

A narrow plane cut near the crystal surface increases the probability of capture into the stable channeling motion up to 99 percent

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It is shown that a narrow plane cut near the crystal surface considerably increases the probability of capture into the stable channeling motion of positively charged particles entering a crystal at angles smaller than a quarter of the critical channeling angle with respect to the crystal planes. At smallest incidence angles the capture probability reaches 99 percent. A pair of crystals with cuts bent in orthogonal planes allows to reach a 99.9 percent efficiency of single-pass deflection of a proton beam with an ultra small divergence. Conditions necessary for efficient single-pass deflection of protons from the LHC beam halo are discussed.

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The phenomenon of positively charged particle channeling in crystals has already found several applications in high energy physics. In particular, the deflection of channeling protons and ions by bent crystals is widely used for beam extraction from high-energy accelerators [1, 2] as well as opens up a possibility to increase the efficiency of beam halo cleaning at the stage of LHC luminosity upgrade [1]. Next, the radiation of channeling particles, in that number, in crystal undulators [3, 4, 5, 6], allows to generate bright gamma-beams. Both planar and axial channeling can be also used for positron radiative cooling [7].

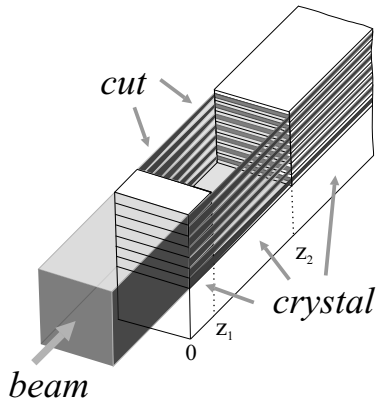


FIG. 1: A narrow cut between the planes $z = z_1$ and $z = z_2$, which preserves a single crystal structure in front and behind itself, allows to considerably reduce the proton transverse energy.

The efficiency of all these applications is restricted by an incomplete beam capture into the regime of stable channeling motion, the probability of which hardly exceeds 85% even for zero beam divergence because of the fast dechanneling of, at least, 15% of protons (positrons,

ions which we will not mention further for short) most intensively scattered by nuclei. To change the situation and to reach a 99% efficiency of proton capture into the stable channeling motion we suggest in this letter to use a narrow plane cut near the crystal entrance surface shown in Fig. 1. Similar cuts, widely used in channel-cut monochromators, preserve a single crystal structure on the cut opposite sides. In other words, atomic planes behind the cut are direct continuations of that ones in front of it.

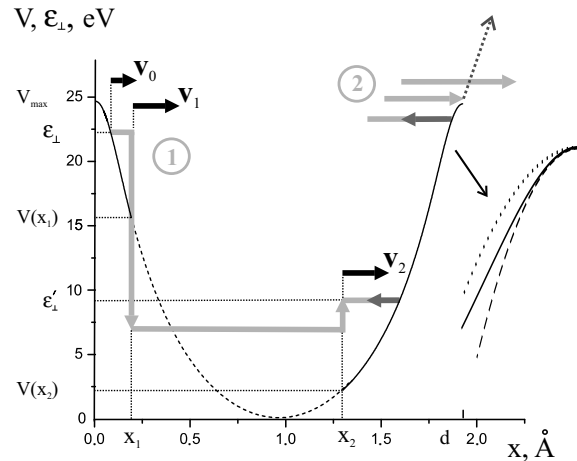


FIG. 2: Dependencies of the averaged planar potential (thin black curves) and transverse proton energy (thick gray lines) on the transverse coordinate, 1 – transverse energy reduction by the crystal cut region (dashed curve), 2 – dechanneling peak formation by the protons with $\epsilon_{\perp} \simeq V_{max}$. Two extreme approximations to the potential near its maximum are shown on the right.

