Volume reflection angle study as a function of crystal curvature

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(Received 25 September 2016; published 27 October 2016)

We compare the volume reflection angles measured for protons and electrons over a wide energy range from 1 to 400 GeV in Si and Ge bent crystals at PNPI, IHEP, SLAC, and CERN with the predictions of FLUX and CATCH simulation codes based on binary collisions (FLUX) and continuum model (CATCH). We show good consistency of the data taken by many experimental groups, in good agreement with earlier published predictions.

DOI: 10.1103/PhysRevAccelBeams.19.101006

I. INTRODUCTION

Interaction of particles with bent crystals [1] has lead to the rise of an interesting technique of beam steering at particle accelerators [2,3]. Recent development in the field is related to so-called volume reflection [4–13] caused by interaction of an incident particle with the potential of the bent crystal atomic planes, which give the particle an angular kick of the order of a critical channeling angle θ_C in the direction opposite to the crystal bending. Bent crystal channeling occurs for those ions incident on the surface within the planar channeling critical angle, $\pm\theta_c$ where

$$\theta_c = \sqrt{\frac{4Z_1Z_2e^2Nd_pCa_{TF}}{pv}}. \quad (1)$$

Here Z_1 and Z_2 are the atomic numbers of the incident and lattice nuclei, N is the atomic density, d_p in the planar spacing, $C \cong \sqrt{3}$, a_{TF} is the Thomas-Fermi screening distance, and p, v are the ion momentum and velocity. The critical radius R_c is given by

$$R_c = \frac{pv}{\pi Z_1Z_2e^2Nd_p}. \quad (2)$$

To a good approximation the value of R_c in silicon is given by

$$\frac{pv}{R_c} \approx 6\ \mathrm{GeV/cm}. \quad (3)$$

For instance, for 400 GeV protons in Si (110) this corresponds to the critical angle of 10.6 μrad and critical radius of 0.68 m. We shall compare the theoretical understanding of volume reflection with the experimental data. In this comparison we limit ourselves only with the calculations performed before the experimental data have appeared.

II. COMPARISON OF EXPERIMENTS WITH PREDICTIONS

A. Theoretical predictions

The subject of our study is the angle of volume reflection of particles in bent crystals as a function of crystal bending radius. Such a study was performed in computer simulations in Ref. [14] using two very different approaches.

Motivations for the study [14] have been to provide a detailed analysis of the angular deflection and dispersion of high-energy ions by multiple volume reflection through several bent crystals' layers and also to devise schemes capable of deflecting with high efficiency a larger range of entrance angles of ions using bent crystal shields. This study is relevant to applications on the use of bent crystals as a means of collimating and extracting beams from accelerators. Two computer codes have been used to simulate 10,000 ion trajectories through several bent layers over a wide range of energies. The Monte Carlo code FLUX [15], which uses a binary collision model in conjunction with the Ziegler-Biersack-Littmark potential [16], has been adapted to simulate ions with energies up to 100 MeV/n through thin layers (several micrometers thick) of bent crystals. The code CATCH [17], based on a continuum-model [18] with Moliere potential and taking into account the single and multiple scattering on crystal electrons and nuclei, has been used to simulate the passage of 400 and 980 GeV protons through much thicker layers (up to many millimeters thick). FLUX considers interactions on an atom-by-atom basis, where CATCH considers them on a plane-by-plane basis. FLUX thus takes more time to simulate trajectories through a given layer thickness but is ultimately more accurate. A combination of these two codes enables multiple volume reflection to be studied from MeV to TeV for beam energies.

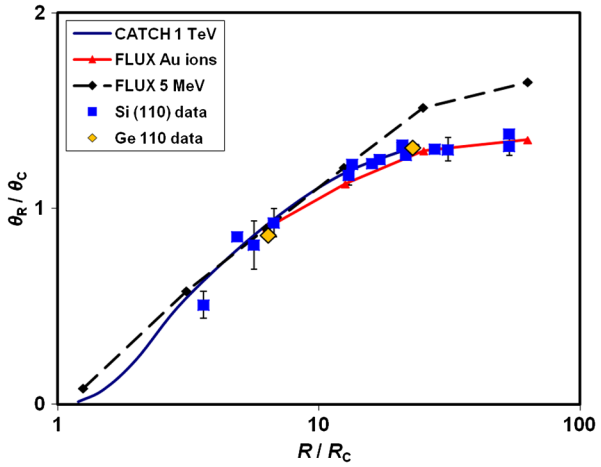

FIG. 1. Reflection angle θ_R/θ_C as a function of crystal curvature radius R/R_C. FLUX and CATCH simulations and Si (110) and Ge (110) experimental data.

