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INFLUENCE OF TEMPERATURE ON THE DECHANNELING IN THE BENT <100> SI CRYSTAL

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Abstract. The influence of temperature on the dechanneling of H^+ ions in the bent <100> Si crystal is investigated. The ion energy is 7 TeV, the bending angle is $\varphi = 0,02\,\text{mrad}$, the reduced crystal thickness is $\Lambda = 2,1$, which corresponds to the crystal thickness of $1\,\text{mm}$, and the temperature range under the investigation is 0 – 400 K.

The number of dechanneled ions is obtained by the computer simulation method using the numerical solution of the ion equations of motion in the transversal plane. The effect of the thermal vibrations of crystal atoms is included using the Debye theory. Effects of the proton energy loss and uncertainties of the proton scattering angle caused by its collisions with the crystal electrons are also taken into account. The analysis of the obtained results shows that the influence of the temperature on the dechanneling of H^+ ions is very small.

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1. DECHANNELING IN A BENT CRYSTAL

Dechanneling is a process by which fraction of the channeled ions is reduced. This process occurs when the scattering angle of the ion ψ is larger than the critical angle for the channeling ψ_C [1].

Increase of the transversal energy $E_\perp$ of the ion, which causes increase of the ion's scattering angle ψ, is a result of the inelastic multiple ion scattering with electrons and nuclei of the crystal. The average rate of change of $E_\perp$ per the penetration depth z can be written as

$$\left\langle \frac{\mathrm{d}E_\perp}{\mathrm{d}z} \right\rangle = E \left\langle \frac{\mathrm{d}\psi^2}{\mathrm{d}z} \right\rangle + \left\langle \psi^2 \left(\frac{\mathrm{d}E}{\mathrm{d}z} \right) \right\rangle, \tag{1}$$

where the average is taken over the area in the transverse plane accessible to particles with energy $E_\perp$ [1]. The first term of equation (1) gives the rate of increase of transverse energy due to multiple scattering of the proton with the electrons of the crystal, and is given by

$$\left(\frac{\mathrm{d}\psi^2}{\mathrm{d}z}\right)_e = \frac{m_e}{p^2}\, n_e\left(r_\perp\right) S_e, \tag{2}$$

where m_e is the electron mass, p is relativistic momentum of the ion, $n_e\left(r_\perp\right)$ is average electron density, and S_e is electronic stopping cross section.

The second term of equation (1) gives the rate of decrease of transverse energy due to electronic energy loss of the proton beam (damping)

$$-\left(\frac{\mathrm{d}E}{\mathrm{d}z}\right)_e = n_e\left(r_\perp\right) S_e . \tag{3}$$

It has been shown that the second term (3) is small in comparison with the first one (2) and its influence will be neglected.

In this paper, we assume that the continuum potential of i-th atomic string ,U_i , is given by the standard Lindhard's expression [1], and, consequently, the average electron density is given by

$$n_e^{\mathrm{th}}\left(r_\perp\right) = \frac{1}{4\pi Z_1 e}\sum_{i=1}^{M}\left(\partial_{xx}U_i^{\mathrm{th}} + \partial_{yy}U_i^{\mathrm{th}}\right) = \frac{Z_2 e C a_{\mathrm{TF}}^2}{\pi d}\sum_{i=1}^{M}\frac{1}{q_i^4}\left[1 + \frac{4\sigma_{\mathrm{th}}^2\left(3r_{\perp i}^2 - q_i^2\right)}{q_i^4}\right], \tag{4}$$

where Z_1 is the projectile atomic number, $U_i^{th} = U_i + (\sigma_{th}^2/2)\Delta U_i$ is the continuum potential of the i-th atomic string with the effect of the thermal vibrations included, σ_{th} is the one-dimensional thermal vibration amplitude of the crystal atoms, Z_2 is atomic number of the crystal atom, C is the screening constant, a_{TF} is the screening radius, d is the distance between the atoms of the atomic strings, $q_i^2 = r_i^2 + Ca_{\mathrm{TF}}^2$, where $r_i^2 = \left(x - x_i\right)^2 + \left(y - y_i\right)^2$; x_i and y_i are the coordinates of the atomic strings in the transverse plane. The formula (4) is valid if $\sigma_{\mathrm{th}} < a_{\mathrm{TF}}$.

For the electronic stopping cross section, we used the following expression [1, 2]

$$S_e = \frac{4\pi Z_1^2 e^4}{m_e v^2}\left(\ln\frac{2m_e\gamma^2 v^2}{\hbar\omega_e} - \beta^2\right), \tag{5}$$

where, m_e is the electron mass, v is ion velocity, $\beta = v/c$, where c is the speed of light, $\gamma^2 = 1 - \beta^2$, and $\omega_e = \left(4\pi e^2 n_e^{th}/m_e\right)^{1/2}$ is the angular frequency of oscillations of the crystal electron gas induced by the ion.