The protons which start their transverse motion from the regions of high nuclear number density, such as $|x| \lesssim 0.2\text{\AA}$ and $|x - d| \lesssim 0.2\text{\AA}$ in Figs. 2 and 3a, efficiently dechannel at any, even zero beam divergence, since such protons recur to the regions of high nuclear density – see Fig. 3d. The cut prevents the recurrence

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by reducing transverse energies of most of the ready to dechannel protons. At first, passing through the crystal plate $0 \leq z \leq z_1$ protons acquire transverse velocities $v_1 = v_x(z_1)$ directed to the channel center $x = d/2$, namely $v_1 > 0$ at $0 < x_0 < d/2$ and $v_1 < 0$ at $d/2 < x_0 < d$, where $x_0 = x(z = 0)$, – see Fig. 3b. Next, passing through the cut, they drift towards the channel center (see Fig. 3c). As a result, entering the crystal behind the cut the protons acquire smaller potential energy $V(x_2)$ than the potential energy $V(x_1)$ they lose at the cut entrance (here $x_{1,2} = x(z_{1,2})$). Moving further with the reduced transverse energy most of the protons are now not able to reach the regions $|x| \lesssim 0.2\text{\AA}$ and $|x - d| \lesssim 0.2\text{\AA}$ of high nuclear density (see Fig. 3e) from which they would dechannel in the cut absence.

Of course, such a transverse energy reduction is possible if the proton incidence angle $\vartheta_0 = v_0/v_{\parallel}$ is sufficiently small. Here $v_0 = v_x(z = 0)$ and v_{\parallel} are, respectively, the initial transverse and average longitudinal velocity components. We will retain the later in the formulas to make them valid both in relativistic and nonrelativistic cases. In order to estimate the necessary ϑ_0 value one can, first, conjecture that to make a transverse kinetic energy $\varepsilon v_1^2/2$ sufficiently small (say, less than a quarter of the planar potential amplitude V_{max} , reserving another quarter for the potential energy), the angle $\vartheta_1 = v_1/v_{\parallel}$ should not exceed a half of the critical channeling angle $\theta_{ch} = \sqrt{2V_{max}/\varepsilon}$, where ε is the total proton energy. Second, in order not to considerably change the angle ϑ_1 , at least, its sign, the incidence angle ϑ_0 should be considerably (say, twice) less than ϑ_1 . Combining these two arguments one comes to the condition

$$\vartheta_0 \lesssim \theta_{ch}/4 \quad (1)$$

of efficient dechanneling probability reduction by the cut.

To obtain Eq. (1) more rigorously let us develop a simple model of the transverse energy reduction by the cut. Consider a proton entering a crystal with a transverse velocity v_0 in a point x_0 located in the high nuclear density region. Such a proton possesses a transverse energy $\varepsilon_{\perp} = \varepsilon v_0^2/2 + V(x_0)$ close to V_{max} – see Fig. 2. After passing through the crystal plate separated by the cut, the proton acquires a coordinate x_1 and a velocity v_1 . Entering then the cut, it loses the potential energy $V(x_1)$, passes freely through the cut with the constant velocity v_1 , and acquires a transverse coordinate

$$x_2 \equiv x(z_2) = x_1 + v_1 \cdot (t_2 - t_1), \quad (2)$$

where $t_1 = z_1/v_{\parallel}$ and $t_2 = z_2/v_{\parallel}$, and an energy

$$\varepsilon'_{\perp} \equiv \varepsilon_{\perp}(x_2) = \varepsilon \frac{v_1^2}{2} + V(x_2) \quad (3)$$

at the second entrance to the crystal at $z = z_2$.

