Energy loss of MeV light ions specularly reflected from a SnTe(001) surface

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Energy losses of specularly reflected MeV protons and He ions from a clean (001) surface of SnTe single crystal are observed. The position-dependent stopping powers near the surface are derived from the observed results. The obtained stopping power is proportional to $E^{-1/2}\exp(-\beta_3 x/2a_{TF})$, where E is the ion energy, a_{TF} is the Thomas-Fermi screening distance, β_3 is 0.3, and x is the distance from the surface. This result is similar to the observed position-dependent stopping power for planar channeled ions.

I. INTRODUCTION

Processes of charge and energy transfer between energetic ions and solid surfaces have recently been the subject of extensive studies.[1] In relatively recent works, the formation of coherent excited states of ions, which lead to the alignment and polarization of emitted photons, has been studied at glancing-angle incidence of energetic ions on flat surfaces of single crystals.[2] In these and related studies on ion scattering at glancing-angle incidence of energetic ions on a clean surface of a single crystal, it is expected from the concept of planar channeling that the ions do not penetrate into the target crystal but are subjected to a specular scattering by the first surface layer of crystal atoms. This is a favorable situation for the study of interaction of energetic ions with solid surfaces, where a number of complex phenomena associated with the penetration of ions through solids can be avoided.

However, the scattering of ions at glancing-angle incidence on a surface of a single crystal depends on the incident beam direction with respect to the surface atomic rows. Surface channeling occurs when the ions are directed towards a low-index crystallographic axis parallel to the surface. In this case, the interaction between ion and surface is slightly complicated because subsurface atomic layers participate in scattering of ion.[3]

The aim of this paper is to present our experimental observations of energy losses of H and He ions reflected from clean (001) surfaces of SnTe single crystals at glancing-angle incidence of MeV protons and He^+ ions. The process of reflection of energetic ions at the surface of a single crystal is discussed and the stopping powers of the solid surface which depend on the distance of the ion from the surface are derived.

II. EXPERIMENTAL PROCEDURE

The experimental setup was described elsewhere.[4] A brief outline is summarized here. A single crystal of KCl with the (001) cleavage surface was mounted on a high-precision goniometer in the scattering chamber whose base pressure was 3×10^{-10} Torr. The single crystal of SnTe(001) was prepared by epitaxial growth *in situ* by vacuum evaporation on the KCl(001) surface. The surface of SnTe(001) showed a sharp 1×1 reflection high-energy electron diffraction (RHEED) pattern. A beam of ions from the 4 MV Van de Graaff accelerator of Kyoto University was collimated by apertures to a divergence angle less than 0.5 mrad. The ions scattered at an angle θ_s in the plane, which contains the incident beam and the normal to the surface, were chosen by a movable aperture. The acceptance angle of this aperture was 0.9 mrad for the scattered ions. The ions passing through the aperture were resolved into their charge states by a magnetic analyzer and measured by a solid-state detector (energy resolution 14 keV).

III. EXPERIMENTAL RESULTS

Figure 1 shows examples of the observed energy spectra of scattered He^+ ions for various scattering angles when 0.7-MeV He^+ ions were incident on the SnTe(001) surface with a glancing angle of 4.9 mrad. The spectra consist of several well-defined peaks separated by equal energy spacings. The dependences of the ion yields of each peak on the scattering angle are shown in Fig. 2. The ion yields show peaks at the scattering angle of specular reflection (twice the glancing angle) and the yield of the first peak (the peak of highest energy) is dominant especially around the angle of specular reflection. The dependence of the energy spacing between adjacent peaks on the ion energy is shown in Fig. 3. The spacing between the first peak and the second peak and that between the second peak and the third peak for scattered He^+ and He^{2+} ions are shown for the glancing angle 2.9 mrad and the scattering angle 6.4 mrad. The spacings are independent of the charge state and increase gradually with increasing energy.

Similar energy spectra, having an oscillatory feature, were observed for the ions transmitted through a planar channel in the crystal.[5] The energy spectra of the planar channeling ions were explained by the fact that well-resolved peaks correspond to particles which made an integral number of oscillations in passing through the crystal. Though the present experimental condition is different from that of the planar channeling, the oscillatory feature of the present energy spectra may be explained by a similar mechanism.

