Stopping power of a KCl(0 0 1) surface for low energy Ne atoms

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Abstract

Energy losses of specularly reflected ions from a KCl(0 0 1) surface at grazing incidence of 15–30 keV Ne⁺ ions are measured in order to investigate the effect of the large band gap on the surface stopping power for low energy projectiles. The position-dependent stopping power of the KCl(0 0 1) surface for Ne projectile is derived from the observed energy losses. Because the direct electron excitation by the projectile–electron collision, which is the dominant stopping mechanism for low energy projectiles at metal or semiconductor surfaces, is almost prohibited at insulator surfaces due to the large band gap, the surface stopping power of the KCl(0 0 1) is expected to be much smaller than those of metals or semiconductors. The obtained stopping power is, however, found to be comparable to that of the SnTe(0 0 1) surface, which is a typical narrow-gap semiconductor. Charge exchange processes probably make an important contribution to the stopping at the KCl(0 0 1) surface for the low energy Ne projectile.

1. Introduction

The mechanism of slowing down of fast ions at solid surfaces has been extensively studied during the last two decades in particular for metal and semiconductor surfaces [1–8]. To investigate the stopping power of a solid surface, the technique of specular reflection of ions is often used. The specular reflection of ions refers to the phenomenon that most of the ions are scattered from the atomically smooth surface in the direction of specular reflection without penetrating into the inside of the solid when the ions are incident on the surface at a glancing angle. This technique enables us to investigate the stopping power in front of the solid surface by measuring the energy loss of specularly reflected ions. Naturally, the stopping power of the surface is dependent on the distance from the surface. However even the position-dependent stopping power can be obtained from the energy loss data for various angles of incidence since one can control the impact parameter from the surface by changing the incident angle of ions.

For swift projectiles with the velocity $V$ larger than the Fermi velocity $v_F$, both the plasmon excitation process and the direct electron excitation process equally contribute to the stopping power [1]. On the other hand, for slow projectiles with $V < v_F$, recently we have demonstrated that the
stopping power of a SnTe(001) surface for slow noble gas atoms is explained by the direct excitation only [8]. Energy losses of 15–30 keV He⁺, Ne⁺, Ar⁺ and Kr⁺ ions specularly reflected from the SnTe(001) surface were measured and the position-dependent stopping powers of the SnTe(001) surface for the noble gas atoms were derived from the observed energy losses. The obtained stopping powers showed good agreement with the calculated stopping powers taking account of the only contribution of the direct electron excitation process. This is because the plasmon excitation process is forbidden at \( V < v_F \).

For insulator surfaces, the situation should be different because the large band gap makes the direct electron excitation process less effective. Energy loss by the direct electron excitation can occur only when energy transfer to a target electron exceeds the band gap. Therefore the energy loss on an insulator surface is expected to have a threshold at the energy of the projectile and the stopping power of the insulator surface is expected to be much smaller than that of metals or narrow-gap semiconductors for slow projectiles. Recently, some interesting results about stopping of slow protons on wide band gap insulators have been reported. Eder et al. [9] measured the energy loss of slow protons (2–10 keV) traversing thin foils made from large band gap insulators (Al₂O₃, SiO₂ or LiF) and no threshold effects are observed. The authors attribute the results to local reduction of the band gap of the target in collisions of the projectiles with target atoms. Auth et al. [10] investigated the stopping of slow protons (300 eV–28 keV) scattered from a LiF(001) surface and concluded from the effect of the outgoing charge state that electron capture and loss are dominant mechanisms for the stopping of the slow protons interacting with a wide-gap insulator.

In this work, we investigate the energy losses of 15–30 keV Ne⁺ ions specularly reflected from the KCl(001) surface and determine the position-dependent stopping powers of the KCl(001) surface for low energy Ne atoms. The velocities of the 30 and 15 keV Ne⁺ ions are 0.25 and 0.17 a.u., respectively. The results are compared with those for the SnTe(001) surface in our previous study. The possible stopping mechanism at insulator surfaces in the low velocity region is also discussed.

2. Experimental

A single crystal of KCl was cleaved in air along the (001) plane to obtain an atomically flat KCl(001) surface and mounted on a five-axis precise goniometer in an UHV scattering chamber (base pressure \( 3 \times 10^{-10} \) Torr). After the crystal was heated at 250°C to prepare a clean surface in situ in the UHV chamber, it was kept at 220°C to maintain a clean surface and to avoid surface charging due to the ion beam irradiation. A beam of 15–30 keV Ne⁺ ions from a 30 kV RF ion source was momentum-analyzed with an analyzing dipole magnet and collimated to 0.3 × 0.3 mm² and a divergence angle to less than 0.2 mrad by a series of slit system. The beam was incident on the KCl(001) at angles of incidence \( \theta \), ranging from 5 to 50 mrad with respect to the surface plane. The azimuthal angle of the incident beam was chosen 200 mrad apart from the [1 0 0] axis in order to avoid surface axial channeling. The energy of the scattered (or primary) ions was measured with an energy-analyzing system consisting of a 120° cylindrical electrostatic spectrometer (\( r = 80 \) mm) and a channel electron multiplier. The system could be rotated around the target KCl(001) crystal in the scattering plane which contains the incident beam and the surface normal of the target. The specularly reflected (primary) ions were selected by an entrance aperture of the spectrometer whose diameter was 0.2 mm and acceptance angle was 2 mrad. The ions accepted in the aperture were energy-analyzed by the spectrometer and detected by the channel electron multiplier. The system was controlled by a personal computer. The energy resolution of the spectrometer, \( \Delta E/E \), was 0.3%.