2. THERMAL VIBRATIONS OF THE CRYSTAL LATTICE

The one-dimensional thermal vibration amplitude of the crystal atoms is equal to the root-mean-square displacement of the crystal atoms, $\sigma_{\mathrm{th}} = \sqrt{\overline{\Delta\xi^2}}$, and its value could be computed by the use of the Debye theory [3]. According to this theory,

$$\overline{\Delta\xi^2} = \frac{1}{12}\frac{1}{N m \pi^2}\int\frac{f(\nu)}{\nu^2}g(\nu)\,\mathrm{d}\nu , \tag{6}$$

where N is the total number of atoms in the crystal, m is the atomic mass, and the distributive function f and the density function g are given by

$$f(\nu)=\frac{h\nu}{2}+\frac{h\nu}{e^{h\nu/k_BT}-1}, \tag{7}$$

where ν is the frequency of the normal mode of vibrations and

$$g(\nu)=\begin{cases}\dfrac{9N}{\nu_{\mathrm{D}}^3}\nu^2, & \nu\le\nu_{\mathrm{D}}\\ 0, & \nu>\nu_{\mathrm{D}}\end{cases}, \tag{8}$$

is the density of the normal modes according to the Debye theory. ν_D is known as the Debye frequency. After some calculations, for one-dimensional thermal vibration amplitude one obtains

$$\sigma_{\mathrm{th}}^2=\frac{3h^2}{4\pi^2k_B}\left[\frac{1}{4}+\frac{\phi(y)}{y}\right]\frac{1}{m\theta_D}, \tag{9}$$

where $\phi(y)$ is the Debye function and θ_D is the Debye temperature [3]. Figure 1 shows the dependence of σ_{th} on temperature according to the Eq. (9) in the case under the consideration.

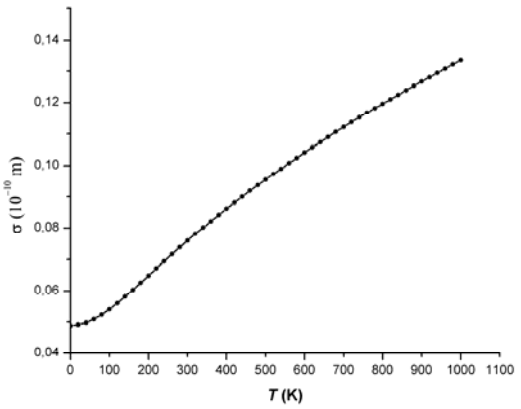

Fig. 1. The dependence of the amplitude of the thermal vibrations of the crystal atoms, σ_{th}, on the temperature, *T*, according to Debye theory.

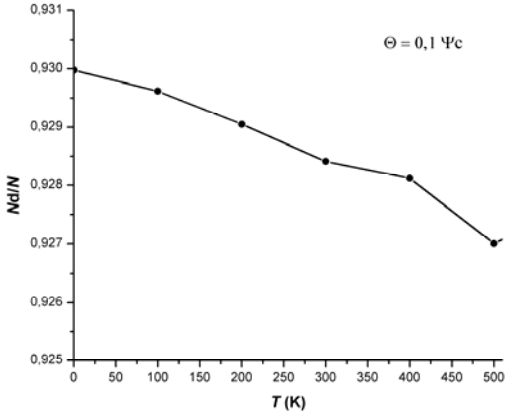

Fig. 2. Dechanneleng curve which show the changes of the number of the dechanneled ions, N_d, as a function of the temperature T.

3. COMPUTER SIMULATION

Here, the number of dechanneled ions is determined numerically by following of the trajectories of channelled ions [2, 4], and using the computer simulation method. We chose the numerical method because it is more accurate than the analytical one [4].

The trajectories of ions are obtained by numerical solving of the equations of motion in the transversal plane

$$\ddot{x}=-\frac{1}{\gamma m}\sum_{i=1}^{n}\partial_x U_i^{\mathrm{th}}=\frac{2Z_1Z_2e^2Ca_{\mathrm{TF}}^2}{d\gamma m}\sum_{i=1}^{n}\frac{1}{q_i^2}\left[\frac{1}{r_i^2}+\frac{4\sigma_{\mathrm{th}}^2}{q_i^4}\right](x-x_i), \tag{9a}$$

$$\ddot{y}=-\frac{1}{\gamma m}\sum_{i=1}^{n}\partial_y U_i^{\mathrm{th}}=\frac{2Z_1Z_2e^2Ca_{\mathrm{TF}}^2}{d\gamma m}\sum_{i=1}^{n}\frac{1}{q_i^2}\left[\frac{1}{r_i^2}+\frac{4\sigma_{\mathrm{th}}^2}{q_i^4}\right](y-y_i), \tag{9b}$$

where $Z_1 = 1$, $Z_2 = 14$, $C = 4,4939$ and $d = 0,543082\,\text{nm}$ is the distance between the atoms along <100> crystallographic direction of Si. For numerical solving of the above system of differential equations, we used the Runge-Kutta method of the forth order [5].

In the computer simulation code, we included effects of the ion's energy loss, the uncertainty of its scattering angle caused by the inelastic scattering with the electrons of crystal, and the divergence of the ion's beam before its interaction with the crystal.