To evaluate the cut coordinates $z_{1,2}$ which minimize the transverse energy ε'_{\perp} analytically let us use the parabolic approximation

$$V(x) = \frac{k}{2} \left(x - \frac{d}{2} \right)^2 \quad (4)$$

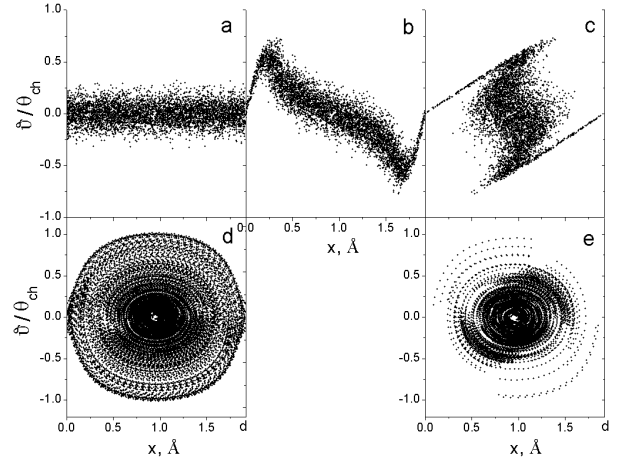


FIG. 3: Proton "phase space" a) at $z = 0$, b) at $z = z_1$, c) at $z = z_2$ and e) at $z = z_2 + \pi v_{\parallel}/2\omega$ in the cut presence and d) at $z = z_2 + \pi v_{\parallel}/\omega$ in its absence.

correctly describing the motion of most part of protons in the planar potential at small incidence angles. Substituting the corresponding x-coordinate

$$x_1 = d/2 + a_0 \cos \omega t_1 + v_0 \sin \omega t_1 \quad (5)$$

and velocity x-component

$$v_1 = -a_0 \omega \sin \omega t_1 + v_0 \omega \cos \omega t_1 \quad (6)$$

one can represent ε'_{\perp} in the form of a bilinear combination of v_0 and a_0 with some coefficients depending on z_1 and z_2 . Here $a_0 = x_0 - d/2$ and $\omega = \sqrt{k/\varepsilon}$ are, respectively, the amplitude and angular frequency of the channeling oscillations. The coefficient by the product $a_0 v_0$ vanishes and Eq.(3) takes the form

$$\varepsilon'_{\perp} = \varepsilon \frac{v_0^2}{2} \cot^2 \omega t_1 + k \frac{a_0^2}{2} \tan^2 \omega t_1 \quad (7)$$

if the cut coordinates satisfy the relation

$$z_2 = z_1 + \frac{2 \cot(2\omega t_1) v_{\parallel}}{\omega}. \quad (8)$$

We find this choice of the coordinate z_2 quite appropriate since Eq. (7) is much simpler than the explicit form of Eq. (3), it satisfies the symmetry conditions $\varepsilon'_{\perp}(a_0) = \varepsilon'_{\perp}(-a_0)$ and $\varepsilon'_{\perp}(v_0) = \varepsilon'_{\perp}(-v_0)$ and reaches a minimum both at $a_0 = 0$ and $v_0 = 0$. In addition, Eq. (7) allows to find the coordinate

$$z_1 = \frac{v_{\parallel}}{\omega} \arctan \sqrt{\frac{\vartheta_0}{\theta(a_0)}}, \quad (9)$$

at which the minimal value

$$\varepsilon'_{\perp} = 2 \frac{\vartheta_0}{\theta(a_0)} V(a_0) \quad (10)$$

of (7) is reached. Here $V(a_0) = ka_0^2/2$ is the initial potential energy and $\theta(a_0) = (1/v_{\parallel})\sqrt{2V(a_0)/\varepsilon}$ is the proton deflection angle. Putting $a_0 = d/2$ one obtains $V(d/2) \simeq V_{max}$ and $\theta(d/2) \simeq \theta_{ch}$. Assuming that protons quickly dechannel at $\varepsilon'_{\perp} > \varepsilon_{\perp dech}$, where $\varepsilon_{\perp dech}$ is an effective dechanneling energy, one indeed comes to the condition (1) of efficient cut use at quite natural value of $\varepsilon_{\perp dech} = V_{max}/2$.