In order to investigate the origin of the oscillatory feature of the present energy spectra, we measured the Rutherford backscattering (RBS) spectra of (100) planar channeling. The energy loss of (100) planar channeled He

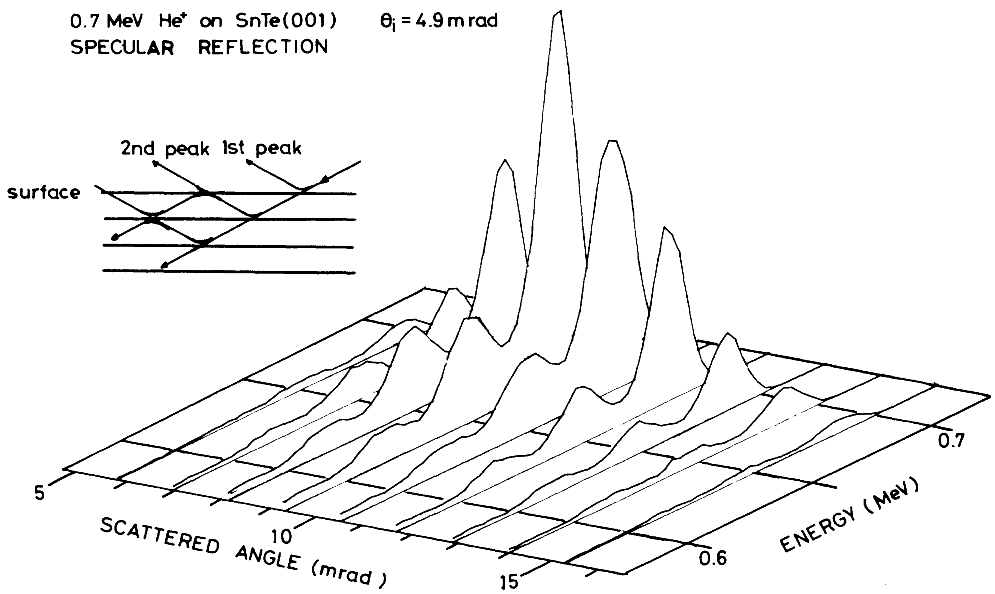

FIG. 1. Energy spectra of scattered He^+ ions for various scattering angles when 0.7-MeV He^+ ions are incident on SnTe(001) surface with a glancing angle 4.9 mrad. The inset shows the reflection of ions at surface atomic planes.

ions in SnTe traveling for one wavelength of the channeling motion was derived from the surface oscillation seen in the RBS spectra. The obtained energy losses are shown in Fig. 3. They coincide with the energy spacing between adjacent peaks. This indicates that the ions of the first peak are reflected from the surface atomic plane, and others penetrate through the surface and travel for a few wavelengths of oscillatory motion in the (001) channel before appearing from the surface as described by the inset in Fig. 1. This penetration of ions through the surface atomic plane is caused by the thermal vibration of surface atoms, electronic scattering, and surface lattice defects.

The feature of the observed energy spectra of the reflected protons at the glancing angle incidence is different from that of He ions. The oscillatory feature is not observed in the energy spectra of scattered protons

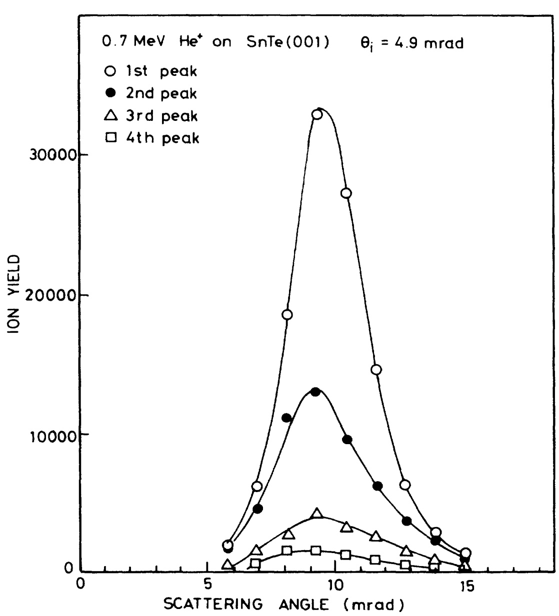

FIG. 2. Dependence of scattered He^+ ion yields of each peaks on the scattering angle when 0.7-MeV He^+ ions are incident on SnTe(001) surface with a glancing angle 4.9 mrad; first peak (○), second peak (●), third peak (△), and fourth peak (□).

