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Neutralization of low-energy D^+ scattered from solid surfaces

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In this study, some of the fundamental aspects of neutralization of low-energy (10–300-eV) D^+ ions have been addressed in comparison with that of He^+ ions. To examine the role of the valence-band structure in determining neutralization rates for D^+, a range of target materials has been studied (Mo, Ta, Ag, Pb, BaF_2, CsCl, LiCl, AgCl, $PbCl_2$, etc.). The surface peak of D^+ is extremely small compared with that of He^+ in scattering from metal surfaces, while the contrary is sometimes true in scattering from ionic compounds such as alkali-metal halides and alkaline-earth halides. It is found that the neutralization of D^+ depends on the local electronic states of the target atom and occurs via the resonant neutralization by *s*- or *d*-band electrons of the metal atoms or via an energy-level-crossing mechanism between D 1*s* and the closed *p* band of the anions. The reason why the neutralization probability for D^+ is very much enhanced compared with that for He^+ is that the surface electronic state relevant to the resonant neutralization of D^+ is not a level but a broad valence band (band effect). It is concluded that the smaller ionization energy of deuterium than helium results in strong coupling of the D 1*s* level with the valence band.

I. INTRODUCTION

Scattering and neutralization of ions at surfaces is one of the well-established fields of physics and of great scientific and technological interest. From a purely applied point of view, the interest in this subject has been related to the generation of ion beams and to plasma-wall interaction problems in fusion devices. So far, many experiments on bombardment of solid surfaces with ions have been made to elucidate the structure and composition of surfaces.[1–4] However, the study of the charge transfer has also attracted considerable attention over the past years because it is closely related to reactive events at surfaces. In fact, it has been illustrated that the low-energy reactive ion bombardment of a metal surface provides a unique opportunity to explore the particle-surface chemical interaction,[5–10] bridging the gap between chemisorption experiments (thermal energy molecules) and high-energy (a few keV) ion-bombardment experiments. Particularly, numerous experimental and theoretical studies have been devoted to the scattering of atomic hydrogen ions from solid surfaces because it is one of the simplest reactive scattering systems.[11–14] However, it cannot be said that the mechanism of the charge exchange between hydrogen ions and solid surfaces is well understood. For He^+ scattering, ions which are scattered by surface atoms are more likely to remain ionized than those emerging from the bulk, and accordingly form so-called surface peaks in their energy distribution. But a surface peak for H^+ scattered from metallic surfaces is usually very small or completely absent.[11,13] These remarkable phenomena could be ascribed to a difference in the charge exchange processes for H^+ and He^+. It is believed that charge capture occurs via both one-electron resonant and two-electron Auger processes in which many states of the surface atoms may be involved simultaneously.[15,16] However, the relative role of these neutralization processes is not well characterized. In addition, the remarkable differences between H^+ and He^+ scattering cannot be well explained on the basis of these processes. Eckstein and co-workers[11,13] have proposed a more localized neutralization model based on the adiabatic maximum rule in which ions are neutralized most effectively when the impact velocity is given by

$$v = a\Delta E/\hbar , \quad (1)$$

where a is a distance of atomic dimensions and ΔE is the difference of the ionization energy of the projectile and the binding energy of the target atoms. According to this model, the maximum of the neutralization probability for H^+ lies at several keV while it is far higher for He^+, and hence the disappearance of the H^+ surface peak in the keV range seems to be attributed to this effect. In the case of He^+ scattering, however, it has recently been claimed that reionization of neutral He atoms can easily occur provided that the He 1*s* orbital is promoted to a molecular state during collision.[17–23] Hence, the criterion of the electronic transition given by Eq. (1) can be satisfied even at fairly small kinetic energies due to the effective reduction of ΔE. Thus, there is still a lack of understanding of the observed phenomena and more experimental data might stimulate further theoretical investigations.