From Eqs. (8) and (9) one easily obtains that

$$\frac{z_2}{z_1} = 1 + \frac{\sqrt{\vartheta_0/\theta_{ch}}}{\arctan \sqrt{\vartheta_0/\theta_{ch}}} \left(\frac{\theta_{ch}}{\vartheta_0} - 1 \right) \quad (11)$$

at $\theta(d/2) \simeq \theta_{ch}$ and $z_2/z_1 \simeq 4.235$ at $\vartheta_0 = 0.25\theta_{ch}$. Putting $k = 8V_{max}/d^2 \simeq 53.1eV/\text{\AA}^2$ one can easily estimate that z_1 value increases from 100\AA at $\varepsilon = 1MeV$, to $0.2\mu m$ at $\varepsilon = 1GeV$ and to $17\mu m$ at the LHC energy of $\varepsilon = 7TeV$. Expressing the equation of transverse motion in the form $\varepsilon v_{\parallel}^2 d^2 x/d^2 z = -V(x)'$ and observing that $z_{1,2} \propto v_{\parallel} \sqrt{\varepsilon}$, one can easily see that the ε_{\perp} evolution from $z = 0$ to $z = z_2$ remains the same for any energy.

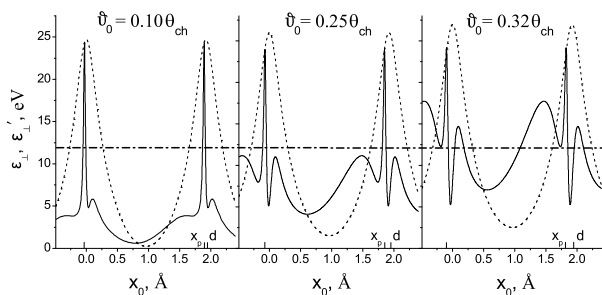


FIG. 4: Dependencies of the proton transverse energy at $z = 0$ (dashed) and $z = z_2$ (solid curves) on the initial proton coordinate at different angles of proton incidence with respect to the (110) *Si* plane.

The results of such an evolution simulated for three incidence angles ϑ_0 using the Moliere approximation for the averaged planar potential are illustrated by Fig. 4. A comparison of the solid and dashed curves demonstrates an efficient ε'_{\perp} reduction by the cut in the regions of high nuclear density. At $\vartheta_0 < \theta_{ch}/4$ this reduction allows to reach $\varepsilon'_{\perp} < V_{max}/2$ and, thus, to avoid fast dechanneling by 98-99% of the protons while the rest 1-2% of them form sharp peaks at $x_0 = x_p$ and quickly dechannel. Though the origin of these "dechanneling peaks" can not be explained using the approximation (4), Eqs. (7) and (10) correctly describe the ϑ_0 dependence of the maximum ε'_{\perp} value reached outside the peaks. In particular, one can see that ε'_{\perp} indeed reaches $V_{max}/2 \simeq 12.2eV$ at ϑ_0 slightly exceeding $\theta_{ch}/4$.

The dechanneling peaks originate from the protons with $x_0 \simeq x_p$ and $\varepsilon_{\perp} \simeq \varepsilon v_0^2/2 + V(x_p) \simeq V_{max}$ which slow down their transverse motion near the potential maxima acquiring very low velocities v_1 and coordinates

$x_1 \simeq nd, n = 0, \pm 1, \pm 2, \dots$, at the cut entrance. Their further motion with very low transverse velocities inside the cut preserves the proton transverse positions $x_2 \simeq x_1 = nd$ near the potential maxima. As a result, entering the crystal behind the cut such protons acquire transverse energies $\varepsilon'_{\perp} \simeq V(x_2) \simeq V_{max}$ corresponding to the dechanneling peak height. A few outermost trajectories in Fig. 3e belong to such protons.

