

## Computer simulation of dislocation dechanneling in bent crystals at tera-electron-volt energies

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The dislocation dechanneling of protons in the high-GeV and TeV energy ranges in long curved crystals has been investigated by means of computer simulation. The prospects for multi-TeV applications of bent crystals are discussed.

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### I. CLASSIFICATION OF LATTICE DEFECTS

Recent studies [1,2] have made impressive progress in efficient steering of high energy charged-particle beams using bent crystal channeling. The CERN experiments on the crystal-assisted beam extraction from the Super Proton Synchrotron accelerator [3] are of particular interest. These studies have in view the possible application of channeling for beam extraction from a multi-TeV machine [4,5], where an extracted beam would open up very interesting possibilities for beauty quark physics [6].

Beam bending by a bent crystal is due to the trapping of some particles in the potential well  $U(x)$  formed by the field of the bent atomic planes; the particles are then steered between two adjacent atomic planes. The channeling effect persists in a bent crystal until the ratio of the beam momentum  $p$  to the bending radius  $R$  becomes as high as the maximal field gradient ( $\sim 6$  GeV/cm in silicon). The efficiency of charged-beam crystal optics is limited by the dechanneling process. Two kinds of dechanneling are well known at present (see, e.g., Ref. [1]): (a) bending dechanneling, due to the centrifugal force in a bent channel, and (b) "diffusion" dechanneling, due to the multiple scattering of the channeled particle. The latter process is characterized by the dechanneling length  $L_D$ , over which most of the beam ( $1 - 1/e$ ) is dechanneled. In a perfect straight crystal the scattering on the electrons and nuclei leads to the proportionality  $L_D \sim pv$  (logarithmic term is omitted here). At multi-TeV energies the  $L_D$  value in a perfect crystal is several meters, therefore there is no problem with it.

In the real crystal various defects disturb the lattice. It is convenient to classify all defects present in the crystal into a few groups—pointlike defects (interstitial atoms and vacancies), linear (dislocations), two-dimensional (stacking faults), and three-dimensional (amorphous clusters) ones—because of their different influence on the particle channeling. This difference is particularly essential for the energy dependence of dechan-

neling on the lattice defects. The book by Feldman *et al.* [7] provides a readable introduction to this field; below we briefly review dechanneling for each group of defects.

*Pointlike defects.* Scattering of a particle with charge  $Z_i e$  on a single isolated atom (of atomic number  $Z_a$  and mass  $M_a$ ) in a channel, Fig. 1, may cause immediate dechanneling, if the impact is close enough. For such a hard scattering event, with angle  $\theta_s$  greater than critical angle of channeling  $\theta_c$  (maximal angle of the channeled particle with respect to atomic plane), one may apply the unscreened Rutherford scattering cross section

$$\frac{d\sigma}{d\Omega} = \frac{4Z_i^2 Z_a^2 e^4}{p^2 v^2 \theta_s^4} \quad (1)$$

written here for scattering with  $\theta_s \ll 1$ . Integration over  $d\Omega = \theta_s d\theta_s d\phi$  for the projection angle  $\theta_s \cos \phi$  greater than  $\theta_c$  gives the cross section of the planar dechanneling

$$\sigma_D = \frac{2\pi Z_i^2 Z_a^2 e^4}{p^2 v^2 \theta_c^2} \quad (2)$$

which decreases with energy as  $1/pv$  (notice that  $\theta_c^2 = 2E_c/pv$  [8], where  $E_c$  is the potential well depth). The length  $L_D$  of dechanneling, if it is defined mainly by this kind of defect,

$$L_D = \frac{1}{n_D \sigma_D}, \quad (3)$$

depends on the defect volume density  $n_D$ , and grows linearly with energy.

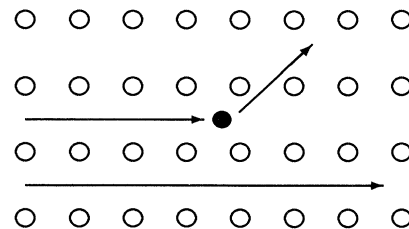


FIG. 1. Scattering of a channeled particle on an interstitial atom.

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Contribution of the multiple Coulomb scattering on the pointlike defects to the diffusion of transverse energy  $E_T$  may be taken into account in the framework of kinetic theory [9]. Assuming the uniform distribution of interstitial atoms across the channel, we take the diffusion factor as  $D = E_T \epsilon^2 Z_i^2 n_a / 2 p v L_R$ ; here  $\epsilon = 14$  MeV,  $L_R$  is the radiation length,  $n_a$  is the volume density of interstitials normalized to its value in amorphous medium. This contribution becomes comparable to the electronic one only at  $n_a \approx 0.01$ . The diffusion-induced  $L_D \approx p v E_c L_R / \epsilon^2 Z_i^2 n_a$  grows as  $p v / Z_i$ , together with Eq. (3).

