV energy range in ideal or distorted crystal lattices are discussed. Monte Carlo predictions for feed-out and feed-in rates, dislocation dechanneling, and deflection efficiencies of bent crystals are compared to the experimental data. The role of multiple interactions with crystal in circular accelerators ("multipass channeling") for the efficiency boost in the crystal-aided extraction experiments is analysed. Possible future applications of the crystal channeling technique are considered.

1 Introduction

The experiments on charge particle beam steering by means of channeling in bent crystals have greatly progressed in recent years, spanning over two decades in energy [1, 2, 3]. The detailed theory of beam steering is essentially based on Monte Carlo simulations, as tracking of a particle through a bent crystal lattice requires not only a calculation of a particle dynamics in this nonlinear field, but also a generation of random events of scattering on the crystal electrons and nuclei.

To track particles through the curved crystal lattices in simulation we apply the approach with a continuous potential introduced by Lindhard. The continuum-model description is disturbed by scattering which could cause the trapped particle to come to a free state (feed out), and an initially free particle to be trapped (feed in). By every step the probabilities of scattering events on electrons and nuclei are computed depending on their local densities which are functions of coordinates. This ensures correct orientational dependence of all the processes in crystal material.
2 Numerical methods

As the channeled particles move far from the nuclei, the transitions between the random and channeled states are mainly due to electronic scattering. It is these processes which have been studied experimentally in detail. Hence, an adequate theory needs an accurate consideration of electronic scattering\cite{4}.

The energy transfer $T$ in a collision has a distribution function:

$$\frac{d^2N}{dTdz} = \frac{D\rho_e(x) \frac{1}{2\beta^2}}{T^2}.$$ (1)

Here $D=0.3071$ MeV cm$^2$g$^{-1}Z_i^2Z/A$; $\beta=v/c$; the local density $\rho_e(x)$ of electrons is normalized on the amorphous one. Deviations from (1) at $T\approx I$ or $T\approx T_{max}$ are of no concern, due to the nature of dechanneling as explained below. The (round) angular kick from collision is

$$\theta_s = \left(\frac{2m_eT(1-T/T_{max})}{p}\right)^{1/2}.$$ (2)

$T_{max} \approx 2m_e\beta^2\gamma^2$ is the maximal transfer to a single electron. The frequent small kicks produce a diffusion-like angular scattering, with mean square

$$\theta_{rms}^2 = \frac{2m_e}{p^2}\left(\sum_i T_i(1-T_i/T_{max})\right).$$ (3)

Relativistic Diffusion Factor

The diffusion approximation for electronic scattering was used by all the authors (e.g. \cite{5,6}). One assumes that scattering on electrons is diffusion-like, i.e. $\theta_s < \theta_c$ in any collision. Then the angle of particle is changed by small steps, with the rms value from Eq.(\ref{3}). Note that $\theta_{rms}$ depends on the total transferred energy, not on the detail of (\ref{3}). In the MeV range this approximation for heavy ions works well, because even the maximal possible angular kick per collision $\theta_s^{max} = \sqrt{m_eT_{max}/p} \approx 1.4m_e/M$ (M for the particle mass) is $< \theta_c$.

At $\sim 100$ GeV (the range of modern applications of bent crystals), $\theta_c$ is greatly reduced to $\sim 10$ $\mu$rad, so rare catastrophic collisions with $\theta_s > \theta_c$ may happen. The problem for the diffusion approach is that the integration up to $T_{max}$ in the diffusion factor (\ref{3}) is no longer justified. The energy transferred with catastrophic collisions ($\theta_s > \theta_c$) is of no importance for dechanneling, and therefore it should not be included into Eq. (\ref{3}). Although $\theta_{rms}^2$ depends on $T_{max}$ via $ln(T_{max}/I)$, the removal of the energy transfers of catastrophic collisions from Eq.(\ref{3}) reduces the diffusion coefficient by a factor of $\sim 2$. Hence, the diffusion approach may overestimate the rate of feed-out and feed-in by about the same factor. Here is an example. For a 100 GeV proton $T_{max}=10$ GeV. However the transfer $T_c$ causing the angular kick (projection) equal to $\theta_c$, is quite moderate:

$$T_c \approx \frac{p^2\theta_c^2}{m_e} = \frac{2M\gamma}{m_e}E_c.$$ (4)

$T_c= 4$ MeV for a 100 GeV proton in Si. From the energy transferred via single collisions, about one half is due to the scatterings with $\theta_s > \theta_c$. For collisions with
The above algorithm, i.e. consideration of electronic scattering as a series of single scattering events instead of the traditional diffusion approach, is the pronounced feature of the computer code CATCH\cite{4}. Other approaches, such as analytical calculations by Gärtnert K. et al.\cite{7}, can nicely describe the effects dominated by the potential of crystalline lattice, notably the lattice distorted by defects, but the matter of our study – the transitions from channelled to random states and backward in perfect bent crystals as induced by electronic scattering, – can be approached most correctly by Monte Carlo methods.