3. Results and discussion

Fig. 1 displays an example of the observed Ne⁺ yield as a function of the scattering angle when 30 keV Ne⁺ ions were incident on the KCl(001) at
\( \theta_s = 16.7 \text{ mrad} \). The ion yield shows a peak at a scattering angle \( \theta_s \sim 2\theta_i \), i.e., at the angle for specular reflection. Similar results were obtained over the whole region of \( \theta_i \) up to 50 mrad for the incidence of 15–30 keV Ne⁺ ions. The energy spectrum of the scattered ions was measured at the angle for specular reflection. Fig. 2 shows an example of the observed energy spectra of specularly reflected ions at glancing-angle incidence of 30 keV Ne⁺ ions on the KCl(0 0 1) surface. The angle of incidence \( \theta_i \) measured from the surface plane is 16.7 mrad. The energy spectrum of the primary 30 keV Ne⁺ ions is also shown by empty circles. The data of the energy spectra are measured with a step width of \( \sim 50 \text{ eV} \) for 30 keV Ne⁺ ions shown in Fig. 2, while the data are measured with a narrower step width of \( \sim 17 \text{ eV} \) for 15 keV Ne⁺ ions. Each of the energy spectra of the primary and reflected ions shows a well-defined peak, which is fitted with a Gaussian depicted by a solid curve. The energy loss \( \Delta E \) of the reflected ions is determined from the difference between the most probable energies of the primary ions and the reflected ions. The obtained energy losses of the specularly reflected ions are shown as a function of the incident angle \( \theta_i \) for the incidence of 30 keV (empty circles) and 15 keV Ne⁺ ions (empty triangles) in Fig. 3. The previous results for 30 and 15 keV Ne⁺ ions specularly reflected from a SnTe(0 0 1) surface are also shown by filled circles and filled triangles, respectively. Typical errors in the energy loss are as small as represented by the size of the symbols in Fig. 3 since the energy loss \( \Delta E \) of the reflected ions is determined from the
difference between the most probable energies of the primary ions and the reflected ions. The fluctuation of the most probable energies of the primary ions which was estimated by repeated measurements was much smaller than the full width at half maximum of the energy peak of the primary ions, for example, seen in Fig. 2. The energy losses at the KCl surface increase roughly in proportion to the incident angle \( \theta \), for both 30 and 15 keV Ne\(^+\) ions. The energy loss for 30 keV Ne\(^+\) ions is about twice as large as that for 15 keV Ne\(^+\) ions over all the region of \( \theta \). The energy loss at the KCl(0 0 1) surface at the small \( \theta \) is much less than that at the SnTe(0 0 1) surface for the corresponding ion incidence.

Utilizing a well-defined trajectory of the reflected Ne projectile, a position-dependent stopping power \( S(x) \) for Ne projectiles at the distance \( x \) from the surface can be derived from the observed energy loss \( \Delta E(\theta) \) [1,5]. The energy loss \( \Delta E(\theta) \) is expressed by integrating \( S(x) \) along the trajectory, which is described by the continuum surface planar potential \( U(x) \).

\[
\Delta E(\theta) = \int_{\text{traj.}} S(x) \, dz
= 2\sqrt{E} \int_{x_m}^{\infty} \frac{S(x)}{\sqrt{U(x_m) - U(x)}} \, dx,
\tag{1}
\]

where \( E \) is the ion energy and \( x_m \) the closest approach distance to the surface. In Eq. (1), the ion trajectory lies on the \( xz \)-plane where the \( x \)-axis is perpendicular to the surface and the origin is on the surface atomic plane. Eq. (1) is an Abel-type integral equation and \( S(x) \) is solved as

\[
S(x) = \frac{U'(x)}{2\pi E} \left[ \sqrt{E} \left( \frac{U(x)}{E} \right) \Delta E(0) \right.
+ \int_0^{\pi/2} \Delta E \left( \sqrt{\frac{U(x)}{E}} \sin u \right) \, du \bigg].
\tag{2}
\]