A small width of the dechanneling peaks takes its origin from the high potential curvature k' near its maxima due to which even a slight x_0 deviation from the peak positions x_p leads either to the fast proton reflection from the potential wall at $\varepsilon_{\perp} < V_{max}$ or to the passage above the potential maximum at $\varepsilon_{\perp} > V_{max}$ – see Fig. 2. In both cases the protons quickly join the process of transverse energy reduction illustrated by Figs. 3 b, c and e.

In order to estimate the fraction of protons contributing to the dechanneling peaks we consider an analytical model of proton motion in the potential $V(x) \simeq V(0) - k'x^2/2$ approximating the realistic one near its maximum. Substituting corresponding x-coordinate

$$x_1 = x_0 \coth \lambda t_1 + v_0 \sinh \lambda t_1, \quad (12)$$

where $\lambda = \sqrt{k'/\varepsilon}$, and velocity $v_1 = dx(t_1)/dt$ into Eqs. (2) and (3) one obtains

$$\varepsilon'_{\perp}(x_0) \simeq V_{max} + \frac{1}{2} \frac{\partial^2 \varepsilon'_{\perp}(x_0)}{\partial^2 x_0} \Big|_{x_0=x_p} (x_0 - x_p)^2, \quad (13)$$

where $x_p = x_p(v_0)$ is the dechanneling peak coordinate fixed by the equation $\partial \varepsilon'_{\perp}(x_0)/\partial x_0 = 0$ and

$$\begin{aligned} \frac{\partial^2 \varepsilon'_{\perp}(x_0)}{\partial^2 x_0} \Big|_{x_0=x_p} &= -1 - \lambda(t_2 - t_1) \\ &\times [\lambda(t_2 - t_1) \sinh^2 \lambda t_1 + 2 \coth \lambda t_1 \sinh \lambda t_1] \end{aligned} \quad (14)$$

is the second ε'_{\perp} derivative which directly determines the dechanneling peak width Δx_p at the level of a dechanneling energy $\varepsilon_{\perp dech}$. This width allows to evaluate the relative number $\Delta x_p/d$ of protons with $\varepsilon_{\perp} > \varepsilon_{\perp dech}$ which we will use as an estimate

$$P_{dech} = 2 \sqrt{\frac{2(V_{max} - \varepsilon_{\perp dech})}{\partial^2 \varepsilon'_{\perp}(x_0)/\partial^2 x_0 \Big|_{x_0=x_p}}} \quad (15)$$

of the dechanneling probability. To evaluate the later one has to substitute the potential curvature k' the choice of which is somewhat ambiguous, as an insert on the right in Fig. 2 demonstrates. Its lower estimate $k'_{min} = E_{max}/x_{in} \simeq 475eV/\text{\AA}^2$ follows from the values of the maximum electric field strength $E_{max} \simeq 6.17GeV/cm$ and inflection point x-coordinate $x_{in} \simeq 0.13\text{\AA}$, while its maximum value $k'_{max} = d^2 V(x)/d^2 x|_{x=0} \simeq 846eV/\text{\AA}^2$ is reached in the point $x = 0$ of potential maximum. At $\varepsilon_{\perp dech} = V_{max}/2$ the probability (15) is equal to 3.24%

at $k' = k'_{min}$ and to 1.24% at $k' = k'_{max}$. The averaged value 2.24% of these estimates is in a good agreement with the values 2.13% and 2.59% obtained by simulations for the cases of, respectively, $\vartheta_0 = 0$ and $\vartheta_0 = 0.5\mu rad$. The probability (15) will be even lower if the protons effectively dechannel in a relatively short crystal at higher $\varepsilon_{\perp dech}$ values, for instance, at $\varepsilon_{\perp dech} = 3V_{max}/4$. Indeed, Eq. (15) predicts in this case that $P_{dech} = 2.29\%$ and 0.91%, respectively, at $k' = k'_{min}$ and $k' = k'_{max}$ while the simulations give 1.13% at $\vartheta_0 = 0$ and 1.34% at $\vartheta_0 = 0.5\mu rad$.