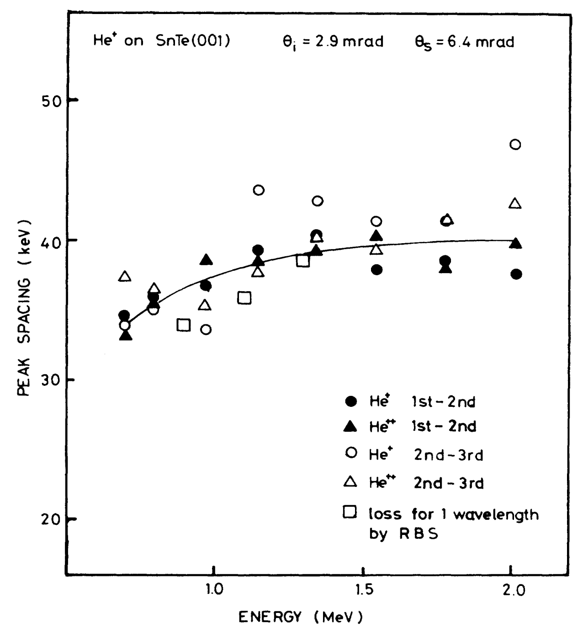

FIG. 3. Dependence of the energy spacing between adjacent peaks on the incident energy for a glancing angle 2.9 mrad and a scattering angle 6.4 mrad. The spacings between the first peak and second peak for scattered He^+ (●) and He^{2+}(▲), those between the second peak and third peak for scattered He^+ (○) and He^{2+} (▲) are shown. The energy loss of (100) channeled He ions in SnTe traveling for one wavelength of the channeling oscillation is also shown by □.

but only one peak is observed at the energy that is slightly smaller than the energy of incident ions. This may be due to the fact that the energy loss of protons for one wavelength of channeling oscillation is smaller than the energy resolution of the detector.

Figure 4 shows the most probable energy loss of the first peak as a function of the scattering angle when 0.7-MeV He^+ ions are incident on a SnTe(001) surface with the glancing angle 4.9 mrad. The most probable energy loss shows a broad peak at the scattering angle of specular reflection and the energy loss of scattered He^{2+} ions is slightly larger than that of He^+ ions especially for the small scattering angle.

The dependence of the most probable energy loss of the specularly reflected He ions on the glancing angle when 0.7 MeV He^+ ions are incident on SnTe(001) surface is shown in Fig. 5. The energy losses of the scattered He^{2+} are slightly larger than those of He^+ ions and both of them are independent of the glancing angle.

Figure 6 shows the dependence of the most probable energy loss of specularly reflected protons on the glancing angle when 0.7 MeV protons are incident on a SnTe(001) surface. The most probable energy loss of protons is also independent of the glancing angle.

Figure 7 shows the dependence of the most probable energy loss of the specularly reflected He ions on the energy when He^+ ions are incident on a SnTe(001) surface with the glancing angle 2.9 mrad. The energy loss is almost independent of the energy of incident ions and slightly smaller than half of the energy spacing between adjacent peaks.