The other possibility of the lack of the surface peak would be the small cross section of H. Indeed, since surface collisions are more important for heavier incoming projectiles at a smaller collision energy, it is expected that the surface scattering is relatively enhanced at smaller kinetic energies although the neutralization might occur more efficiently. These arguments suggest that the surface peak is possibly too small or too narrow to be detected in the experimental conditions used so far. Despite these interesting aspects, very little work has been done on the interactions of H^+ with solid surfaces for the primary energy E_0 ranging below a few hundred eV. In this paper, we discuss the mechanism of the charge transfer between low-energy (10 eV $< E_0 <$ 300 eV) D^+ ions and solid surfaces and demonstrate the band effects on the electronic transition probability. Specifically, the D^+ scattering experiments have been performed at metallic surfaces as well as ionic compound surfaces in order to investigate effects of the band structure on the neutralization probability of D^+. It is found that D^+ scattered from metallic elements such as Ag, Pb, Ba, Ta, and Mo is neutralized with an extremely high probability due to the resonant electronic transition from a broad valence band to the empty D 1*s* level, while neutralization by the Cl 3*p* band electrons, occurring mainly due to the energy-level crossing mechanism above a threshold energy of 20 eV, is fairly small in probability compared with the resonant process.

II. EXPERIMENTAL

The experimental method has been described earlier[18] and only the features important to this experiment are briefly summarized. The sample chamber was evacuated down to an ultrahigh vacuum (UHV) condition (3×10^{-9} Pa) and equipped with facilities for low-energy ($10-10^4$ eV) ion-scattering spectroscopy (ISS), low-energy electron diffraction (LEED), ultraviolet photoelectron spectroscopy (UPS), and a differentially pumped sample evaporator. The D^+ and He^+ ions were generated in a discharge-type ion source and were mass analyzed by a Wien filter. Ion intensities of 1×10^{-8} A/cm^2 are currently used in ISS experiments so as to minimize surface decomposition due to the ion bombardment. The energy spread of the beam was measured to be about 1 eV. The ion source was attached to the sample chamber through two differentially pumped vacuum chambers containing lens systems so that the pressure in the sample chamber was kept below 1×10^{-8} Pa during the measurements. The ion beams were incident upon a surface with a glancing angle of $\alpha=80°$ and ions reflected with a scattering angle of $\theta_L=160°$ were analyzed by a hemispherical electrostatic energy analyzer operating with a constant energy resolution of 1 eV by retardation or acceleration of the ions. The potential difference between the exit slit of the analyzer and the entrance of the channel electron multiplier is kept at a constant value of 1 keV in order to avoid effects arising from the energy dependence of the detector efficiency.

As described in the following sections, specimens with different electronic band structures were carefully selected to investigate the band effects on the neutralization probability. The experiments were made both with pure elements such as Mo, Ta, Ag, Pb, and C, together with compounds like AgCl, $PbCl_2$, BaF_2, CsCl, and LiCl. The single crystals with (111) faces of Mo, Ta, and BaF_2 and a (110) face of diamond were prepared following sample cleaning procedures described in the literature.[24–27] The other samples were polycrystalline thin films *in situ* deposited on graphite in thermal evaporation. It is known from the electron microscopy,[28] optical studies,[29,30] UPS,[31–33] and ISS,[18] that an evaporated thin film of these compounds is a good system for studying bulk chloride properties. The cleanliness of these samples was ensured by the preliminary ISS measurements. The single-crystalline samples showed very sharp 1×1 structures in LEED patterns.

III. RESULTS

Figure 1 shows the energy distributions of D^+ ions (E_0 = 100 eV) backscattered from (a) a clean Mo(111) surface and (b) an oxygen-adsorbed Mo(111) surface. These data are normalized in intensity through beam currents. The ideal binary-collision energies corresponding to Mo and O are indicated by arrows on the abscissa. In contrast to the previous work in which no special feature for scattering from a surface atom is observed,[11,34] a clear surface peak of D^+ ions scattered from surface Mo atoms is observed at the clean surface. We assigned this peak to

