Acceleration of convoy electrons by surface wake produced at glancing-angle scattering of fast ions from a single-crystal surface

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Convoy electrons produced at glancing-angle scattering of MeV H, He, Li, and C ions from a clean (001) surface of SnTe single crystal are studied. Acceleration of the convoy electrons is observed. The observed acceleration increases with increasing atomic number of the projectile ion as predicted by the surface-wake-acceleration model. The classical-trajectory Monte Carlo simulation is performed with the surface-wake-acceleration model in order to study the acceleration of the convoy electrons. The agreement between the calculated results and the experimental ones is reasonably good.

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I. INTRODUCTION

Convoy electrons produced at glancing-angle scattering of fast ions from solid surfaces have been investigated for the past several years [1-9]. It was found that the observed most-probable velocity of the convoy electrons is faster than the velocity of the projectile ion [2,4-8]. This acceleration was explained in terms of the surface wake induced by the projectile ion near the surface [2]. Rough estimations of the acceleration were performed with the surface-wake-acceleration model [2,6-8]. Although the calculated results explained qualitatively the observed acceleration, the quantitative agreement was not satisfactory. Recently, Iitaka et al. performed a classicaltrajectory Monte Carlo simulation in order to explain the experimental results quantitatively [10]. However, they used a simple ion-image dipole potential instead of the surface-wake potential and they neglected the surfacewake potential induced by the convoy electron itself. In the present work, we perform a classical-trajectory Monte Carlo simulation using the surface-wake potential in order to calculate the acceleration of the convoy electrons produced at glancing-angle scattering of fast ions from solid surfaces. The calculated results are compared with our observations of convoy electrons produced at glancing-angle scattering of 0.05-0.65-MeV/amu H⁺, He⁺, Li^{+-3+} , and C^{+-4+} ions from a clean (001) surface of SnTe single crystal.

II. EXPERIMENT

A single crystal of SnTe(001) was prepared by epitaxial growth *in situ* by vacuum evaporation of pure SnTe (99.999%) on a cleavage (001) surface of KCl in an UHV chamber. The crystal was mounted on a five-axis highprecision goniometer. Beams of 0.05-0.65-MeV/amu H⁺, He⁺, Li⁺⁻³⁺, and C⁺⁻⁴⁺ ions from the 1.7-MV Tandetron accelerator of Kyoto University were collimated to 0.1×0.1 mm² by a series of apertures. The beam current was monitored by a vibrating beam chopper installed before the scattering chamber. The energy spectrum of secondary electrons emitted at the glancing-angle scattering of the ions was measured by a 30° parallel-plate electrostatic analyzer ($\Delta E / E = 0.023$, acceptance half-angle is 25 mrad), which was able to rotate around the target. The entrance focus of the analyzer was placed on the center of the crystal surface. The glancing incidence angle of the ions was 6 mrad, which was smaller than the critical angle for the specular reflection.

The ions reflected from the target surface at the scattering angle of the specular reflection were selected by an aperture ($\phi 0.2 \text{ mm}$) placed 400 mm downstream the target. The ions passing through the aperture were resolved into their charge states by an analyzing magnet and the charge-state distribution was measured.

III. EXPERIMENTAL RESULTS

Figure 1 shows examples of the observed energy spectra of the secondary electrons emitted at the glancingangle scattering of 0.3-MeV/amu H⁺, He⁺, Li⁺, and C^{2+} ions. All spectra show a broad convoy electron peak around 200 eV. The energy of the electron isotachic to the incident ion is shown by a vertical line. Although the peak energy of the convoy electrons coincides with the vertical line for the incidence of H⁺ ions, the peak energies are larger than the energy shown by the vertical line for the other ions. The peak energy and the width of the peak increase with increasing atomic number of the projectile ion, Z_1 . Figure 2 shows the ratio of the observed peak energy to the energy of the electron isotachic to the incident ion as a function of the ion energy. The ratio does not depend on the incident charge state and decreases with increasing ion energy. Figure 3 shows the emission-angle dependence of the convoy electron yield at the glancing-angle incidence of 0.3-MeV/amu Li⁺ ions. The yield shows a broad peak at an emission angle \sim 150 mrad. As compared with the foil-transmission experiment, the emission-angle distribution is very broad. This cannot be attributed to the angular distribution of the reflected ions, because the scattering angle distribution of the reflected ions has a peak at the scattering angle of the specular reflection (12 mrad in the present case) and the width is about 5 mrad [11].