*Linear defects.* The long defects of the crystal structure (such as dislocation lines, loops, and walls) disturb the long-range order of the crystal lattice. For this reason, the channeled particle could enter the region with a high density of nuclei and be scattered, and/or pass through the region with high local bend. This may lead to a considerable change of the transverse energy or dechanneling. In general, this could result both in bendinglike dechanneling, and in the diffusionlike dechanneling. The former determines some “intrinsic acceptance” defined by a maximal local curvature; the latter means an additional diffusion in the phase space. In terms of the kinetic equations, these are the new boundary condition and the new diffusion coefficient, respectively.

In the neighborhood of linear dislocations the lattice planes are inclined by an angle of order  $b/r$ , where  $r$  is the distance to dislocation and  $b$  is the Burgers vector value [10]. This angle exceeds the critical value  $\theta_c$  at distances of up to  $r_D \approx b/\theta_c$  from the dislocation. The disturbed space is a cylinder of thickness  $\sigma_D \approx r_D$  (“dechanneling cylinder”) coaxial with the dislocation. Taking into account the dislocation density  $n_D$  (total length of dislocations per unit volume, measured in  $\text{cm}^{-2}$ ), we may estimate the probability of a particle to enter the dechanneling cylinder as  $n_D \sigma_D \approx n_D b / \theta_c$  per unit length. The dechanneling length

$$L_D \approx \frac{1}{n_D \sigma_D} \approx \frac{\theta_c}{b n_D} \quad (4)$$

decreases  $\sim 1/\sqrt{p v}$ , as the centrifugal effects become increasingly important with higher energy.

*Two-dimensional defects.* There may be a discontinuity in the positions of the atomic rows and planes (Fig. 2), called a stacking fault. The fault boundary, separating the perfect blocks, is a planar defect. Its area defines the probability for a particle to meet this discontinuity. The

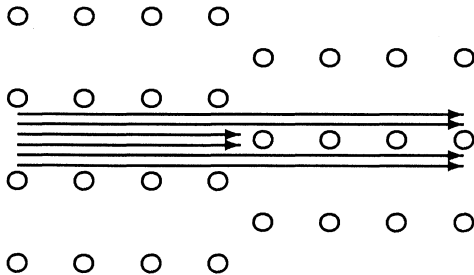


FIG. 2. Stacking fault.

dechanneling probability per crossing this defect is similar to that at the crystal surface,  $\approx (\pi/4)(2x_c/d_p) \approx 0.6$  (“surface transmission”); here  $d_p$  is the interplanar spacing and  $x_c$  is the maximal allowed amplitude of channeled particle. Its value is practically independent of energy.

*Three-dimensional defects.* Volume defects, where the crystal structure is different from that outside (amorphous clusters, twins, etc.), contribute to the dechanneling in the same manner as the interstitial atoms do. This contribution vanishes with energy as  $1/E$ . If the size of the defect is comparable to the period of particle oscillation in channel  $\lambda \approx 2\pi x_c / \theta_c$ , the behavior approaches that of a stacking fault.

We see that of all the various defects present in crystal the dislocations are of most interest, because the contribution of other defects to dechanneling decreases with energy or remains constant. At the present energies (hundreds of GeV) and high perfection of the silicon crystals the defects do not affect the efficiency of beam deflection. There is good agreement between theory for the perfect crystals and the experiments with real silicon crystals at the energies of up to  $\sim 450$  GeV [1,2,11]. Therefore we need to consider only dislocations. Below we analyze the dechanneling theory for defects of dislocation nature, giving emphasis to the multi-TeV energy domain.

## II. DISLOCATIONS

### A. The linear dislocations

Linear edge dislocation may be viewed as the edge of an extra half-plane of atoms in the crystal lattice (Fig. 3). It is characterized by the Burgers vector  $\mathbf{b}$  which is shown in Fig. 3 normal to the surplus (interstitial) half-plane, with the value equal to the interatomic distance (lattice period in the direction of  $\mathbf{b}$ ). The atom displacement in the surrounding lattice, caused by this defect, is equal [10] to

$$u_x = \frac{b}{2\pi} \left( \arctan \frac{y}{x} + \frac{1}{2(1-\nu)} \frac{xy}{r^2} \right), \quad (5)$$

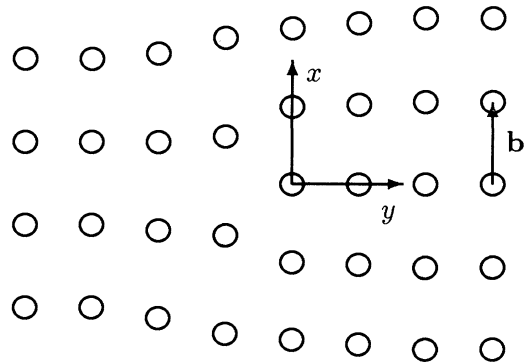


FIG. 3. Linear edge dislocation.