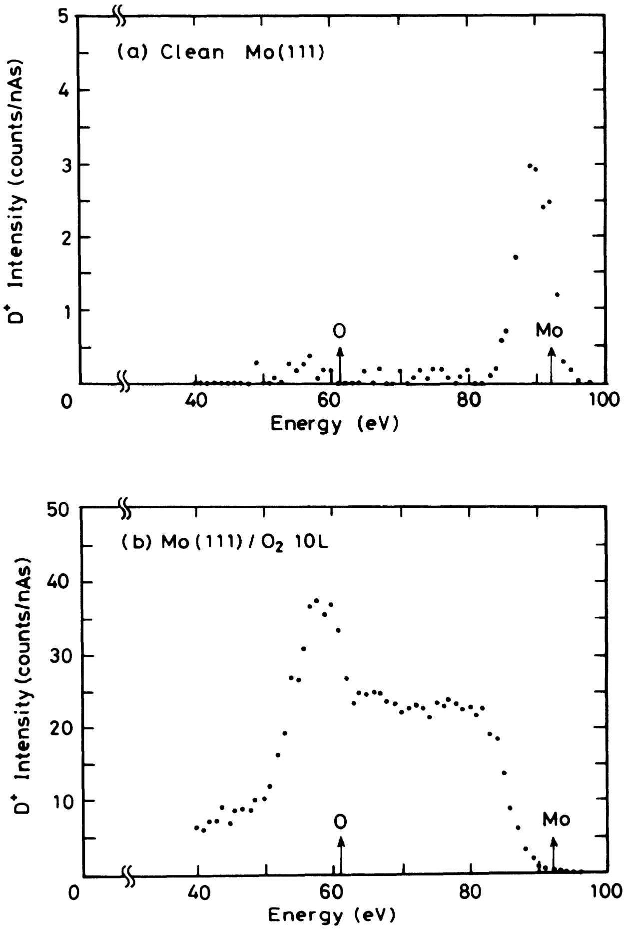

FIG. 1. Energy spectra of D^+ ions scattered from (a) the clean Mo(111) surface and (b) the Mo(111) surface exposed to a 10-L O_2 gas. The intensity is normalized through beam currents. The measurements were made using a E_0=100-eV D^+ beam at a fixed scattering geometry, $\alpha=80°$, $\theta_L=160°$. The energies corresponding to elastic binary collision are indicated by arrows on the abscissa.

a surface peak from the fact that the spectral peak shape and the angular dependence of the intensity are quite similar to those of He^+ scattering.[35] If this surface is saturated with oxygen exposure of 10 L (1 $L=1$ langmuir$=1\times10^{-6}$ Torr s$=1.3\times10^{-4}$ Pa s), the D^+ spectrum changes drastically: a large increase in the D^+ intensity with increasing oxygen exposure was observed.[11] The spectrum is broad, extending from a maximum energy down to zero energy. Although the surface peak corresponding to oxygen is clearly observed, the Mo surface peak disappears completely. The disappearance of the Mo surface peak cannot be accounted for only due to the shadowing effect by the adsorbed oxygen atoms because a Mo surface peak is observed twice as large as an O surface peak in the case of the He^+ scattering under the same conditions. This example clearly shows that the probability for detecting deuterium as an ion depends strongly on the chemical state of the surface. The extended background intensity comes from D^+ scattered after significant penetration into the solid. Comparing the experiments of ionization of a neutral D^0 beam, we can assign this background to reionization of D^0 neutralized somewhere in the path. The experimental details will be presented elsewhere.[35]

From the above result, it is found that the appearance of the surface peak is strongly dependent on the species of target element or the chemical state of the surface. In the following, therefore, we shall focus on these subjects. As described in Sec. I, one of the most interesting points should be the difference between D^+ and He^+ scattering. Listed in Table I are the intensity ratios of the surface peaks for D^+ scattering [I(D^+)] to those for He^+ scattering [I(He^+)]; the intensities, taken at $E_0=100$ eV, are normalized relative to each other through beam currents. The surface peaks appear with high intensity in He^+ scattering from all these target elements while they are below the detection limit in D^+ scattering from Ta, Ag, and Pb. Even for the case of Mo(111) shown in Fig. 1(a), the surface peak is exceedingly small compared with that for He^+ scattering. On the contrary, the surface peak for each element of $BaF_2(111)$ is larger in D^+ scattering than in He^+ scattering. This is the case not only for BaF_2 but also for other ionic compounds such as CsCl and LiCl. This remarkable contrast implies that an electronic state of the metallic surface contributes significantly to the neutralization of D^+.