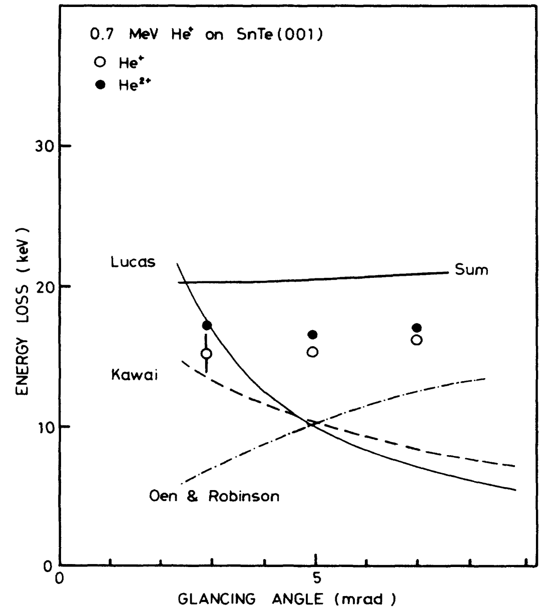

FIG. 5. Dependence of the most probable energy loss of the specularly reflected He^+ ions (○) and He^{2+} ions (●) on the glancing angle when 0.7-MeV He^+ ions are incident on SnTe(001) surface. The typical experimental error is shown. The energy loss calculated from the model of Lucas (——), that of Kawai *et al.* (— — —), and that of Oen and Robinson scaled by the stopping power of Ziegler (—·—·—·) are shown. The sum of the energy loss of Kawai *et al.* and that of Oen and Robinson is also shown by a solid line.

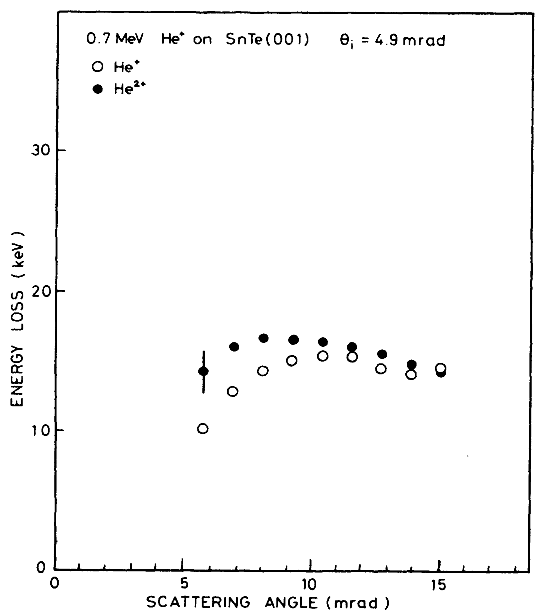

FIG. 4. Dependence of the most probable energy loss of the first peak on the scattering angle when 0.7-MeV He^+ ions are incident on SnTe(001) surface with a glancing angle 4.9 mrad. The typical experimental error is shown. The result of the scattered He^+ ions (○) and that of scattered He^{2+} ions (●) are shown.

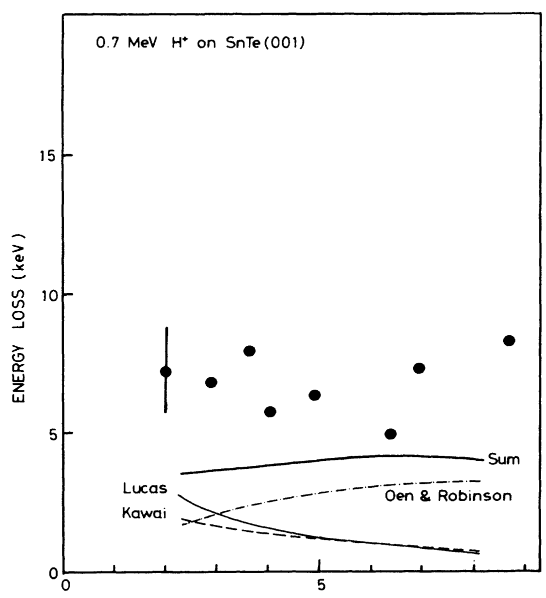

FIG. 6. Dependence of the most probable energy loss of the specularly reflected protons on the glancing angle when 0.7 MeV protons are incident on SnTe (001). The typical experimental error is shown. The calculated results similar to Fig. 5 are also shown.