$$u_y = \frac{b}{4\pi(1-\nu)} \left( (1-2\nu) \ln r + \frac{x^2}{r^2} \right), \quad (6)$$

in the reference frame shown in Fig. 3: the  $z$  axis is along the dislocation line  $\xi$ , the  $x$  axis is along the Burgers vector  $\mathbf{b}$ ;  $r^2 = x^2 + y^2$ . Poisson ratio  $\nu$  is 0.42 in Si. In the case of a screw dislocation, the dislocation line  $\xi$  and vector  $\mathbf{b}$  are parallel (let it be  $z$  axis). The only nonzero displacement takes place in the  $z$  direction:

$$u_z = \frac{b}{2\pi} \arctan \frac{y}{x}. \quad (7)$$

Here the stress field is radially symmetric and  $u_z$  does not contain Poisson ratio. The above formulas are discussed in detail in any standard textbook on the theory of elasticity.

The particle motion in the disturbed lattice must be considered taking into account the changed positions of the atoms. The equivalent approach is to go to the reference frame related to the lattice atoms. In this frame, instead of displacements, the centrifugal force appears. This approach is widely used to describe the particle motion in curved crystals. The equation of particle motion becomes

$$pv \frac{d^2x}{dz^2} + U'(x) + pv \frac{\partial^2 u}{\partial z^2} + \frac{pv}{R(z)} = 0. \quad (8)$$

The local curvature  $\partial^2 u / \partial z^2$  in the plane of channeling depends on the mutual orientation of a dislocation  $\xi$ , Burgers vector  $\mathbf{b}$ , and the particle momentum  $\mathbf{p}$ , as well as on the distance  $r$  from the defect. The global curvature (if present) of a crystal slab is represented with  $1/R(z)$ .

The centrifugal force has the order of  $pvb/r^2$ ; it may remove the particle from the channeling mode, if that approaches the dislocation at too small  $r$ . This consideration was performed by Quéré [12]. Assuming that a particle dechannels if (and only if) the maximal local curvature along its path exceeds the critical value  $1/R_c$ , Quéré has derived the following cross section for the planar dechanneling on a straight dislocation line:

$$\sigma_D = K \sqrt{\frac{bpv}{2Z_i Z e^2 N d_p}} = K \sqrt{\frac{\pi}{2} b R_c}. \quad (9)$$

The critical radius is found from the balance of the centrifugal force  $pv/R_c$  and the maximal planar field gradient  $U'(x_c)$ . For  $\sigma_D$  averaged over possible orientation of  $\xi$  and  $\mathbf{p}$ , the constant  $K$  is  $\simeq 0.34$  for a screw dislocation and 0.56 for an edge one. The  $\sigma_D$  is the diameter of a cylinder (coaxial to  $\xi$ ), which is opaque to the channeled particles in Quéré's consideration. For a 1-TeV proton in Si,  $\sigma_D$  is of the order of 10  $\mu\text{m}$ . The probability of dechanneling per unit length is  $\sigma_D n_D$ ; the dechanneling length

$$L_D = \frac{1}{n_D \sigma_D} \quad (10)$$

decreases with energy as  $1/\sqrt{pv}$ .

The  $\sigma_D$  value is about one order of magnitude smaller than the oscillation period  $\lambda$ . This means that a particle does not make even one oscillation in a curved channel. Hence, the Quéré's criterion of the critical curvature is a poor approximation. Instead of considering the static balance of two forces,  $U'(x_c)$  and  $pv/R$ , one should solve Eq. (8) taking into account the flux distribution in the channel.

The approach of Eq. (8) was employed by many authors [13–17]. They followed the particle trajectory and applied the dechanneling criterion,  $x > x_c$ , along the path  $x(z)$  or just at  $z = +\infty$ ; this drops from consideration the nuclear scattering in the dislocation core, respectively overestimating or underestimating it. Several [18,19] computer simulations included the scattering. These investigations confirmed the  $\sigma_D \sim \sqrt{E}$  scaling law predicted by Quéré. This  $\sqrt{E}$  law was also found in the experiments [20,7] with MeV ion beams. As compared to the observations, the Quéré's formula underestimates  $\sigma_D$  for planar channels by a factor of  $\sim 2$  [16] or less [14,7], and overestimates it for axial channels by a factor of  $\sim 4$  [17]. All the theorists [13–18] report good agreement of their calculations with the experiments. There are few measurements of dechanneling in imperfect crystals in the high-GeV range, to be discussed later.