Figure 2 shows energy spectra of D^+ ions of $E_0=100$ eV measured at (a) the $BaF_2(111)$ surface, (b) the metallic Ba surface, and (c) the Ba surface exposed to 100-L oxygen gas, the intensity of each spectrum being normalized through beam currents. It is found that the spectral peaks from Ba and F atoms in Fig. 2(a) consist of two peaks, *A* and *B*. These peaks originate from surface scattering and are not attributable to multiple scattering because the energy differences between the two peaks are independent of E_0 over a wide range from 50 to 500 eV.

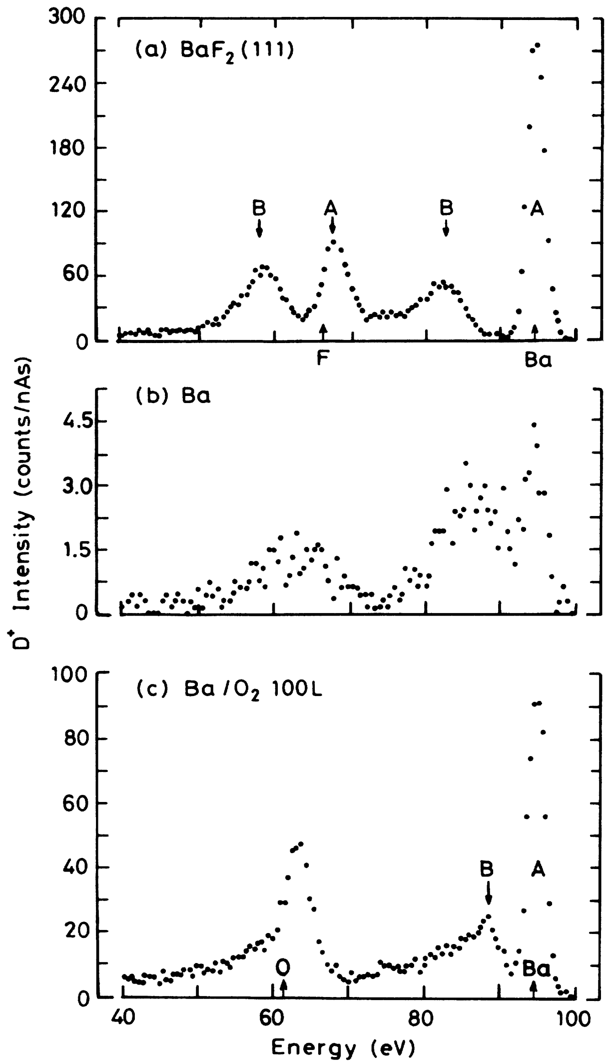

FIG. 2. Energy spectra of $E_0=100$ eV D^+ scattered from (a) the $BaF_2(111)$ surface, (b) the metallic Ba surface obtained by electron beam bombardment, and (c) the oxygen-saturated Ba surface. The measurements were made under the same condition as in Fig. 1.

TABLE I. The surface peak intensity of D^+ relative to that of He^+ for six target elements at $E_0=100$ eV. The intensities determined by integrating the areas under the surface peak are normalized relative to each other through beam currents.