The predictions of CATCH were testified by the recent experiments, where feeding-out, feeding-in, high-efficiency bending, energy loss spectra, dislocation dechanneling, and crystal extraction from accelerators have been studied\cite{4}.

3 Crystal extraction: multi-pass channeling

In the extraction mode, circulating particles may pass through the crystal many times. Another major point: the first incidence of particles may occur very close to the crystal edge. The scattering of unchanneled beam in crystal, and the accelerator optics become important.

3.1 The SPS Experiments

Before the CERN SPS studies of crystal extraction\cite{1}, theoretical comparisons\cite{8} with extraction experiments\cite{9,10} were restricted by analytical estimates only, which gave the right order of magnitude. The computer simulations considered idealized models only and predicted the extraction efficiencies always in the order of 90–99% while real experiments handled much smaller efficiencies, in the order of 0.01%.

The considered-below theoretical work has been the first comparison between the realistic calculation from the "first principles" (computer simulation) and the experiment. The simulation was performed\cite{11} with parameters matching those of the SPS experiment. Over $10^5$ protons have been tracked both in the crystal and in the accelerator for many subsequent passes and turns until they were lost either at the aperture or in interaction with crystal nuclei. In the simulation two options were considered. The first one assumed near-surface irregularities (a ‘septum width’) of a few µm. With impact parameter below 1 µm, it excluded the possibility of channeling in the first pass through the crystal. The second option assumed perfect crystal surface. Table\cite{11} shows the expected extraction efficiencies for both options from the first simulation run and the measured lower limit of extraction efficiency as presented at the 19-th meeting on "SPS Crystal Extraction"\cite{12} held at CERN.

Though the efficiency comparison, theory to measurements, was not possible at that time, from the analysis one could see that the perfect-surface simulation predicted narrow peaks for the angular scans (30 µrad fwhm) and extracted-beam profiles, which were not observed. The imperfect-surface option was consistent with the experiment: wide (~200 µrad fwhm) angular scan and sophisticated profiles of the
Table 1: SPS crystal extraction efficiencies from the early runs, Monte Carlo and experiment

| Option          | Monte Carlo | Experiment |
|-----------------|-------------|------------|
| Poor surface    | 15%         | lower limit of 2-3% |
| Ideal surface   | 40%         | only known |

extracted beam (dependent on the crystal alignment). The efficiency was then measured in the SPS with that first tested crystal to be 10±1.7%. Detailed simulations have shown that efficiency should be a function of beam vertical coordinate at the crystal, and be from 12 to 18% at peak, with imperfect-surface option.

The simulation studies for a new crystal with “U-shaped” geometry, performed prior to the measurements, predicted just slight increase in efficiency and much narrower angular scan in the option of edge imperfection. Fig. 1 shows one of measured scans in rather good agreement with prediction. Further simulation took more realistic details into model [13], and studied the dependence of crystal efficiency on septum width, Table 2. These simulations have been repeated with the energies of 14 and 270 GeV, where new measurements have been done at the SPS. The results are shown in Table 3 vs measured data.

Table 2: Peak efficiency $F$ vs septum width $t$. The statistical error is 0.6%.

| $t$ ($\mu$m) | 1   | 20  | 50  | 100 | 200 |
|-------------|-----|-----|-----|-----|-----|
| $F$ (%)     | 13.9| 12.4| 12.9| 10.9| 8.2 |

3.2 The Tevatron Experiment

The Tevatron extraction experiment has provided another check of theory at a substantially higher energy of 900 GeV. A detailed report of predictions for this experiment from the Monte Carlo simulations was published [4] two years before the measurements were taken [2].

We have investigated three options: a crystal with ideal surface, one with a septum width (amorphous layer) of $t=1\ \mu$m, and one with $t=50\ \mu$m. The crystal bending
shape and other details were as used later in the experiment. Figure 2 shows that there is little difference between the three options; the peak efficiency is about 35-40%, and the angular scan fwhm is 50-55 µrad. This insensitivity to the crystal surface quality is due to the set-up different from that used in other experiments; as a result, the starting divergence of incident protons at the crystal was not small and hence less sensitive to edge scattering.

The measured peak efficiency was about 30%. This value, together with the measured angular scan, is superimposed in Figure 2 on the theoretical expectation, showing a rather good agreement.

3.3 Crystal optimisation

The length of the Si crystals used in the SPS and Tevatron experiments was about optimal to bend protons with a single pass. The efficiency of the multi-pass extraction is defined by the processes of channeling, scattering, and nuclear interaction in the crystal, which depend essentially on the crystal length \( L \). The length optimisation was a subject of a simulation, with results shown in Fig. 3.
3.4 Protvino crystal extraction experiment

This experiment, started at the end of 1997, aims to test crystals as short as possible in order to gain in the extraction efficiency from an increased number of proton encounters with crystal, as promised by simulations. In the first run of 1998 this experiment established world record of efficiency of crystal extraction, over 40% \[3\]. The silicon crystal was just 5 mm along the beam direction, and only 3 mm long central part was bent to give the 70 GeV protons a deflection of 1.5 mrad. Figs. 4,5 show the extraction efficiency and the angular scan, Monte Carlo vs measurement.