Equation (8) can be solved with the harmonic potential [21]. In the final state ( $z = +\infty$ ) the solution is a harmonic oscillation with the amplitude [14,17]

$$x_f = (x_m^2 + x_d^2 + 2x_m x_d \cos \phi)^{1/2}, \quad (11)$$

where  $x_m$  is the amplitude at  $z = -\infty$ ,  $\phi$  depends on the initial phase and will be averaged later. The  $x_d$  is determined by the dislocation; for  $\mathbf{p} \perp \xi$  it is equal to

$$x_d = \frac{b}{2} e^{-2\pi r/\lambda} \quad (12)$$

for the screw dislocation; and

$$x_d = \frac{b}{2} e^{-2\pi r/\lambda} \left( \frac{1-2\nu}{2(1-\nu)} + \frac{\pi r}{(1-\nu)\lambda} \right), \quad (13)$$

$$x_d = \frac{b}{2} e^{-2\pi r/\lambda} \left( 1 + \frac{\pi r}{(1-\nu)\lambda} \right), \quad (14)$$

for the edge dislocation,  $\mathbf{p} \parallel \mathbf{b}$  and  $\mathbf{p} \perp \mathbf{b}$ , respectively. Equations (12)–(14) show that the influence of dislocation is limited to the distance of  $\approx \lambda/2\pi$ , which grows as  $\sqrt{pv}$ . The difference of transverse energy  $E_T$  of the final and initial states is

$$\delta E_T = \frac{E_c}{x_c^2} (x_d^2 + 2x_m x_d \cos \phi). \quad (15)$$

A particle dechannels if  $\delta E_T \geq E_c - E_T$ . Since  $\phi$  is random, we find the dechanneling probability for a particle with  $E_T$  and impact parameter  $r$  as

$$q(E_T) = \frac{1}{\pi} \arccos \left( \frac{x_c^2 E_c - x_c^2 E_T - x_d^2 E_c}{x_d x_c \sqrt{E_c E_T}} \right) \quad (16)$$

for  $E_T + \sqrt{E_c E_T} x_d / x_c > E_c (1 - x_d^2 / x_c^2)$ , and zero for smaller  $E_T$ . The net probability is  $\int_0^{E_c} q(E_T) f(E_T) dE_T$  for the particle distribution function  $f(E_T)$  (which is roughly flat just at the incidence for divergent beams, but different in the depth of crystal). Finally, the dechanneling cross section is the integral over impact parameters:

$$\sigma_D = \int_0^\infty dr \int_0^{E_c} q(r, E_T) f(E_T) dE_T. \quad (17)$$

Above we considered only interactions with a single dislocation. The particles that were not dechanneled in a single event have experienced some change of  $E_T$  (due to the long range of the displacement field). As a result, the dechanneling may be caused by the multiple interactions with dislocations. A consistent theory should include all the contributions. Here we shall derive an analytical estimate following the diffusion approach. It is applicable only if  $\delta E_T \ll E_c$ . Then we may estimate Eq. (15) as  $\delta E_T \approx 2E_c x_m x_d \cos \phi / x_c^2$ . The diffusion factor is

$$\left\langle \frac{(\delta E_T)^2}{\delta z} \right\rangle = \frac{2E_c E_T n_D}{x_c^2} \int_{r_{\min}}^\infty x_d^2 dr \quad (18)$$

as the diffusion approach is valid starting with  $r_{\min} \approx \lambda / 2\pi$ , according to (12)–(14).

In order to feel the contribution of the soft multiple interactions, we could assume, for the moment, that dechanneling is solely due to them, and then derive a “partial” dechanneling length corresponding to (18) (details to be found in Ref. [9]). For example, in the case of a screw dislocation this length [for (18) averaged over the angle between  $\mathbf{p}$  and  $\xi$ ] equals

$$L_{\text{diff}} \approx \frac{6\pi e^{2\pi r_{\min}/\lambda}}{j_{0,1}^2} \frac{\theta_c d_p}{b^2 n_D} \approx 25 \frac{\theta_c d_p}{b^2 n_D}. \quad (19)$$

The contribution of the soft multiple collisions is, thus, a fraction of that from the single hard scatterings (9), and grows as  $b^2$ . The estimate for the edge dislocation leads to the same conclusion. Although the quantitative predictions should take into account both single and multiple scatterings (in the Monte Carlo approach), we see that both mechanisms provide similar dependence. The results of this analysis may be expressed with a simple formula

$$L_D \approx \frac{\theta_c}{bn_D} \quad (20)$$

which gives the right order of magnitude. The correct quantitative factor (of the order of unit), as well as the dependence on the distortion geometry, should be obtained with a more detailed theory.