The position-dependent stopping powers \( S(x) \) of the KCl(0 0 1) surface for 15 and 30 keV Ne projectiles is obtained from the observed energy losses with the Molière approximation to the Thomas–Fermi screening function for the continuum surface planar potential \( U(x) \) in Eq. (2). The potential \( U(x) \) is represented as

\[
U(x) = 2\pi n_p Z_1 Z_2 \rho e^2 a_{TF} \sum_{i=1}^{3} \frac{x_i}{\beta_i} \exp \left( - \beta_i x / a_{TF} \right),
\]

\[
a_{TF} = 0.4685 (\sqrt{Z_1} + \sqrt{Z_2})^{-2/3},
\tag{3}
\]

where \( Z_1, Z_2 \) are the atomic numbers of the projectile and the target atoms, \( n_p \) is the atomic density of the surface plane and \( a_{TF} \) is the Thomas–Fermi screening radius. \( \{x_i\} = \{0.35, 0.55, 0.1\} \), \( \{\beta_i\} = \{6.0, 1.2, 0.3\} \). The potential \( U(x) \) is obtained as the sum of the potentials due to the surface K and Cl atoms. The image potential is neglected since almost all the projectiles are expected to be neutralized and stay neutral near the surface even if re-ionized on their outgoing trajectories. The obtained stopping powers are shown in Figs. 4(a) and (b), respectively. The previous results for the stopping powers of the SnTe(0 0 1) surface for 15 and 30 keV Ne projectiles are also depicted by dashed curves for comparison. The stopping powers of the KCl(0 0 1) surface decrease exponentially with the distance from the surface as the case of the SnTe(0 0 1) surface. Contrary to the expectation discussed above, the obtained stopping power of the KCl(0 0 1) surface is comparable to that of the SnTe(0 0 1) surface. Comparing Figs. 4(a) and (b), it can be seen that the stopping power for 30 keV Ne is about 1.4 times as large as that for 15 keV Ne, indicating that the stopping power is proportional to the projectile velocity.

In our previous study, the stopping power of the SnTe(0 0 1) surface for low energy noble gas projectiles was explained by the direct electron excitation by the projectile–electron collision [8]. This mechanism is responsible for the stopping powers of metals or narrow band gap semiconductors, but is no longer effective for large band gap insulators at low projectile energies because the energy gain of the target electron by the projectile–electron collision cannot exceed the band gap. The maximum energy gain of the electron which takes place in the case of the head-on collision is \( m[(2V + v_i)^2 - v_i^2]/2 \), where \( v_i \) is the velocity of the target electron. In the present case where \( V = 0.17 \) a.u. for 15 keV Ne and \( v_i = 0.81 \)
a.u. for 3p electrons in Cl atoms, the maximum energy gain is calculated to be 9 eV, which is of the same order of the KCl band gap energy, 8.7 eV [11,12]. Therefore the direct electron excitation is expected to make little, if any, contribution to the stopping power. However, the experimental stopping power of the KCl(001) surface is comparable to that of the SnTe(001) surface, indicating existence of another stopping mechanism at the KCl(001) surface.

Firsov [13] proposed a stopping mechanism for slow projectiles in terms of capture and loss of electrons between the projectile and the target atoms during the collision (Firsov model). The energy loss during the collision at the impact parameter $b$ is given by

$$W(b) = \frac{0.35(Z_1 + Z_2)^{5/3} V}{\left[1 + 0.16(Z_1 + Z_2)^{1/3} b\right]^5},$$

in atomic units. Summing up the energy loss $W(b)$ due to the surface atoms, the position-dependent stopping power for a projectile traveling parallel to the surface at the distance $x$ from the surface atomic plane is given as

$$S_p(x) = 2n_p \int_0^\infty W\left(\sqrt{x^2 + y^2}\right) dy,$$

$$= 2n_p \int_0^{\pi/2} W(x/\cos \theta) \frac{x}{\cos^2 \theta} d\theta. \quad (5)$$

The stopping power of the KCl(001) surface is obtained as sum of stopping powers due to surface K atoms and Cl atoms. The calculated stopping powers of the KCl(001) with Eq. (4) are shown by dotted curves in Fig. 4. Although the calculated stopping power decreases more slowly than the experimental result, the calculated result agrees roughly with the experimental one, in particular near the surface ($x \sim 1$ A), suggesting that the stopping power of the KCl(001) surface can be explained in terms of charge exchange processes.

Recently, Eder et al. [9] measured the electronic stopping cross section of slow hydrogen projectiles in large band gap insulators at a few keV where the direct electron excitation is prohibited. They found no influence of the large band gap on the velocity dependence of the stopping cross section. They suggested that the electron promotion process due to the formation of molecular orbitals (MO) contributes substantially to the stopping power for slow protons. Although the Firsov model described above contains an idea of the formation of
a pseudo-molecule consisting of the slow projectile and the target atom, Eq. (4) is derived on some assumptions that each electron distribution of the projectile and the target atom is given by the Thomas–Fermi model even in the collision. Better agreement between the present experimental result and theoretical calculation might be obtained if detailed calculation is performed with the MO process taken into account.

4. Conclusions

Energy losses of specularly reflected ions from a KCl(0 0 1) surface at grazing incidence of 15–30 keV Ne$^+$ ions are measured. Position-dependent stopping powers of the KCl(0 0 1) surface for Ne projectiles are derived from the observed energy losses. The obtained stopping powers are comparable to those of the SnTe(0 0 1) surface although the large band gap of KCl forbids the direct electron excitation process which is the dominant stopping mechanism for SnTe at the present energy region. The surface stopping power calculated with the Firsov model gives rough agreement with the present experimental result, suggesting that the stopping due to the charge exchange processes is responsible for the present result.

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References