					$BaF_2(111)$	
	Mo(111)	Ta(111)	Ag	Pb	Ba	F
$I(D^+)/I(He^+)$	0.017	$<5\times10^{-4}$	$<5\times10^{-3}$	$<3\times10^{-3}$	14.8	1.7

Therefore, peak *A* is due to quasielastic single scattering and peak *B* is due to inelastic single scattering. Accordingly, the energy difference between peaks *A* and *B* is the inelastic energy loss which is hereafter referred to as *Q*. The *Q* value for Ba (F), measured to be 10.5 eV (9 eV), is comparable to the band-gap energy of BaF_2 or the ionization energy of D^0, so that peak *B* is suggested to be due either to excitation of a valence electron to the conduction band or to reionization of D^0. The similar energy-loss structure has been observed in the He^+ spectra from the same surface except for an additional third loss peak in the F peak.[18]

As shown in Fig. 2(b), the spectral peaks decrease in intensity by irradiation of a $E_0=500$-eV electron beam with a dose of about 10 mC/cm^2. It is well known that the electron bombardment removes the fluorine atoms from the (111) surface of the alkaline-earth fluorides and leaves a metallic surface.[36] If this surface is exposed to 100-L oxygen, the surface peak of Ba increases again by a factor of about 20 and a clear oxygen surface peak appears. The small surface peak in Fig. 2(b) at about 60–65 eV, resembling that in Fig. 2(c) in the peak position, may be due to oxygen contamination from the residual gas, so that the D^+ intensity at the entirely clean Ba surface is far smaller than that shown in Fig. 2(b). Two peaks *A* and *B* are clearly observed in the Ba peak at the oxidized surface; the *Q* value (6 eV) is smaller than that at the $BaF_2(111)$ surface, corresponding instead to the band gap of BaO. This result clearly indicates that loss peak *B* is not due to reionization but due to the interband electronic transition.

The experimental result that the surface peak of D^+ scattered from the metal atoms appears in Fig. 2(c) but not in Fig. 1(b) can be ascribed to the differences in the neutralization effect and/or the shadowing effect, depending on the arrangement of the surface oxygen atom. As described earlier, however, the complete absence of the surface peak in Fig. 1(b) is not ascribed only to the steric shadowing effect.[35] In terms of the ion neutralization effect, there are the following two possibilities: (1) The neutralization probability is dependent on the species of the target elements. (2) Existence of the band gap for ionic compounds breaks an important neutralization process of D^+. In order to investigate these possibilities, we have measured energy spectra of $E_0=100$-eV D^+ ions scattered from ionic compounds of Ag and Pb for which no surface peak appears in the elemental surfaces. The results taken for evaporated thin films of chlorides such as (a) AgCl, (b) $PbCl_2$, and (c) CsCl are shown in Fig. 3. The surface peaks corresponding to Cl and Cs appear intensely while those of Ag and Pb disappear even for the chloride surface. It should be noted that in He^+ scattering surface peaks of these elements have been observed clearly.[18] These results might suggest that a local electronic transition process is responsible for the disappearance of the Ag and Pb surface peaks.

Figure 4 shows the D^+ energy spectra from the polycrystalline LiCl film measured at kinetic energies of (a) 100 eV and (b) 50 eV. The spectra are composed of two clearly separated peaks *A* and *B* with a very small background intensity. This is because D^+ scattered from Li, which would contribute to the background intensity, has such a small energy, shown by the arrow, that the background overlaps with a large tail of the secondary ions. One may think that the surface peak of Li disappears similar to that for Ag or Pb. However, this assumption is discarded because the Li peak is clearly observed in the H^+ scattering. Because of the simple structure of the spectral peaks, we can readily measure the energy dependence of the D^+ peak intensities for scattering from Cl and the results are shown in Fig. 5. Both peaks *A* and *B* have broad maxima around 150 and 200 eV followed by monotonically decreasing regions. This type of yield curve has been explained by Smith[37] using a monotonically decreasing differential scattering cross section and a monotonically increasing probability of the scattered ion remaining ionized. Of greater interest is the smaller energy region where the behavior of the two peaks contrasts sharply; the threshold energy for appearance of the loss