The theory was originally developed for MeV energies, and possible changes may be necessary to apply it in the TeV range. Both the distortion size  $\sigma_D$  and the particle oscillation period  $\lambda$  have the same dependence on energy. So there is no change in the character of particle motion. On the other hand, scattering is strongly suppressed. For example, the scattering angle along  $\lambda$  in amorphous sili-

con is one order higher than  $\theta_c$  at 1 MeV, but it is two orders lower than  $\theta_c$  at 1 TeV. Hence, contribution of nuclear scattering in the dislocation core, substantial at 1 MeV, is negligible at 1 TeV. The estimates of the continuum model become even more justified in the  $\sim$ TeV domain. For the applications foreseen at the highest energies,  $\sim 7$  TeV, the crystal purity required is  $n_D \ll \theta_c / bL$ , in order to use the crystals with length  $L$ . This means that a “perfect” crystal should have not more than one linear dislocation per square centimeter. The quality of crystals is steadily improving; dislocation-free examples ( $n_D \leq 1/\text{cm}^2$  [22]) can be produced in principle.

### B. The crystal mosaicity and dislocation loops

Linear dislocations may be not isolated. Because of interactions between them in crystal, they can produce some more complicated structures. One example of such a structure is the crystal mosaicity, which may be the most visual defect of a lattice. The crystal consists of a number of perfect blocks slightly disoriented to each other.

The crystal splitting is due to an arrangement of edge dislocations in a pattern (dislocation wall), separating the crystal into blocks. To produce such a pattern, the dislocations should be mobile; for this reason this defect is more typical for metal crystals than for semiconductors.

For the available Si crystals of high quality and  $\sim$ cm in size, the very low values of  $\theta_m$  (down to  $0.05 \mu\text{rad}$  [23]) were measured. This mosaic spread makes a negligible effect for the channeling even at  $\sim 10$  TeV, where  $\theta_c \simeq 2 \mu\text{rad}$ . Some dechanneling may occur at the dislocation cores in the wall.

The dislocation-loop defect can be imagined as an interstitial (vacant) piece of atomic layer. In other words this is a closed edge dislocation. Their typical size (from  $0.06$ – $0.08$  to  $1$ – $3 \mu\text{m}$  in Si [24]) is essentially smaller than  $\lambda$  in the near-TeV range ( $\sim 0.1$  mm). For this reason, their influence on TeV channeling is rather similar to that of pointlike defects; that is, the small loops cause a lower effect with higher energy [25].

### III. COMPUTER SIMULATION OF DISLOCATION DECHANNELING

In what follows we study the planar dechanneling on the linear dislocations by means of a Monte Carlo simulation. For this purpose we have upgraded the computer code CATCH [26], in order to include Eqs. (5)–(8) into the equations of the particle motion in crystal (we refer to this code version as CATCH 2.0). This code uses Lindhard’s continuous-potential approach to the field of atomic planes, and takes into account the processes of both single and multiple scattering on electrons and nuclei. The particles are tracked through the curved crystal lattices with the steps of a few  $\mu\text{m}$  at near-TeV energy. Further details on the code may be found in [26].

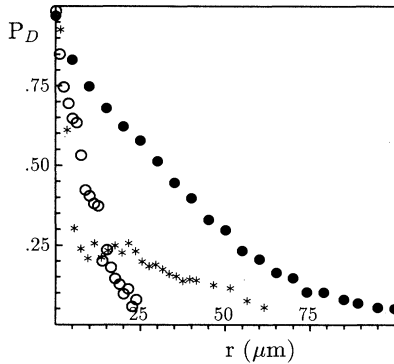


FIG. 4. The probability of dechanneling by a single dislocation as a function of the impact parameter for the edge ( $\bullet$ ) and screw ( $*$ ) type at 7 TeV, and for the edge type at 450 GeV ( $\circ$ ).

We concentrate on the high energy (GeV and TeV) case, which means divergent beams (with respect to  $\theta_c$ ) and the long bent crystals (multiple interactions are involved); in contrast, the MeV case studied in Refs. [12–18] implied a parallel beam and a single interaction.

First we investigate the dechanneling from a single interaction with a linear dislocation. In the simulation the proton beam with the divergence greater than  $\theta_c$  was incident onto the Si (110) crystal. Soon after the incidence the particles meet a single dislocation. In order to distinguish easier between the channeled and random particles in the crystal, and to provide the starting particle distribution typical for the high energy applications, we have applied a slight bending of the crystal with  $pv/R = 0.1$  GeV/cm. The channeled particles with  $E_T < 18$  eV have been selected upstream of the dislocation, and those with  $E_T > 22.8$  eV downstream were considered as dechanneled; 22.8 eV is the depth of the Si(110) Molière potential (the gap 22.8–18 eV was to suppress the contribution from an “ordinary dechanneling” caused by scattering in a perfect crystal). The dechanneling probability obtained in this simulation is plotted in Fig. 4 as a function of the impact parameter (the minimal distance between the particle and dislocation), for the edge and screw dislocations with  $b = 3.84$  Å at 450 GeV and 7 TeV. The probability in Fig. 4 is averaged over the incident angles of the proton with respect to  $\mathbf{b}$  and the dislocation line. The scattering of points in Fig. 4 is statistical.