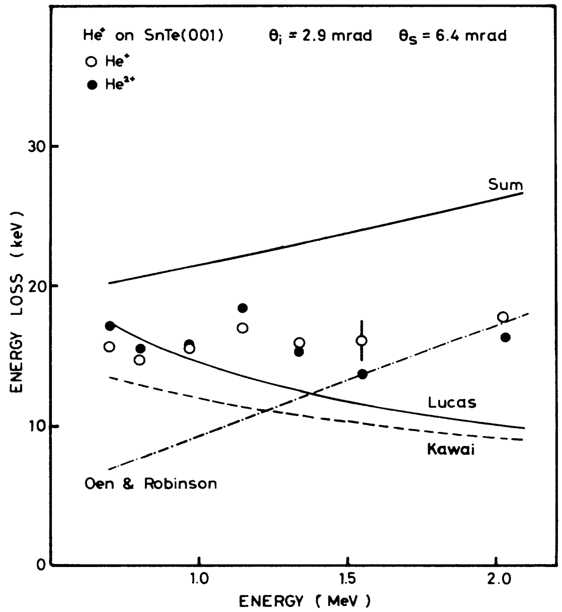

FIG. 7. Dependence of the most probable energy loss of the specularly reflected He^{+} ions (○) and He^{2+} ions (●) on the incident energy when He^{+} ions are incident on SnTe(001) surface with the glancing angle 2.9 mrad. The typical experimental error is shown. The calculated results similar to Fig. 5 are also shown.

IV. DERIVATION OF THE POSITION-DEPENDENT STOPPING POWER NEAR THE SURFACE

The energy loss of specularly reflected ions can be written by

$$\Delta E = \int s(x)\,dz \ , \tag{1}$$

where $s(x)$ is the position-dependent stopping power at distance x from the surface and the trajectory of ions lies on the x-z plane. The integration is performed along the ion trajectory. The trajectory of specularly reflected ions can be calculated with the use of continuum surface potential constructed by surface atoms. Molière potential is employed in the calculation of the continuum potential and the first and second terms of Molière potential are neglected because the closest approach of the specularly reflected ions to the surface is larger than $4a_{\mathrm{TF}}$ for the present experimental conditions. The error of this approximation is less than 2%. The image potential is neglected in the calculation of trajectory as it is very small for MeV-light ions.[6] Using these approximations and assuming the apex of the trajectory is at zero on the z axis, the trajectory of the ion can be written as

$$x(z) = \frac{a_{\mathrm{TF}}}{\beta_3} \ln \left[\frac{2\pi n_p Z_1 Z_2 e^2 a_{\mathrm{TF}} \alpha_3}{E\theta_i^2 \beta_3} \cosh^2 \left[\frac{\beta_3 \theta_i z}{2a_{\mathrm{TF}}} \right] \right] , \tag{2}$$

where a_{TF} is the Thomas-Fermi screening distance, n_p is the atomic density of the surface, Z_1 is the atomic number of the incident ion, Z_2 is that of the target atom, E is the ion energy, θ_i is the glancing angle, and α_3, β_3 are the constants for the Molière potential. Substituting Eq. (2) into Eq. (1), the energy loss of a specularly reflected ion can be written as

$$\Delta E = \frac{4a_{\mathrm{TF}}}{\beta_3 \theta_i} \int_{X_1}^{\infty} S(X/\theta_i)(X^2 - X_1^2)^{-1/2} dX \ , \tag{3}$$

where $X = \theta_i \exp(\beta_3 x / 2a_{\mathrm{TF}})$, $X_1 = (2\pi n_p Z_1 Z_2 e^2 a_{\mathrm{TF}} \alpha_3 / E\beta_3)^{1/2}$, and $S(X/\theta_i) = s(x)$. The observed energy losses are independent of θ_i as can be seen in Figs. 5 and 6, so $S(X/\theta_i)$ must be proportional to $(X/\theta_i)^{-1}$, i.e.,

$$s(x) = A(E) \exp \left[-\frac{\beta_3 x}{2a_{\mathrm{TF}}} \right] . \tag{4}$$

Substituting Eq. (4) into Eq. (3), the integration can be performed,

$$\Delta E = A(E) \left[\frac{2\pi a_{\mathrm{TF}} E}{\alpha_3 \beta_3 n_p Z_1 Z_2 e^2} \right]^{1/2} . \tag{5}$$

Since the observed energy loss is independent of the ion energy as can be seen in Fig. 7, $A(E)$ must be proportional to $E^{-1/2}$. Thus the stopping power near the surface of SnTe(001) is derived as

$$s(x) = CE^{-1/2} \exp \left[-\frac{\beta_3 x}{2a_{\mathrm{TF}}} \right] , \tag{6}$$

where C is $\Delta E(\alpha_3 \beta_3 n_p Z_1 Z_2 e^2 / 2\pi a_{\mathrm{TF}})^{1/2}$. The constant C is determined to be 7700 $\mathrm{MeV}^{3/2}\,\mathrm{cm}^{-1}$ for He ions and 2000 $\mathrm{MeV}^{3/2}\,\mathrm{cm}^{-1}$ for protons from the experimental results. The obtained position-dependent stopping power for 0.7-MeV He ions is shown in Fig. 8.