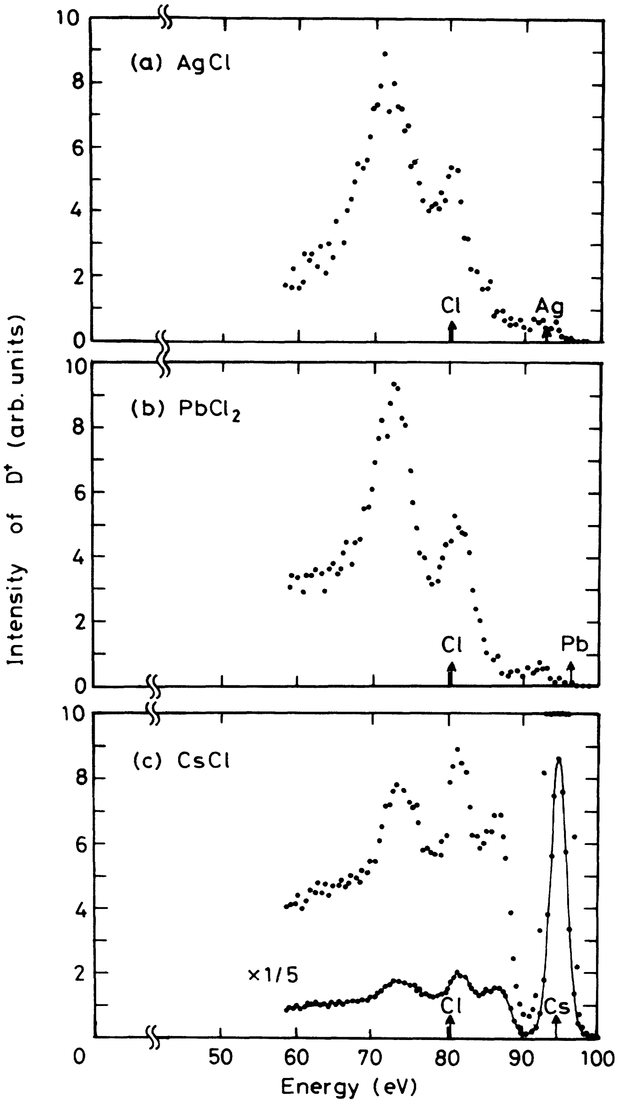

FIG. 3. Energy spectra of $E_0=100$-eV D^+ scattered from evaporated thin films of (a) AgCl, (b) $PbCl_2$, and (c) CsCl.

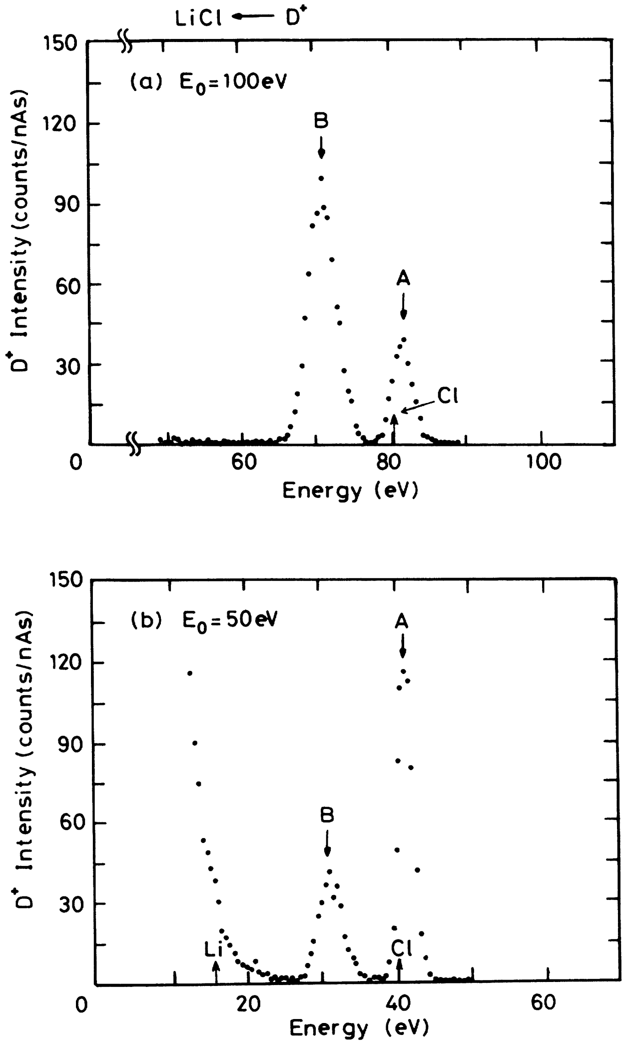

FIG. 4. Energy spectra of D^+ scattered from an evaporated thin film of LiCl at a primary beam energy of (a) 100 eV and (b) 50 eV.