Thus, the cut reduces the transverse energy of 98-99% of protons of a beam with divergence (1) down to the level securing their stable channeling motion. The rest 1-2% of the protons avoid efficient energy reduction and dechannel fast. This picture manifests itself independently of the proton energy provided the cut coordinates which are, naturally, energy dependent, are chosen according to Eqs. (8) and (9). Thus, to illustrate the general features of the cut functioning by Monte Carlo simulations any proton energy may be chosen. Let us therefore consider the LHC proton deflection by bent crystals as the most challenging channeling application.

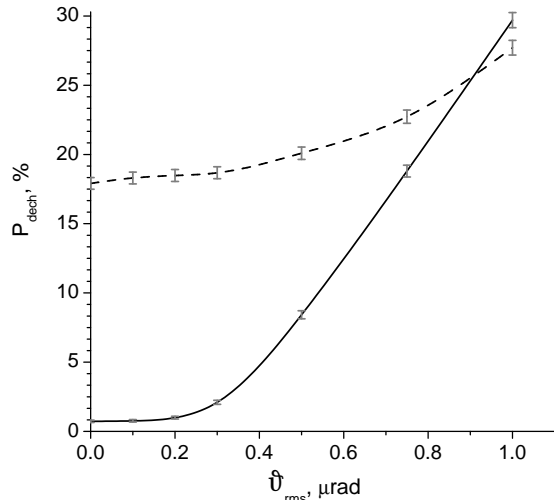


FIG. 5: Dependence of the 7 TeV proton dechanneling probability in a 1 cm bent *Si* crystal with (solid) and without (dashed curve) the cut on the r.m.s. incidence angle.

In previous deflection experiments the low capture probability was predetermined simultaneously by the high incident beam divergence, relatively thick amorphous near-surface crystal layer and fast dechanneling of protons moving in the regions of high nuclear density. At low capture probability a high deflection efficiency could be realized only in the multi-pass mode [1, 2]. However the divergence of the beam fraction encountering a crystal placed in the beam halo of a high energy proton accelerator can, in fact, be made very low [8, 9]. The amorphous layer also can be made as thin as $0.01\mu m$ [1].

In the circumstances the fast dechanneling becomes the only obstacle impeding an efficient single pass proton deflection and since the cut drastically reduces the number of quickly dechanneling protons, its use has to make an efficient single pass deflection possible.

To demonstrate this we simulated the 7TeV LHC proton deflection by a 1 cm *Si* crystal with 100m bending radius and cut coordinates $z_1 = 17\mu m$ and $z_2 = 71\mu m$ evaluated using Eqs. (8) and (9). To make the simulation process more adequate and efficient we treated the large-angle single Coulomb scattering separately from the small-angle multiple one. The angular distribution of protons in the incident beam was assumed to be both Gaussian and cylindrically symmetric. The simulated dependence of the dechanneling fraction on the root mean square (r.m.s.) divergence angle ϑ_{rms} is given in Fig. 5. On the average the cut begins to suppress the dechanneling process starting from $\vartheta_{rms} \simeq 0.9\mu rad \simeq 0.34\theta_{ch}$ while the highest efficiency of its use is reached at $\vartheta_{rms} \leq 0.3\mu rad \simeq 0.1\theta_{ch}$ when the dechanneling probability decreases down to 1% as predicted by the analytical model.

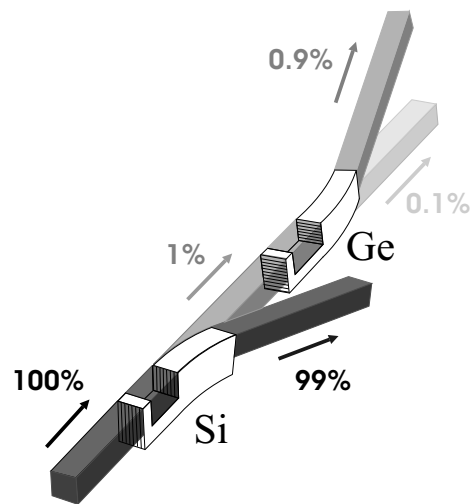


FIG. 6: A pair of 1 cm *Si* and *Ge* crystals with cuts bent in orthogonal planes with 100m bending radii allows to reach a 99.9% single-pass proton deflection efficiency at the LHC.