FIG. 1. Energy spectra of secondary electrons emitted in the forward direction at a glancing-angle incidence of 0.3-MeV/amu H⁺, He⁺, Li⁺, and C²⁺ ions on the SnTe(001). The glancing incidence angle was 6 mrad and the electrons emitted in the direction at 100 mrad from the surface plane were energy analyzed. The energy of the electron isotachic to the incident ion is shown by a vertical line.



FIG. 2. Energy dependence of the observed most-probable energy of the convoy electrons produced at a glancing-angle incidence of $H^+(+)$, $He^+(\blacksquare)$, $Li^+(\odot)$, $Li^{2+}(\bullet)$, $Li^{3+}(\circledcirc)$, $C^+(\blacktriangle)$, $C^{2+}(\bigtriangleup)$, $C^{3+}(\blacktriangledown)$, and $C^{4+}(\nabla)$ on the SnTe(001). The ordinate shows the ratio of the most-probable energy of the convoy electrons to the energy of the electron isotachic to the incident ion. Calculated results for H ions (thin solid curve), He ions (dashed curve), Li ions (dot-dashed curve), and C ions (thick solid curve) are also shown.



FIG. 3. Emission-angle distribution of the convoy electrons produced at a glancing-angle incidence of 0.3-MeV/amu Li⁺ ions on the SnTe(001). The typical experimental error is shown by a bar. Calculated result is also shown by a histogram.

IV. MONTE CARLO SIMULATION

The response of surface electrons to the charged particle traveling near the surface has been studied by many authors [12]. The projectile induces an oscillatory electric field, called "surface wake potential" or "dynamic image potential" behind it. Using a plasmon-pole approximation for the dielectric function, the surface-wake potential induced by a projectile ion with a charge +qe moving parallel to the surface (x direction) at z_i outside the solid can be written as [13]

$$\phi = -(qe\omega_{s}/v)\int_{0}^{v/v_{F}} d\zeta J_{0}(\omega_{s}\zeta\sqrt{y^{2}+(z_{i}+z)^{2}}/v) \\
\times \exp(-\omega_{s}\zeta x/v)/(1+\zeta^{2}) \\
+(2qe\omega_{s}/v)\sin(\omega_{s}x/v)\Theta(-x) \\
\times \int_{0}^{v/v_{F}} d\zeta J_{0}(\omega_{s}\zeta\sqrt{y^{2}+(z_{i}+z)^{2}}/v)/(1+\zeta^{2}),$$
(1)

where ω_s is the surface-plasmon frequency (0.386 a.u. for SnTe), v the ion velocity, v_F the Fermi velocity, J_0 denotes the zero-order Bessel function, $\Theta(x)$ the unit-step function, and the origin of the coordinates system is on the electronic surface and moves with the ion. The electronic surface is taken outside of the atomic surface by half of the atomic plane separation [14], which is 3.0 a.u. for the SnTe(001) surface. An example of the calculated surface-wake potential is shown in Fig. 4. It can be seen from Fig. 4 that the surface wake decelerates the projectile ion itself. This is one of the origins of the surface stopping power for the ion. If there is a convoy electron around the ion, the convoy electron is accelerated by the surface wake. It should be noted that the electron receives the force not only in the x direction (parallel to the surface) but also in the z direction (perpendicular to the surface,), although it cannot be seen from Fig. 4.



FIG. 4. Surface-wake potential induced by a 1-MeV H^+ ion traveling parallel to the SnTe(001) surface at a distance 2 a.u. from the electronic surface. The potential on the plane, which contains the ion and is parallel to the surface plane, is shown.

The motion of the convoy electron produced by the ion traveling near the surface can be numerically calculated within the framework of the classical mechanics taking account of the surface wakes induced by both the ion and the electron itself and the Coulomb interaction between the ion and the electron. In the previous study [4], it was shown that the convoy electron is produced when the He ion is at a distance \sim 4 a.u. from the atomic surface on the outgoing trajectory of the ion. As the surface potential for the electron is sufficiently small at 4 a.u. from the atomic surface, it can be neglected in the calculation of the motion of the convoy electron and the straight line approximation can be used for the outgoing ion trajectory. The observed mean charge of the scattered ions was used as the ion charge qe. The classical-trajectory Monte Carlo simulation was performed with the following initial conditions. (i) the electron is produced when the ion is at 4 a.u. from the atomic surface on the outgoing trajectory. (ii) the energy of the electron in the ion rest frame is zero. (iii) the electrons are distributed uniformly on a sphere of radius r_0 with its origin at the ion. The value of r_0 used in the simulation will be discussed later. (iv) the velocity distribution of the electrons is isotropic in the ion-rest frame.