The integration of the dependences shown in Fig. 4 gives the following dechanneling cross sections  $\sigma_D$ : 20  $\mu\text{m}$  and 7  $\mu\text{m}$  for the edge and screw dislocations, respectively, at 450 GeV, and 77  $\mu\text{m}$  (edge) and 27  $\mu\text{m}$  (screw) at 7 TeV. The ratio  $\sigma_D(7 \text{ TeV})/\sigma_D(450 \text{ GeV})$  is equal to 3.85, in accord with that expected from the  $(pv)^{1/2}$  law, i.e.,  $(7 \text{ TeV}/450 \text{ GeV})^{1/2} = 3.94$ . The found cross sections are rather close to those predicted by Eq. (9): 47  $\mu\text{m}$  (edge) and 29  $\mu\text{m}$  (screw) for the 7-TeV case. With the similar procedure repeated for the stronger bending (1 GeV/cm) of the crystal,  $\sigma_D$  increased by the order of 10%.

Further we have studied the multiple interactions of

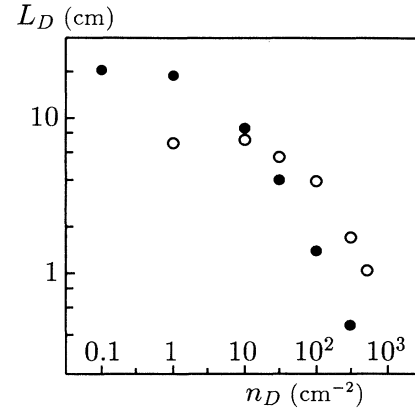


FIG. 5. The dechanneling length in the 3-cm-long Si(110) crystal bent with  $pv/R = 1$  GeV/cm, as a function of the dislocation density. For 450 GeV ( $\circ$ ) and 7 TeV ( $\bullet$ ).

the channeled particles with linear dislocations in the long bent silicon crystals. The same proton beam was incident onto the 3-cm-long Si (110) crystal. The crystal bending was uniform, with the  $pv/R$  value varying in the range from 0.2 to 3.0 GeV/cm.

The dislocations were distributed randomly in the crystal bulk with some density  $n_D$ , with the uniform distribution of the position and orientation angles. There was an equal number of the dislocations of the edge and screw type. For simplicity, we kept the same Burgers vector value  $b = 3.84$  Å independent of the dislocation orientation.

Two energies, 450 GeV and 7 TeV, have been studied with the dislocation density varying from 0.1 to 500  $\text{cm}^{-2}$ . The usual scattering on electrons and nuclei was also taken into account. The dechanneling lengths obtained in this simulation by fitting the particle angular distribution downstream of the crystal are plotted in Fig. 5. For nearly perfect crystal ( $n_D = 0.1\text{--}1 \text{ cm}^{-2}$ ) the dechanneling distribution along the crystal length  $L$  was not truly exponential (because  $L$  was essentially shorter than  $L_D$ ; see Refs. [27,28]), and the  $L_D$  value should be considered as a “local” estimate; it was defined by the rapid dechanneling of the particles with highest amplitudes of channeling (of order and above  $x_c$ ).

For the higher values of  $n_D$  the dechanneling over the 3-cm-long crystal was exponential, and the corresponding length  $L_D$  was well defined. The influence of the dislocations starts to be seen for  $n_D \geq 30 \text{ cm}^{-2}$  at 450 GeV, and for  $n_D \geq 3 \text{ cm}^{-2}$  at 7 TeV. For much higher densities the defect dechanneling dominates, and  $L_D$  is well described by the formula

$$L_D = 1/n_D \sigma_{\text{eff}}. \quad (21)$$

The effective dechanneling cross section  $\sigma_{\text{eff}}$ , obtained from the fit of the simulation results, is equal to 19  $\mu\text{m}$  at 450 GeV and 72  $\mu\text{m}$  at 7 TeV. As it includes all the possible contributions from the single and multiple collisions with dislocations in the crystal bulk, the  $\sigma_{\text{eff}}$  value may be somewhat higher than the average (edge and screw)

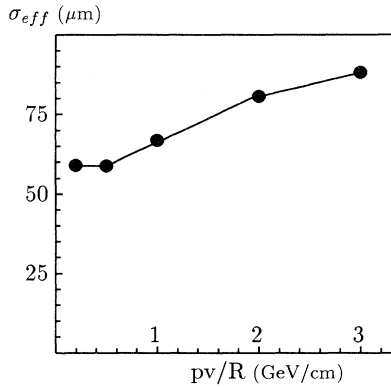


FIG. 6. The effective dechanneling cross section as a function of  $pv/R$ , for 7 TeV protons channeled in a long Si (110) crystal.