The authors of Ref. [14] have studied the volume reflections of protons and Au ions in the energy range from 5 MeV up to 1 TeV in crystals of Si(110) (using FLUX) and Si(111) (using CATCH), with bending radii spanning from 0.001 to 3000 cm. The results are shown in Fig. 1 for the most probable angle of volume reflection as a function of crystal curvature radius. Reference [4] suggested that the function for the reflection angle $\theta_R = F(R, E)$ must be of the form

$$\theta_R = \theta_C \cdot f(R/R_C) \tag{4}$$

for any crystal at any energy range and bending radius R, where f is a function which depends only on the ratio R/R_C while θ_C sets the scale for θ_R. Therefore, it is natural to plot the results θ_R/θ_C vs R/R_C on the plane $(\theta_R/\theta_C, R/R_C)$ as done in Fig. 1, which shows variation of reflection angle θ_R/θ_C with lattice curvature radius R/R_C for different ion types and energies. The silicon layer thicknesses are 0.44 μm for 5 MeV protons, 7 μm for 100 MeV/n Au ions and 1 mm for 1 TeV protons.

The agreement between FLUX and CATCH was good over all the range of R/R_C studied. This agreement confirms that the function $f(R/R_C)$ is invariant for a broad range of energies from MeV to TeV and a broad range of crystal bending radii. The computed function thus can be used for predictions of experiments and design of applications.

B. Silicon (110) data

In the following decade many experimental results were obtained by several groups at IHEP, PNPI, CERN, MAMI, and SLAC [5–13] in the energy range from ~1 to 400 GeV with protons, electrons, and negative pions in crystals of Si(110), Si(111), Ge(110), and Ge(111). Figure 1 shows the data measured for Si(110) and protons, compared to the prediction of Ref. [14]. The data used for Fig. 1 are also listed in Table I.

We find good agreement between the data and prior published predictions. It is remarkable that a computer study of binary collisions of MeV Au ions is able to predict the results of future experiments with 400 GeV protons with such good precision.

The agreement of theory with experiment is important as the simulation code CATCH was used to predict the performance of several crystal channeling applications at the LHC, in particular crystal collimation [19,20].

TABLE I. Experimental data for (110) lattice.

		E (GeV)	R (cm)	$\theta_R(\mu\text{rad})$	R/R_C	θ_R/θ_C	$\lg(R/R_C)$
CERN	Si (110)	400	241	5.43	3.6	0.51	0.56
CERN	Si (110)	400	324	9.14	4.9	0.86	0.69
CERN	Si (110)	400	376	8.68	5.6	0.81	0.75
CERN	Si (110)	400	449	9.89	6.7	0.93	0.83
CERN	Si (110)	400	870	12.48	13.1	1.17	1.12
CERN	Si (110)	400	895	13.1	13.4	1.23	1.13
CERN	Si (110)	400	1065	13.13	16.0	1.23	1.20
CERN	Si (110)	400	1143	13.35	17.1	1.25	1.23
CERN	Si (110)	400	1391	14.03	20.9	1.31	1.32
CERN	Si (110)	400	1393	14.15	20.9	1.33	1.32
CERN	Si (110)	400	1433	13.57	21.5	1.27	1.33
CERN	Si (110)	400	1852	13.91	27.8	1.30	1.44
CERN	Si (110)	400	2085	13.9	31.3	1.30	…
CERN	Si (110)	400	3571	14.08	53.6	1.32	…
CERN	Si (110)	400	8720	14.41	130.8	1.35	…
CERN	Si (110)	120	1072	26.9	53.6	1.38	…
CERN	Si (110)	13	281	69.4	129.7	1.17	…
CERN	Ge(110)	400	230	11.4	6.4	0.86	0.81
CERN	Ge(110)	400	820	17.3	22.9	1.31	1.36

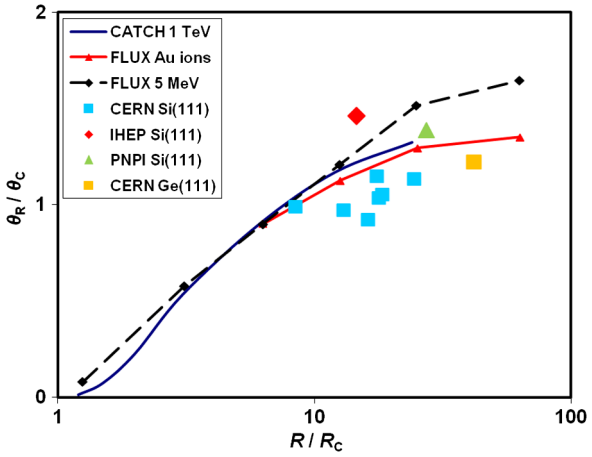

FIG. 2. Same theoretical curves as in Fig. 1 with the experimental data for Si (111) and Ge (111) added.