The simulations also show that the protons dechanneled in the crystal which is bent in horizontal xz plane acquires a r.m.s. divergence angle of about $0.7\mu rad$ in the vertical yz plane. Such a divergence allows to use a second crystal bent in the yz plane to deflect about 90% of these protons, as is shown in Fig. 6. Though the high beam divergence impedes the dechanneling suppression by the cut, a combined single-pass deflection efficiency by a pair of *Si* and *Ge* crystals with cuts approaches 99.9%. Both the single passage through the crystal and the proton moving off the high nuclear density regions will drastically diminish the rate of nuclear reactions accompanying the proton deflection by crystals with cuts.

Thus, to reach a really high single-pass deflection efficiency the beam divergence angle has not to exceed much $0.1\mu rad$. The angle which the proton beam axis forms with the crystal planes must be of the same order of value. Since the best goniometers allow to position a crystal only with a microradian accuracy, the necessary beam alignment along the crystal planes can most easily be reached by a proton deflection by a magnetic field with the typical integral value of only $0.01T \cdot m$ which should be adjusted to maximize the deflection probability.

The symmetry of the cut region from Fig. 1 prevents the disturbance of ε_{\perp} reduction process by a distortion accompanying the cut formation. However the crystal bending in the horizontal plane violates the symmetry and can distort the cut region upsetting the ε_{\perp} reduction process. The simplest possibility to avoid such a distortion is to leave the cut region straight, starting the crystal bending at $z > z_2$. To prevent the distortion of the cut region if it is nevertheless bent we suggest to tightly fix a crystal plane or set of planes with random crystal structure orientation and elastic properties identical to that of the removed crystal plane inside the cut. The method of high-resolution x-ray scattering [10] can be used to check both the crystal plane matching and alignment on the opposite sides of the cut.

Note briefly that the reduction of both the dechanneling probability and averaged transverse energy by the cut fabricated in the crystals used to generate either usual channeling radiation or channelled positron radiation from crystal undulators [3, 4, 5, 6] will diminish the intensity of radiation from non channelled positrons, make the radiation spectrum more narrow, increase the effectively used crystal length and reduce the rate of positron interaction with nuclei.

The positron transverse energy reduction by the cut also allows to increase the number of positrons involved in the process of radiative cooling being effective only in the

regions of negligible nuclear density [7]. Note that the cut can be used to improve the efficiency of radiative cooling both in the planar and axial cases. At that the two-dimensional distribution of both the nuclear density and averaged potential allows to reach even higher reduction of the quickly dechanneling proton or positron fraction in the axial case than in the planar one.

Note also that the cut application to the case of negatively charged particles will, on the opposite, several times and more increase the dechanneling and nuclear reaction probabilities both in planar and axial cases.

In principle, dechanneling probability reduction by the cut can both increase the depth and modify the profile of non relativistic ion implantation. However the small lengths $z_{1,2} \sim 10 - 100nm$ will seriously complicate the cut production. A crystalline surface layer with low average atomic number can be used instead of such narrow cuts. The crystal planes of this layer also have to be the direct continuations of that in the crystal. A vast experience in heterostructure growth [11] allows one to argue that a high quality *GaAl* layer can be produced on a *Ge* crystal most readily.

To summarize, the fabrication of a narrow plane cut near the crystal surface allows to ten times and more decrease both the dechanneling probability and nuclear reaction rate of positively charged particles in crystals. This possibility can many times increase the efficiency of both the beam deflection and halo cleaning at proton and ion colliders, of the gamma-quantum emission by positrons in crystal undulators and of the positron beam cooling.

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