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Estimate of the Influence of Dislocation Defects on Crystal Deflector Efficiency at 20 TeV*

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Abstract

Dechanneling in bent crystals due to dislocation defects in the lattice is considered. The effect of these defects in commercially available silicon crystals for the proposed crystal extraction scheme at the Superconducting Super Collider (SSC) is estimated. Future needed investigation is discussed.

1.0 INTRODUCTION

The efficiency of charged-beam crystal optics is limited by the dechanneling process. Two kinds of dechanneling are well known at present:[1]

- bending dechanneling, due to the centrifugal force in a bent channel, and
- 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 $pv = 20$ TeV the L_D value in a perfect crystal is of the order of 10 m, so there is no problem with it.

In the real crystal, various defects disturb the lattice perfection. Of all the various defects present in crystal—point-like (interstitial atoms and vacancies), linear (dislocations), two-dimensional (stacking faults), and three-dimensional (amorphous clusters)—dislocations are of most interest, because the dechanneling cross-section for the other defects decreases with energy or remains constant. (For a good review of this field, see Ref. 2.)

Since the present application of commercially available crystals is successful (as a rule), we should take care of the dislocation defects only. The long defects of the crystal structure (such as dislocation lines, loops, and walls) induce local distortions of the planar channels. For this reason, the channeled particle could enter the region with a high density of nuclei and scatter, and/or pass through the region with high local bend, leading to a considerable change of the transverse energy or dechanneling.

In general, this could result both in bending-like dechanneling and in the diffusion-like 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 a previous discussion[3] on this subject, some limit cases were estimated.

Below we shall consider the channeled beam interaction with some defects, and make a few estimates for the crystal extraction scheme with commercially available silicon crystals proposed for the Superconducting Super Collider (SSC).

2.0 THE CRYSTAL MOSAICITY

Mosaicity should be the most visible defect of the lattice. The crystal consists of a number of perfect blocks slightly disoriented from one another. This is due to an arrangement of edge dislocations in a pattern (dislocation wall), separating the crystal into blocks. This defect is more typical for metal crystals. The angle of misalignment of the crystal blocks for each side of the wall[4] equals

$$\theta_m = \frac{b}{h} \,, \tag{1}$$

where $h = b/\theta_m$ is the spacing between dislocations in the wall and b is the Burgers vector value. Channel orientation differs on θ_m along the distance of order h. If $z_0 << h$, where z_0 is the oscillation period of the channeled particle, the dechanneling is determined by the maximal curvature along the distance h. If z_0 and h are comparable, the result of the particle interaction with the wall depends on the phase of its oscillation; its random character leads, in addition, to some diffusion in phase space. Finally, for $z_0 >> h$, there would be only diffusion and no bending-like dechanneling. The same approach could also be useful in other cases.

For commercially available Si crystals of high quality, the extremely low value of θ_m (about 0.05 μrad[5]) leads to the b/θ_m value one order of magnitude higher than the oscillation period at 20 TeV. For this reason we will estimate here the bending-like dechanneling only. As discussed above, the "intrinsic" bend leads to some "intrinsic" acceptance. The channel bent by angle θ_m along the distance b/θ_m corresponds to the radius of curvature b/θ_m^2. The ratio $pv/R_{loc} = pv\theta_m^2/b$ determines the bent channel acceptance A in the model of Kudo and Ellison.[6] It should be added to the global curvature pv/R_{glob}, if present.

For a 4-cm Si crystal bent on 0.1 mrad, a 20 TeV beam (the SSC case), and a mosaic spread $\theta_m = 0.05\,\mu$rad, the additional loss due to mosaicity is equal to

$$A(pv/R) - A(pv/R + \frac{pv\theta_m^2}{b}) \simeq -A'(pv/R)\frac{pv\theta_m^2}{b} \simeq 10^{-3} \,. \tag{2}$$

So, the preliminary analysis states that the mosaic spread of approximately 0.05 μrad is not dangerous for the proposed crystal application at the SSC. The beam loss is proportional to the $pv\theta_m^2$ value (until it gets too high).

Some dechanneling also occurs due to the dislocation cores in the wall. (See Section 4 for discussion.)

3.0 THE DISLOCATION LOOPS

The dislocation-loop defect can be imagined as an interstitial (vacant) piece of atomic layer. In other words, this is a closed-edge dislocation. It is characterized by its size (radius R, if it is circular). The Si crystal, used for the 1-GeV beam deflection, was tested in Gatchina for the dislocation contamination.[7] It was found that there are two types of clusters associated with dislocation loops: A-type of size 1–3 μm, and B-type of size 0.06–0.08 μm. Their density depends on position: in the center of the crystal it equals 100/cm^2 (A-type) and 10^4/cm^2 (B-type).