C. Silicon (111) data

Figure 3 shows the measured volume reflection angles of protons in Si(111) crystals from the experiments performed at PNPI, IHEP, and CERN. The data used for Fig. 2 are also listed in Table II. The (111) data look more scattered compared to (110) data but still agree with the predictions.

One can speculate on the origins of an increased scatter of (111) data compared to (110) data. The first factor is clear: while for the (110) case all data come from CERN experiments, for (111) they also come from IHEP and PNPI where different methods (e.g., photo emulsions in IHEP) were used with possible different systematic errors. As shown in Fig. 2, the IHEP and PNPI data points are the highest in the (111) sample, adding to the scatter. The second factor shows the crystal bending schemes were different for (110) and (111) cases. The (111) case has often used a "quasimosaic" bending that may increase variation in curvature over the crystal piece and thus variation in reflection angle.

From a theoretical point of view, one should remember that (111) orientation means the double plane. While under (110) orientation a particle sees a series of equal potential wells resulting from equidistant atomic planes, the case of (111) orientation is different. Here the interplanar spacing alternates between the narrow one d_S and wide one $d_L = 3 \cdot d_S$. For protons, this results in a series of two kinds of potential wells—one is narrow and shallow, another one is wide and deep. These two potential wells or channels in Si(111) correspondingly have two different critical angles and two different critical radii. Usually we normalize the results on the characteristics of the larger channel. Under channeling condition the probability for a proton to enter the narrow channel is 1 to 4, which makes a significant effect on the outcoming distribution [21]. Under reflection conditions, the existence of two planes with different θ_C and R_C affects the picture.

TABLE II. Experimental data for (111) lattice.

		E (GeV)	R (cm)	$\theta_R(\mu\text{rad})$	R/R_C	θ_R/θ_C
CERN	Si (111)	400	562	11.21	8.4	0.99
CERN	Si (111)	400	866	11	13.0	0.97
CERN	Si (111)	400	1078	10.45	16.2	0.92
CERN	Si (111)	400	1191	11.7	17.9	1.03
CERN	Si (111)	400	1225	11.9	18.4	1.05
CERN	Si (111)	400	1637	12.85	24.6	1.14
CERN	Si (111)	400	17 670	13.82	265.1	1.22
IHEP	Si (111)	70	170	236	14.6	1.46
PNPI	Si (111)	1	7,9	39.5	27.4	1.39
CERN	Ge(111)	400	1500	15.9	41.8	1.22

D. Germanium (110) and (111) crystals

Further experiments were done with germanium crystals. They have the same diamond-type lattice structure as silicon, with atomic number $Z = 32$ instead of 14, but the lattice spacings and unit cell size are slightly different. This results in stronger atomic fields, with correspondingly larger critical angle (about a factor of 1.5 larger compared to silicon) and smaller critical radius. The experiments with Ge(110) and Ge(111) crystals were done at CERN with 400 GeV protons [11,12]. Figures 1 and 2 show three germanium data points Ge (110) and (111) on the same plots compared to FLUX and CATCH predictions. Despite the fact that the computer simulations were done with Si(110) and Si(111) crystals, the similarity of Ge and Si lattices results in good agreement between the new Ge data and the prior published predictions. The agreement between germanium and silicon measurements looks also quite good. The shape of the predicted function $\theta_R = \theta_C \cdot f(R/R_C)$ appears universal indeed serving for Ge as well as for Si. Again, it is encouraging that a study of binary collisions of MeV ions of Au in silicon can predict the results of future experiments with 400 GeV protons in germanium.

E. Empirical formula for the reflection angle

The dependence of θ_R/θ_C on R/R_C is obtained with numerical (and then with experimental) methods. It would be useful to have an easy formula for this dependence for some reasons: (a) for quick comparison of future experimental data with the established dependence known from past studies; (b) for analytical estimates and possible optimization of experiments and applications. The authors of Ref. [14] noticed that the numerical predictions can be roughly approximated by the empirical formula

$$\theta_R = \theta_C \cdot \lg(R/R_C) \tag{5}$$

in the part of the plot for $R/R_C = 1$ to 30. This is not valid for $R/R_C > 30$ where θ_R saturates.