V. DISCUSSION

The crystal surfaces used in the present experiment were not ideal surfaces. They had a few macroscopic steps, which were introduced during the cleavage of the substrate KCl crystal. These steps have no effect on the trajectories of the observed specularly reflected ions, because the ions incident on the side surfaces of the steps penetrate inside the crystal and hardly escape from the crystal with small energy losses. Steps with atomic height also existed on the surface. The ions which encounter such step risers are scattered so strongly that they are not detected in the direction of specular reflection. Thus, the observed energy losses are due only to the ions which are specularly reflected at the surface.

It is known that the energy loss of fast ions in solids consist of two parts, one is the loss due to the collective collision with valence electron gas and the other is that due to the single collision with core electrons. It was pointed out that the collective collision plays an important role in the energy loss of fast ions at the surface.[7,8] Lucas has given a formula of energy loss of ions reflected at a solid surface due to the excitation of the surface plasmon.[7] The calculated energy losses of specularly reflected ions are shown in Figs. 5–7 with the use of the surface plasmon energy 10.5 eV for SnTe. The calculated losses are smaller than the experimental results and the dependence on the glancing angle and that on the energy differ

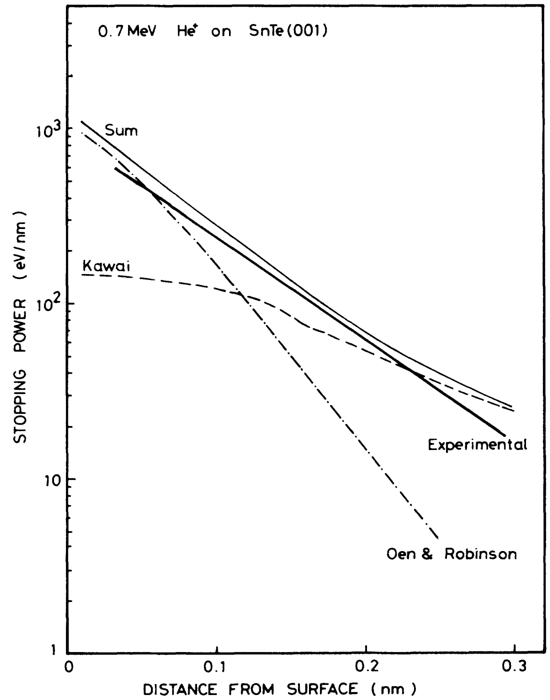

FIG. 8. Position-dependent stopping power of 0.7-MeV He ions near the surface of SnTe(001) derived from the experimental results. The calculated one with the model of Kawai *et al.* (— — —), that of Oen and Robinson scaled by the stopping power of Ziegler (—·—·—·) and the sum of those (——) are also shown.

from those of experimental results.

Kawai *et al.* have derived the position-dependent stopping power of ions near the surface taking account of the excitation of both the bulk and surface plasmons.[8] The position-dependent stopping power calculated from their model is shown for 0.7-MeV He ions in Fig. 8. The electronic surface is taken outside of the surface atomic plane by half of the interplanar separation as carried out by Kawai *et al.* The calculated stopping power is smaller than the experimental one and the deviation is large for small x. The calculated energy losses of specularly reflected ions are also shown in Figs. 5–7. The calculated losses are almost equal to those calculated with the model of Lucas and do not agree with the experimental results.