The lattice in the vicinity of the loop is displaced by approximately the Burgers vector b value (interatomic spacing). The atom displacement at a distance r, large compared to the loop size, is equal[4] (in isotropic matter approximation) to

$$u_i = \frac{\gamma^2}{4\pi r^3}((d_{ik} + d_{ki})x_k - d_{kk}x_i + \frac{3(1-\gamma^2)}{\gamma^2 r^2} d_{kl}x_i x_k x_l) \ , \tag{3}$$

where $\gamma^2 = \frac{\mu}{\lambda+2\mu}$, λ and μ are the Lame coefficients, $d_{ik} = S_i b_k$, and S_i and b_k are the projections of the loop area S and the Burgers vector b onto the coordinate planes.

Displacement falls very fast, as $1/r^2$, so the channel curvature decreases as $1/r^4$. The curvature becomes a critical one at about the distance $(bR^2R_c)^{1/4}$.

For the 20-TeV channeled beam interaction with such a defect, it is essential that the oscillation period of the channeled particle (about 0.5 mm in Si) is much larger than the disturbed lattice region size. The usual criterion of dechanneling (applied at lower energies)—that is, when the channel curvature is larger than the critical one—is not valid here, because the channeled ion does not make an oscillation in the distorted channel. However, we must take into account a "kick" due to the pass through the channel with the disturbed potential (long-range influence of the loop), as well as the multiple scattering of the ion passing through the loop core.

Probability of dechanneling due to a single collision is small; a change of the transverse energy per one interaction with such a defect is also not large, because of the small size of the distorted region.[3] For this reason the consideration could be in terms of the kinetic theory.

We shall make a simple estimate below. We divide the distorted region in two parts: a "core" (with size D_{core} of order R), where the atom displacement is larger (roughly) than the screening radius a_{TF}, and an "outer part." Collisions in the core we consider to be uncorrelated (amorphous approximation); for the outer part no multiple scattering is assumed, only the potential perturbation.

Consider at first a high-energy particle interacting with the core. The transverse energy change is defined by the coordinate changes δx and $\delta\theta$:

$$\delta E_x = pv\theta\delta\theta + U'(x)\delta x \ . \tag{4}$$

We shall consider the second term first:

$$\delta E_x \simeq U'(x)\theta D_{core} \ . \tag{5}$$

The cross section of particle interaction with distortion is $\sigma_D \simeq D^2_{core}$, and the interaction length $\delta z = 1/n'\sigma_D$, where $n' = n_D/2\pi R$ is a volume density of the dislocation loops. Diffusion coefficient (averaging is made over both the oscillation period and the defect size distribution) is of the form:

$$< \frac{(\delta E_x)^2}{\delta z} >= 2 < (U'(x))^2(E_x - U(x)) > \frac{< n' D^4_{core} >}{pv} \ . \tag{6}$$

The noncoherent scattering on nuclei leads to the following diffusion coefficient:

$$< \frac{(\delta E_x)^2}{\delta z} >= 2 < E_x - U(x) > \frac{\epsilon^2}{L_R pv} < n' D^3_{core} > , \tag{7}$$

where $\epsilon = 14.1\,\mathrm{MeV}$ and L_R is the radiation length. Possible correlated collisions in the core would lead here to the transverse energy change:

$$\delta E_x = \int U'(x(z), z)\theta dz \tag{8}$$

of the same order as Eq. (5).

The core size, as defined above, is independent of the beam momentum; for this reason the above diffusion coefficient is inversely proportional to pv.

The long-range contribution can be estimated here as follows. Note that the atom displacement u at the distance r is of the order of $b(R/r)^2$ (Eq. (3)), so its range is much less than z_0. The particle interaction with the distortion may be considered like a "kick" at some point. The interplanar force can be expanded in the following way:

$$U'(x+u) \simeq U'(x) + U''(x)u \ . \tag{9}$$

The angle change over interval dz is

$$\delta\theta = \frac{U''(x)udz}{pv} , \tag{10}$$

and the E_x change, integrated by z over the trajectory, is

$$\delta E_x = pv\theta \int \delta\theta = \theta(x)U''(x) \int u(r,z)dz \ . \tag{11}$$

As mentioned above, we keep x and θ constant during the interaction; a generalization is possible.