Many trajectories of the electrons were calculated with the above initial conditions. Some electrons penetrate inside the solid mainly due to the surface-wake potential induced by the electron itself (e.g., 20% for the incidence of 0.3-MeV/amu He ions). These electrons cannot be observed as convoy electrons. The trajectory calculation was stopped when the electron leaves 20 a.u. away from the electronic surface, where the surface-wake potential is negligibly small. At this final position, some electrons have negative energies in the ion-rest frame and so they are bound to the ion. Thus only some fraction of the electrons (e.g., 40% for the incidence of 0.3-MeV/amu He ions) are observed as convoy electrons. The energies of the convoy electrons produced by 0.3 MeV/amu He ions are calculated with various r_0 (0.5 < r_0 < 4 a.u.). The calculated mean energy hardly depends on r_0 . Therefore we used $r_0 = 2$ a.u. throughout the simulation.

Figure 5 shows the calculated energy distribution of the convoy electrons at the glancing-angle scattering of 0.3-MeV/amu H, He, Li, and C ions from the SnTe(001) surface. The results for the electrons emitted at an emission angle 100 mrad within a window 100×100 mrad² are shown. The observed mean charges of the scattered ions, which were used in the calculation, were $q = 3.9 \pm 0.3, 2.4 \pm 0.2, 1.9 \pm 0.1, and 0.99 \pm 0.05$ for C, Li, He, and H ions, respectively. All distributions have a broad peak at energies larger than the energy of the electron isotachic to the ion (which is shown by a vertical line in Fig. 5) showing that the electrons are accelerated by the surface wake. The peak energy increases with increasing ion charge, because the surface-wake potential is proportional to the ion charge, as can be seen from Eq. (1). Although the agreement between the calculated peak energies and the observed ones is fairly good, the calculated peak widths are narrower than the observed results especially for the ions of large Z_1 . This is partly attributed to the neglect of the charge-state distribution of the projectile ions. The electrons produced by ions with different charge states receive different accelerations. Consequently, the energy distribution becomes broader. Taking account of the charge-state distribution, the agreement between the calculated and observed results can be improved.

The energy spectra of convoy electrons emitted at an emission angle 100 mrad within a window $50 \times 50 \text{ mrad}^2$ were calculated with various ion energies. Because it was difficult to determine the peak energy due to the poor statistics (see Fig. 5), we calculated the mean energy of the convoy electrons, which is considered to be almost



FIG. 5. Calculated energy distributions of the convoy electrons produced at glancing-angle scattering of 0.3-MeV/amu H ions, He ions, Li ions, and C ions. The energy of the electron isotachic to the incident ion is shown by a vertical line.

equal to the peak energy as can be seen from the observed energy spectra (Fig. 1). Calculated ion-energy dependence of the mean energy of the convoy electrons produced by the glancing-angle scattering of H, He, Li, and C ions is shown by curves in Fig. 2. The acceleration decreases with increasing ion energy because the surfacewake potential decreases with increasing ion energy, as can be seen from Eq. (1). The agreement between the calculated and observed results is reasonably good.

Calculated emission-angle distribution of the convoy electrons for the 0.3-MeV/amu Li incidence is shown by a histogram in Fig. 3. The distribution shows a broad peak around 120 mrad and the characteristic features of the calculated distribution reproduce the observed result. The peak angle ~ 120 mrad is much larger than the exit angle of the specularly reflected ion (6 mrad in the present case). This difference is also attributed to the surface-wake potential. The convoy electron is accelerated not only in the x direction but also in the z direction by the surface-wake potential, as mentioned above. Consequently, the emission angle of the convoy electron becomes larger than the exit angle of the ion.

In the present simulation, we neglected elastic- and inelastic-scattering processes of the convoy electrons with target electrons. It is known that these scattering pro-

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cesses play an important role in the transport of convoy electrons in solids [15]. As the convoy electron interacts with the target electrons even outside the solid, these scattering processes can affect the behavior of the convoy electrons studied in the present paper. The modification of the simulation code including these scattering processes is now in progress.

In summary, we have observed the acceleration of convoy electrons produced at glancing-angle scattering of MeV H, He, Li, and C ions from the SnTe(001) surface. The classical-trajectory Monte Carlo simulation with the surface-wake-acceleration model is performed in order to explain the experimental results. The calculated results reproduce the characteristic features of the experimental results.

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