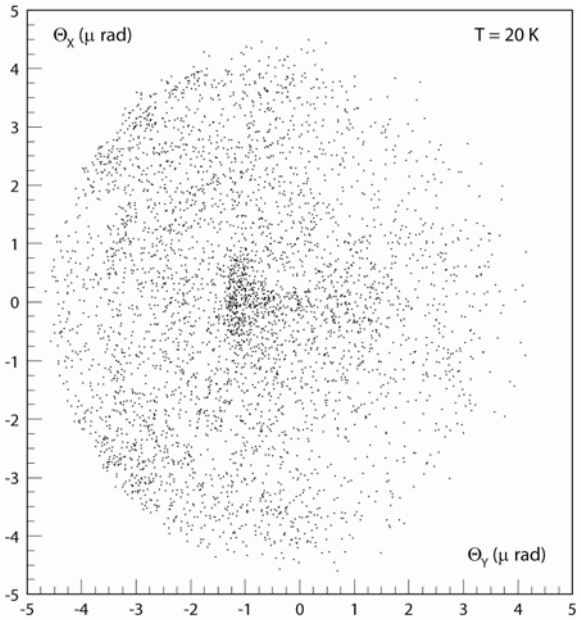

Fig. 3. Angular distribution of H^+ ions when $T = 20$ K.

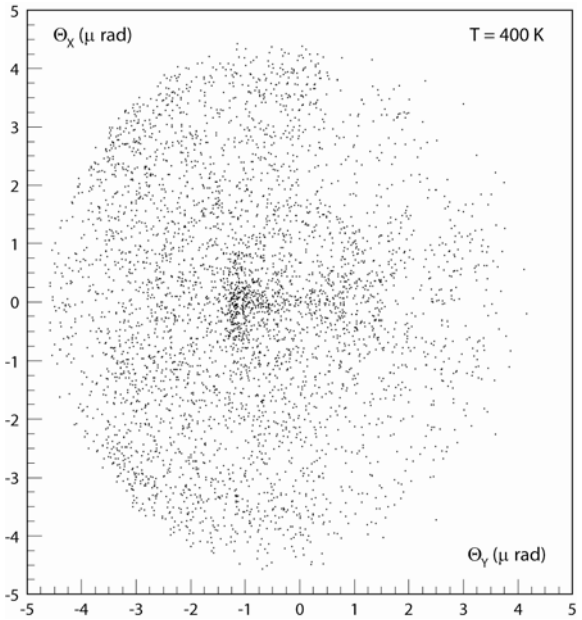

Fig. 4. Angular distribution of H^+ ions when $T = 400$ K.

4. RESULTS AND DISCUSSION

In this work, the influence of temperature on the dechanneling of H^+ ions in the bent <100> Si crystal is investigated. The ion energy is 7 TeV, the bending angle is $\varphi = 0,02\,\text{mrad}$, the reduced crystal thickness is $\Lambda = 2,1$, which corresponds to the crystal thickness of $1\,\text{mm}$, and the temperature range under the investigation is 0 – 400 K. Initial number of ions (trajectories) is $N_p = 101761$, and they are chosen uniformly within the region of the crystal channel.

Figure 2 shows the dechanneling curve for H^+ ions when the divergence of the ion beam is $\Theta = 0,1\psi_C$. One can clearly see that the number of dechanneled ions decreases as the temperature increases, and this decreasing of the number of dechanneled ions is very small in the temperature range under the investigation.

Figures 3 and 4 show the angular distributions of channeled H^+ ions when the temperature of the Si crystal is 20 K and 400 K, respectively. One can see that the changes in the angular distributions of the ions are very small.

It should be mentioned that for $T < 400\,\text{K}$, the amplitude of the thermal vibrations of the crystal, $\sigma_{th} < 0.00862\,\text{nm}$ (see Figure 2), and since the screening radius $a_{TF} = 0,01795\,\text{nm}$, we can conclude that the use of the formulas (4) and (9) is justified.

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ВЛИЈАНИЕ НА ТЕМПЕРАТУРАТА ВРЗ ДЕКАНАЛИРАЊЕТО ВО <100> ЗАКРИВЕН КРИСТАЛ НА Si

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Апстракт. Во овој труд е истражувано влијанието на температурата врз деканалирањето на H^+ јони во <100> закривен кристал на Si. Енергијата на јоните е 7 TeV, аголот на закривување е $\varphi = 0,02\,\text{mrad}$, а редуцираната дебелин на кристалот е $\Lambda = 2,1$, што соодветствува на реална дебелина од 1mm. Температурниот интервал во кој е направено истражувањето се движи од 0 – 400 K.

Бројот на деканалирани јони е добиен со метод на компјутерска симулација, користејќи нумеричко решавање на равенките на движење на јоните во трансверзалната рамнина. Ефектот на термални вибрации е вклучен користејќи ја теоријата на Дебај. Во симулацијата се вклучени и ефектите на енергетските загуби и неопределеноста на аголот на расејување на јоните заради судирите со електроните на кристалот. Анализата на резултатите покажа дека влијанието на температурата врз деканалирањето на H^+ јоните е многу мало.