4 Future Applications

To understand further possible applications of the technique it is useful to recall the analytical theory of multipass crystal extraction \[4\]. Few simple assumptions were taken as an input to the theory: any particle always crosses the full crystal length; pass 1 is like through an amorphous matter but any further pass is like through a crystalline matter; that there are no aperture restrictions; particles interact only with the crystal not a holder.

The overall multipass channeling efficiency is then derived to be

\[
F_C = \left( \frac{\pi}{2} \right)^{1/2} \frac{\theta_c x_c}{\sigma_1 d_p} \times \Sigma(L/L_N)
\]

(5)

where

\[
\Sigma(L/L_N) = \sum_{k=1}^{\infty} k^{-1/2} \exp(-kL/L_N) \approx (\pi L_N/L)^{1/2} - 1.5
\]

(6)

may be called a "multiplicity factor" as it just tells how much the single-pass efficiency is amplified in multipasses. A fraction \((1-G)\) of the channeled particles is to be lost along the bent crystal due to scattering processes and centripetal effects. Then the
Figure 3: Extraction efficiency vs crystal length as simulated with imperfect surface. Tevatron (top) and SPS (bottom). Also shown is the measured efficiency at 4 cm.

The multipass extraction efficiency is

\[ F_E = F_C \times G = \left( \frac{\pi}{2} \right)^{1/2} \frac{\theta_{xc}}{\sigma_{d_\rho}} \times \Sigma(L/L_N) \times G \]  

(7)

The theory check against the CERN SPS data [15] shows good agreement (Table 3).

Table 3: Extraction efficiencies (%) from the SPS experiment, theory [17], and detailed simulations.

| \(pv\) (GeV) | SPS  | Theory | Monte Carlo |
|-------------|------|--------|-------------|
| 14          | 0.55±0.30 | 0.30   | 0.35±0.07   |
| 120         | 15.1±1.2 | 13.5   | 13.9±0.6    |
| 270         | 18.6±2.7 | 17.6   | 17.8±0.6    |

From (7) we see that multiplicity factor can be huge if \(L\) is very small or \(L_N\) big.

**MeV extraction.** One opportunity (small \(L\)) is inspired by the recent successful experiment [16] on bending 3-MeV proton beam by means of graded composition \(Si_{1-x}Ge_x/Si\) strained layers. This invention allows to cover the whole spectrum of accelerator energies (from MeV to multi-TeV) by bent crystal channeling technique.
Figure 4: Efficiency of Protvino crystal extraction as a function of the fraction of beam store incident on the crystal; the measurements (crosses) and simulations (open circles).

Figure 5: Angular scan of Protvino crystal extraction: prediction (●) and measurement (○).
Now one can consider extraction from accelerators starting with MeV energies, by crystals as short as from 1 µm. Eqs. (5-6) predict that channeling efficiency over 99% can be achieved in sub-GeV (and up to several GeV) range, thus opening a new world for bent crystals applications. With traditional bent crystals, it was common to think that highest efficiencies are achievable at highest (TeV) energies as multiple scattering angles vanish with energy faster than channeling angle does. It is very interesting now to find that channeling efficiency can be even more boosted at lower energies due to huge multiplicity factors. One can build a very efficient system to extract beams from accelerators with crystals.

**Muon extraction.** The other opportunity (big $L_N$) for huge multiplicity factor is muons which have formally $L_N = \infty$. Theory then says that efficiency of muon channeling should be 100%. Actually the multiplicity factor for muons is limited by muon lifetime (mostly) and muon outscattering of the aperture. With a muon mean lifetime of 1000 turns, the number of encounters with crystal may be big.

At muon machine, the backgrounds "have the potential of killing the concept of the muon collider" [17]. As muons cannot be absorbed, it was proposed to extract 2-TeV muon beam halo with electrostatic septum as a primary element. Positive muons can be easily steered away by bent channeling crystals. Short analysis says that we could steer negative muons also, e.g. by the same bent planes as used for positive particles, Si(110) [18]. In same crystal Si(110), dechanneling length $L_d$ is shortened by factor of $\sim 100$ for negative particles. However, at 2 TeV $L_d$ is huge ($\sim 1$ meter) for positives and modest ($\sim 1$ cm) for negatives. The required deflection angle is only 64 µrad [16] and can be ensured by a Si crystal $\sim 1$ mm long—quite shorter than $L_d$. Again, multiplicity factor greatly favors muons of both sign. One can build a very efficient system to handle halos at muon colliders.

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