Averaging over the impact parameters and defects distribution, we have

$$< \frac{(\delta E_x)^2}{\delta z} >= \frac{2 < (U''(x))^2(E_x - U(x)) >}{pv} < n' \int d\sigma (\int u dz)^2 > \ . \tag{12}$$

For example, for the loop parallel to the plane of channeling and the b vector orthogonal to it, integration of Eq. (12) gives

$$< \frac{(\delta E_x)^2}{\delta z} >= \frac{2 < (U''(x))^2(E_x - U(x)) >}{pv} < n'\Gamma \frac{\gamma^2 S^2 b^2}{4\pi} \log \frac{z_0}{D_{core}} > , \tag{13}$$

where

$$\Gamma = 1 + \frac{3(1-\gamma^2)}{4\gamma^2} + \frac{5(1-\gamma^2)^2}{8\gamma^4} \ . \tag{14}$$

The result depends logarithmically on the limits of the integration over the impact parameters. The upper limit is set to be z_0, since above this value the loop influence is suppressed by the oscillation of the particle.

Let us estimate now the values of Eqs. 6, 7, and 12 at 20 TeV for the defect densities mentioned above. The result depends strongly on the D_{core} choice; according to the criterion discussed above, we choose $D_{core} = 7R$.

For the large (A-type) loops, in the considered approximation, the Eq. (6) diffusion coefficient value is about $0.6\,\mathrm{eV}^2/\mathrm{cm}$, the Eq. (7) value is $0.002\,\mathrm{eV}^2/\mathrm{cm}$, and the Eq. (12) value is $0.2\,\mathrm{eV}^2/\mathrm{cm}$. The total diffusion coefficient is about $0.8\,\mathrm{eV}^2/\mathrm{cm}$. With a potential well depth of about 10 eV, that means that the length L_D, over which a significant amount of dechanneling occurs, should be of the order of 100 cm.

The diffusion coefficient is proportional to $n_D R^3$, so the dechanneling on the small (B-type) loops is smaller by about 200 times.

With the above estimates we should expect the dechanneling fraction in a crystal of a few centimeters length to be of the order of 10%. All this contribution is from the large (A-type) loops. The small loops' contribution is $10^{-3} - 10^{-4}$. The beam loss is roughly proportional to $n_D R^3$, for sizeable dechanneling.

The most important result of the above analysis is that there is no more saturation in the dechanneling on the loops (contrary to the famous situation in the MeV and GeV region). The dechanneling length becomes a linear function of the energy.

Note that we have estimated only the order of the problems to be encountered. The detailed analysis or MC simulation could change considerably the above estimates. For this reason the 10% value of dechanneling is too high; a better quality of the crystal is needed at 20 TeV.

4.0 THE LINEAR DISLOCATIONS

The channel curvature $1/R$ around the linear dislocation decreases as $1/r^2$, the inverse square of the distance r to it.[2] For this reason the radius of the distorted region is proportional to the square root of the critical radius, i.e., the square root of the beam energy. The particle oscillation period is the same function of the energy. So there will be no change in the character of dechanneling with the energy increase. One can expect that the formulae valid at low energies are also good at 20 TeV.

The dechanneling here occurs when the channel curvature is larger than the critical one. The dechanneling cross section for the rectilinear dislocations was derived first by Quere:[2,8]

$$\sigma_D = K\sqrt{\frac{bpv}{2Ze^2Nd_p}} \, , \tag{15}$$

where N is the atom density, d_p is the interplanar spacing, Ze is the nucleus charge, and $K \simeq 0.34$ for screw dislocation and 0.56 for edge dislocation. The cross section has the meaning of the radius of a cylinder surrounding the dislocation line, inside which dechanneling occurs; its value is about $50\,\mu$m in our case (silicon, 20 TeV). The σ_D is derived under the assumption that every particle inside the cylinder is dechanneled and every particle outside it is not influenced. Dechanneling length is equal to

$$L_D = \frac{1}{n_D \sigma_D} \sim \theta_c \, , \tag{16}$$

and is proportional to the critical angle. The cross section increases with the energy, because the critical bend of channels occurs at a larger distance from the dislocation line.

Further investigation, including experiments, simulation, and more detailed analysis[9] indicates that Eq. (15) overestimates the dechanneling cross section by a factor of about 5. A particle having crossed the cylinder retains the ability to channel again.