The difference between the experimental and calculated results may be due to the single collision between the ion and electrons near the surface. However, the theory is not satisfactory for the single collision energy loss near the surface so far. Oen and Robinson have given the inelastic energy loss of ions scattered by an atom with impact parameter r,

$$Q(r)=(0.045KE^{1/2}/\pi a_{\mathrm{TF}}^2)\exp(-0.3r/a_{\mathrm{TF}}) , \quad (7)$$

where K is a parameter.[9] This formula was not derived from a rigorous theoretical model but was chosen to follow approximately the electron density around the atom and describes the single collision of ions with electrons. They used this formula in the computer simulation of the reflection of low-energy light ions at solid surface. This formula is applicable to the ions moving fast enough to apply the impulse approximation, but still slow enough that velocity-proportional stopping power is appropriate. It is not adequate to use this formula without any modification in the energy region of the present experiment. In order to compare this formula with the present experimental results, the pre-exponential factor is changed so that the stopping cross section calculated from this formula coincides with that calculated from Ziegler's semiempirical formula.[10] Taking account of this modification, the position-dependent stopping power for the specularly reflected ions can be written as

$$s(x)=\frac{0.09n_p Sx}{\pi a_{\mathrm{TF}}^2}K_1(0.3x/a_{\mathrm{TF}}) , \quad (8)$$

where S is the stopping cross section of the crystal atom and $K_1(z)$ is a modified Bessel function. The calculated result is shown in Fig. 8 for 0.7-MeV He ions. The calculated result is nearly equal to the experimental one for small x, but the deviation becomes large for large x.

The sum of the stopping power derived by Kawai *et al.* and that derived by Oen and Robinson is shown in Fig. 8. The agreement between this sum and the experimental result is good. The energy losses of specularly reflected ions calculated from the sum of the position-dependent stopping power of Kawai *et al.* and that of Oen and Robinson are shown in Figs. 5–7. The dependence of the calculated energy loss on the glancing angle is similar to the experimental one, but that on the ion energy is different from the experimental one.

The position-dependent stopping power for planar channeled ions was derived from the energy loss spectra of planar channeled He and I ions transmitted through a thin gold single crystal,

$$s(y)=s_0+s_1[\cosh(\beta_3 y/2a_{\mathrm{TF}})-1] , \quad (9)$$

where y is the distance from the channel center and s_0 and s_1 are constants. Assuming that the present results describe the stopping power of the single atomic plane the position-dependent stopping power for the planar channeled ions is derived from the present results as

$$s(y)=s'\cosh(\beta_3 y/2a_{\mathrm{TF}}) , \quad (10)$$

where s' is a constant. This stopping power is similar to Eq. (9) except for the constant term s_0-s_1. This constant term may be due to the collision with valence electrons.

VI. CONCLUSION

It has been observed that the energy spectrum of scattered MeV He ions from a clean (001) surface of SnTe single crystal at glancing angle incidence consists of several well-defined peaks. The peak of the highest energy corresponds to the ions reflected at the first atomic layer. The observed energy losses of specularly reflected MeV light ions are independent of both the glancing angle and the incident energy. The position-dependent stopping powers at the surface have been derived from the observed energy losses for protons and He ions. The obtained position-dependent stopping power is similar to the position-dependent stopping power for the planar channeled ions. The obtained stopping power can be almost explained by the theoretical models with suitable choice of a fitting parameter, though the energy dependence of it is slightly different from the prediction by the theoretical models.

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[1]M. Hou and C. Varelas, Appl. Phys. A **33**, 121 (1984).

[2]H. Winter, Nucl. Instrum. Methods Phys. Res. B **2**, 286 (1984).

[3]K. Morita, Rad. Eff. **52**, 235 (1980).

[4]M. Mannami, K. Kimura, K. Nakanishi and A. Nishimura, Nucl. Instrum. Methods Phys. Res. B **13**, 587 (1986).

[5]S. Datz, C. D. Moak, T. S. Noggle, B. R. Appleton, and H. O. Lutz, Phys. Rev. **179**, 315 (1969).

[6]Y. H. Ohtsuki, K. Koyama, and Y. Yamamura, Phys. Rev. B **20**, 5044 (1979).

[7]A. A. Lucas Phys. Rev. B **20**, 4990 (1979).

[8]R. Kawai, N. Itoh, and Y. H. Ohtsuki, Surf. Sci. **114**, 137 (1982).

[9]O. S. Oen and M. T. Robinson, Nucl. Instrum. Methods **132**, 647 (1976).

[10]J. F. Ziegler, *The Stopping and Ranges of Ions in Matter* (Pergamon, New York, 1980), Vol. 4.

[11]M. T. Robinson, Phys. Rev. **179**, 327 (1969).