$\sigma_D$  (52  $\mu\text{m}$  for 7 TeV) computed for the single interactions from Fig. 4.

The results in Fig. 5 are given for  $pv/R = 1$  GeV/cm. However, repeating the simulation for  $n_D = 100 \text{ cm}^{-2}$  at 7 TeV with different  $pv/R = 0.2, 0.5, 1, 2,$  and  $3$  GeV/cm, we observed only minor effect of the global curvature on  $L_D$  (which was 1.69, 1.70, 1.50, 1.24, and 1.14 cm, respectively); of course, the number of the initially trapped particles was very different in each case. The dependence of the effective dechanneling cross section on  $pv/R$  is shown in Fig. 6, for 7 TeV protons channeled in the long Si (110) crystal. The qualitative explanation for the fact that the dependence is weak (found also for a single collision) may be as follows. The net local curvature is the sum of  $1/R$  and of the dislocation contribution  $\partial^2 u / \partial z^2$ . The sign of the latter varies in the vicinity of dislocation. Therefore, the  $1/R$  term may either enhance or cancel the contribution of  $\partial^2 u / \partial z^2$ , making a rather small effect in average.

The highest energy of the channeling applications so far is 900 GeV of the protons circulating in the Tevatron accelerator of Fermilab, where the crystal extraction experiment is being prepared [22]. Our simulations show that the influence of the dislocations would be seen for  $n_D \geq 10\text{--}20 \text{ cm}^{-2}$  here. For much higher densities,  $L_D$  can be described by the formula  $L_D = 1/n_D \sigma_{\text{eff}}$ , with  $\sigma_{\text{eff}} \simeq 26 \mu\text{m}$  for the same setting as used above.

The only measurements of dislocation dechanneling in a high-GeV range with the long bent crystals were made by Chesnokov *et al.* [11] at 70 GeV. There were tested several crystals of germanium as long as up to 45 mm. The best examples had less than  $1000/\text{cm}^2$  for the dislocation density, according to the information supplied by the manufacturer. From comparing the fraction of the bent particles with theoretical predictions and also from comparison with the silicon crystals in the same conditions, the estimates  $L_D \simeq 5$  mm have been made.

In the CATCH simulations for this experiment we studied two cases. First, both edge- and screw-type dislocations were present in the Ge crystal with an isotropic distribution in angle. With  $b = 4 \text{ \AA}$  and  $n_D = 1000 \text{ cm}^{-2}$ , the dislocation length over the 3 cm crystal was found to be  $11 \pm 2$  mm. In the second case, the edge disloca-

tions only were present, all of them aligned normally to the beam. The dislocation length decreased to 4 mm. In both cases a linear dependence of  $\sigma_D$  on  $b$  was found. Since no more detailed data on the crystals quality are available, we can conclude that the agreement is better than a factor of 2.

#### IV. RADIATION DAMAGE

An important consideration in accelerator applications is the resistance of crystals to radiation damage [29,30]. Although the damage itself is practically independent of energy in the  $> \text{GeV}$  range [see Eq. (22) below], the effect of it on the crystal channeling may be a strong function of the energy. The behavior of this function is determined by the kind and size of the accumulated defects. For this reason the study of the defects produced in irradiated crystals would be interesting. From the theory we see that the produced defects are more dangerous if they are ordered in an extended pattern. The radiation damage resistance must be scaled as  $E$  in the case of pointlike defects or small dislocation loops [25], as  $1/\sqrt{E}$  in the case of linear dislocations, and as  $1/E$  in the case of mosaicity [25].

However, it seems unlikely that interstitials or vacancies (produced initially) may organize themselves in any extended patterns in Si. For pointlike defects, an elementary estimate of the radiation damage resistance may be given (see also Ref. [29]). Let  $\epsilon_d$  be the minimal energy transfer required for a displacement of the lattice atom. The corresponding momentum transfer is  $q = \sqrt{2Am_p \epsilon_d}$ , with  $Am_p$  being the atom mass. The cross section of knocking the atom from the lattice site is given by the formula similar to (2):

$$\sigma_{\text{def}} = \frac{2\pi Z_i^2 Z^2 e^4}{m_p A \epsilon_d v^2}. \quad (22)$$