We can suppose also that with an energy increase the K constant could decrease, because the contribution of the multiple scattering in the distorted region becomes insignificant in the multi-TeV domain.

The particles that are not dechanneled have experienced some change of the transverse energy (due to long range of the displacement field). The diffusion coefficients for the rectilinear dislocations (in the harmonic approximation) are given[10] for edge dislocation and screw dislocation, respectively:

$$B(E_x) = \frac{b^2}{d_p}\sqrt{2pvE_c}\,n_D E_x \tag{17}$$

$$B(E_x) = \frac{\pi}{12\sqrt{2}} b\sqrt{pv}\,n_D E_x^{3/2} \ . \tag{18}$$

The diffusion coefficient $B = B_0 E_x^k$ leads to a considerable dechanneling along the following length:[11]

$$L_D = \frac{4E_c^{2-k}}{(2-k)^2 j_{m,1}^2 B_0} \ . \tag{19}$$

Here $j_{m,1}$ is the Bessel function I_m zero, and $m = |(1-k)/(2-k)|$. Dechanneling lengths in the considered interactions, with coefficients of Eqs. (17) and (18), for edge dislocation and screw dislocation, respectively, are:

$$L_D = \frac{2d\theta_c}{j_{0,1}^2 b^2 n_D} \tag{20}$$

and

$$L_D = \frac{192\theta_c}{\pi j_{1,1}^2 b n_D} \ . \tag{21}$$

Note that extrapolation of a diffusion-like view to our case should be done with care. With the crystal purity required, $n_D \simeq 1 - 10\,\mathrm{cm}^{-2}$, the average distance between dislocation lines, $1/\sqrt{n_D}$, is a few millimeters. Since the area of the crystal surface in touch with the beam is only a fraction of a square centimeter, $S \simeq 0.3\,\mathrm{cm}^2$, the number of dislocations "on the way of the beam," Sn_D, is of the order of one! So the situation becomes concrete; in particular we can vary the transverse coordinate of the crystal (tangential to the beam) to find the optimum.

At 20 TeV the single-scattering formulae (Eqs. (15) and (16)) give the dechanneling length of a few tens of centimeters at the density of the linear dislocations n_D of the order of $10/\mathrm{cm}^2$. The diffusion estimates (Eqs. (20) and (21)) give lower values. So the crystal, perfect enough, should not have more than one linear dislocation per square centimeter. The quality of commercial crystals is increasing; the dislocation-free examples can be produced now, in principle.

5.0 CONCLUSION

The very preliminary analysis given above estimates the expected problems with the silicon-crystal lattice imperfection to be not too severe. Detailed analysis of the dechanneling at 20 TeV, including an MC simulation, is needed. Measurement of the densities of the dislocation defects of all types is very important. An accurate measurement of imperfection-induced dechanneling at the highest energy in the crystal with the well-known structure would be very useful, especially in comparison with the simulation.

Another important part of this problem is radiation damage resistance. Its value may be a strong function of the energy, in principle. The behavior of this function is determined by the kind and size of the accumulated defects. For this reason the investigation of the defects accumulated in the radiation-damaged crystal would be interesting.

There is another important point. In the proposed bent crystal extraction schemes, most of the beam-crystal interaction occurs in a very thin layer with a thickness of 1 μm order. A simple estimate for this layer lifetime:

$$Lifetime \simeq \frac{10^{19}\,\mathrm{cm}^{-2}\ 1\,\mathrm{mm}\ 1\,\mu\mathrm{m}}{10^{8}\,\mathrm{sec}^{-1}} \simeq 10^{6}\,\mathrm{sec} \simeq 1\ \mathrm{Week}\ , \tag{22}$$

with $10^{19}\,\mathrm{cm}^{-2}$ as a limit of integrated dose and $10^8/\mathrm{sec}$ as a beam intensity.

At this time, the highest irradiation achieved in bent crystals with high-GeV beams is of the order of $10^{19}\,\mathrm{protons/cm}^2$, with no substantial degradation of channeling properties observed. In the experiment,[12] this value was achieved with 70-GeV fast-extracted beam and 13-mrad bent Si crystal, where the crystal also experienced large dynamical and heating shocks. This value could change considerably at the energy two orders higher. Do the defects migrate from the damaged layer? This is also important to understand.

The two-crystal scheme[13] of extraction, with a thin crystal added as a scatterer, would provide the impact parameters of a few hundred microns order. That could solve the problem of radiation damage.

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