We compared the predictions of Eq. (5) with the (110) data in Table I; see the last column. There, we do not show

TABLE III. SLAC experimental data for electrons and Si(111).

	E (GeV)	R (cm)	$\theta_R(\mu\text{rad})$	R/R_C	θ_R/θ_C
SLAC e- Si (111)	3.35	15	129	26.4	1.05
SLAC e- Si (111)	4.2	15	101	21.1	0.92
SLAC e- Si (111)	6.3	15	84	14.0	0.94
SLAC e- Si (111)	10.5	15	50	8.4	0.72
SLAC e- Si (111)	14	15	35.6	6.3	0.59

the predictions for $R/R_C > 30$ where Eq. (5) is not valid. For the sample of all Si(110) and Ge(110) experimental data the ratio of measured θ_R to $\theta_C \cdot \lg(R/R_C)$ equals 1.03 ± 0.09 for $R/R_C = 1$ to 30:

$$\theta_R = (1.03 \pm 0.09) \cdot \theta_C \cdot \lg(R/R_C). \quad (6)$$

Notice that precise computations in crystal channeling may differ between each other by an order of 10% when different models are used, for instance Hartree-Fock, Moliere, etc. The rms accuracy of 9% may be sufficient to open the way for the use of Eq. (5) for analytical estimates, design, and optimization of future applications and so on.

For the (111) data we do not show Eq. (5) predictions, because the experimental data for (111) is limited in span and not sufficient for checking the formula.

III. NEGATIVE PARTICLES

The predictions in Fig. 1 are solely for positive particles. We know from simulations that for negative particles the volume reflection angles should be lower than ones for protons. However, we do not have the plot of theory predictions for the dependence of θ_R/θ_C on R/R_C for negative projectiles. Nonetheless, a good new experimental work is in progress from electron accelerators. The most complete data have come recently from SLAC [13]. It is interesting to compare the electron data with those for protons on the same plot; see Fig. 3. The data used for Fig. 3 are also listed in Table III. It looks like SLAC electron data follow the same slope on the $(\theta_R/\theta_C; R/R_C)$ plot in parallel with protons but lower in absolute values.

If we try to approximate their slope with the same $\lg(R/R_C)$ function, we obtain for SLAC electrons a relation

$$\theta_R = (0.75 \pm 0.06) \cdot \theta_C \cdot \lg(R/R_C). \quad (7)$$

The SLAC data is roughly a factor of 1.3 lower than the proton data. The electron Si(111) data almost overlap with proton Si(111) data in some regions. Meanwhile, some theories expected a factor of 1.8–2.0 ratio between volume reflection angles of positive and negative projectiles [4,22]. It looks as though all of these theory expectations were published for equidistant planes, Si(110). This may need further clarification from both sides—theory and experiment.

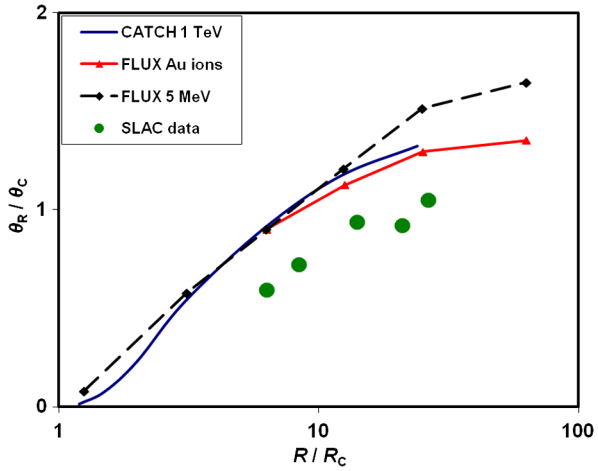

FIG. 3. Same theoretical curves as in Fig. 1 with the SLAC experimental data for electron reflection in a Si (111) crystal shown.

IV. CONCLUSION

Both simulation codes, FLUX based on binary collisions and CATCH based on the continuum model, turned out to be very successful in the prediction of the results of the decade-long experimental study of volume reflection at several high-energy accelerator centers across the world. The codes use no free parameters at all. Only the lattice of silicon crystal and models of atom potential in approximation Ziegler-Biersack-Littmark (FLUX) and Moliere (CATCH)are used. The code predictions were published a decade ago advancing the experimental work. The agreement found is encouraging for future applications of the technique of volume reflection.

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