As  $v^2$  approaches  $c^2$  for a relativistic particle, the value of Eq. (22) saturates. We do not take into account cascade effects. On the other hand, we do not take into account the probability of recombination of the produced interstitial-vacancy pair. Both effects may be important. For a relativistic proton in Si the  $\sigma_{\text{def}}$  value is of the order of  $10^{-23} \text{ cm}^2$ . The maximal allowable fluence  $F_{\text{max}}$  of protons per  $\text{cm}^2$  is then  $F_{\text{max}} = n_a / \sigma_{\text{def}}$ , where  $n_a$  is the allowable relative density of interstitials. As we have seen earlier, the dechanneling on interstitials is comparable to the electronic one at  $n_a \approx 0.01$ . This corresponds to  $F_{\text{max}}$  of order  $10^{21}$  protons/ $\text{cm}^2$  in Si. Above 1 TeV, even the electronic dechanneling is negligible; therefore the practical threshold for  $F_{\text{max}}$  should become higher with energy.

Notice the factor  $Z_i^2$  in (22). The number of atoms knocked from the lattice sites is very much increased for heavy ions. For example, in the case of fully-ionized ions of Pb, this is the factor of 6700. Independently of what is the final structure of the produced defects (amorphous clusters, dislocation loops or lines, etc.),  $Z_i^2$  is the over-

all factor in the production rate of defects. Therefore, we have to conclude that the crystal resistance to radiation damage is decreased by the factor of  $1/Z_i^2$  for heavy ion beams. However, the typical beam intensity at accelerators is lower for heavy ions than for protons. For instance, at the 7-TeV large hadron collider under construction at CERN (Geneva) the heavy ion (lead) option implies an intensity nearly the same factor of  $\simeq 6000$  lower than intensity for the proton option.

At this time, the highest irradiation achieved in the bent crystals with high-GeV beams is of the order of  $10^{19}$  protons/cm<sup>2</sup>, with no substantial degradation of channeling properties observed. In the experiment [31] this value was achieved with a 70-GeV fast-extracted beam and a 13-mrad bent Si crystal, where the crystal also experienced large dynamical and heating shocks. The studies of the crystal irradiated to  $4 \times 10^{20}$  [30] at 28 GeV, protons per cm<sup>2</sup>, are in progress. The crystal retained almost all of its ability to channel 2 MeV He ions after this record exposure, although a measurable radiation-induced effect was seen. How one could extrapolate this from MeV to TeV energies is not clear for the moment.

## V. CONCLUSION

The theory of channeling in imperfect crystals has the same well-known foundations, which are employed in the theory of particle motion in the perfect bent crystals. The theoretical predictions have been confirmed experimentally, wherever it was possible. However, a principal problem is the precise measure of the crystal imperfections. Ideally, one needs to know separately the densities and characteristics of all kinds of defects present in crystal. But normally the detailed measurement procedure should destroy the crystal, in order to study its bulk. . . . An accurate measurement of the imperfection-induced dechanneling at the highest energy in a crystal

with the well-known structure would be very useful, especially in comparison with the simulation.

The lattice perfection of the modern silicon crystals seems to be so good that they probably do not need this theory at all. Long Si crystals with the purity of  $<1$  dislocation per cm<sup>2</sup> are available for the high energy bending experiments [22]; this purity would be sufficient for channeling even at  $>20$  TeV. From the experiments, one of the best reference points is provided by the works [2] with the H8 beam at CERN. The measured bending efficiency of nearly 50% is in excellent agreement with the theory and implies that the contribution of any defect to dechanneling was certainly (much) less than 10%. For the only dangerous lattice defect, linear dislocation, this contribution may grow not faster than  $\sqrt{E}$ ; that is, at the  $\sim 7$ -TeV large hadron collider of CERN their contribution would be (much) less than 40% in the same crystal (possibly sizable but not crucial). Note that from the above theory the purity of this crystal should have been  $n_D < 30/\text{cm}^2$ . Nevertheless the theory is indispensable for application of the crystals of heavier materials, such as tungsten; high- $Z$  crystals are attractive because of their stronger fields, but have a poor-quality lattice at present [32]. We see from Eqs. (9) and (22) that, with  $Z$  increase, the dechanneling cross section is reduced as  $\sim Z^{-1/2}$  while the damage cross section is increased as  $\sim Z$  (for  $Z/A \simeq \text{const}$ ). However, what matters more is the defect density which is very different in semiconductor and metal crystals. The technology of growing big silicon crystals has been highly developed (because of a big market). This practical reason causes the accelerator physicists to normally use the cheap and perfect silicon crystals for bending particle beams. The review of progress in growing high- $Z$  crystals is in Ref. [32].

We have discussed the influence on channeling of the microscopic defects of the crystal lattice. For practical applications, the macroscopic distortions of a crystal body are also important, induced by the processes of cutting and bending the crystal [33].

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