peak *B* is measured to be about 20 eV, and the maximum in intensity of peak *A* is seen around this energy. A similar energy dependence of the peak intensities has been reported in He^+ scattering and attributed to the electronic transition due to the molecular overlap mechanism.[19–21]

IV. DISCUSSION

The dependence of the scattered D^+ intensity upon surface electronic structures has been obtained under identical experimental conditions. Comparison of metal surfaces with ionic compound surfaces allows the discussion of the neutralization mechanism of D^+ ions. Schematically shown in Fig. 6 are band structures of the surfaces examined in the present study. Two fundamental mechanisms by which ion neutralization can occur are Auger neutralization (AN) and resonant neutralization (RN). The resonant tunneling described so far is relevant to the excited 2*s* or 2*p* state,[38,39] but it may not be responsible for the remarkable differences between D^+ and He^+ scattering which are detailed in Sec. III. This is because the excited states of D^+, located at a farther energy position from the Fermi level than those of He^+, are probably not relevant to the preferential neutralization of D^+. On the other hand, the Auger process can contribute to neutralization of the D^+ ions similar to that of the He^+ ions. The appearance of the D^+ surface peak at the ionic compound surfaces can be attributable to the breakdown of AN since AN of D^+ is forbidden at the ionic compound surfaces due to the remarkable band-gap energy and the small ionization energy of deuterium. It is certain that AN is one of the main causes for the disappearance of the surface peak in the D^+ energy spectra, but the target-material dependence of the neutralization probability cannot be explained only by AN and should be ascribed to a more localized neutralization process; that is, the experimental result that the surface peaks of Ag and Pb are not observable even in the ionic compound while those of O, F, Cl, Cs, and Ba appear intensively at the compound surfaces indicates that electronic states localized at each target element are relevant to neutralization of D^+. This is also supported by the facts that the surface peak of Ba is observed with a considerable intensity only in its compound form in which the Ba 5*s* electrons are completely transferred to the anion *p* state, and that the surface peak of carbon cannot be observed in D^+ scattering from both graphite and diamond despite the fact that diamond has a large band-gap energy of 6 eV. From this context, the neutralization of D^+ on Ag^+ (AgCl) and Pb^{2+} ($PbCl_2$) is caused by the Ag 4*d* and Pb 6*s* electrons, respectively, since the Ag 5*s* and Pb 6*p* states become essentially empty conduction bands for their compound form. The D^+ scattering from the oxidized

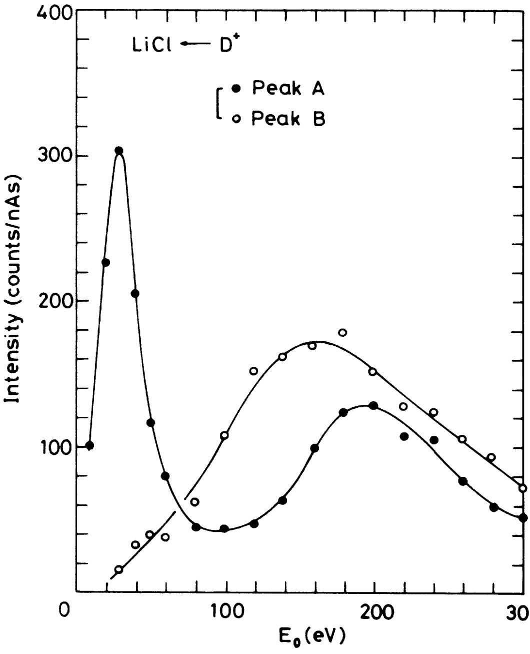

FIG. 5. Intensity of spectral peaks *A* and *B* in D^+ scattering from Cl at LiCl as a function of the primary beam energy.

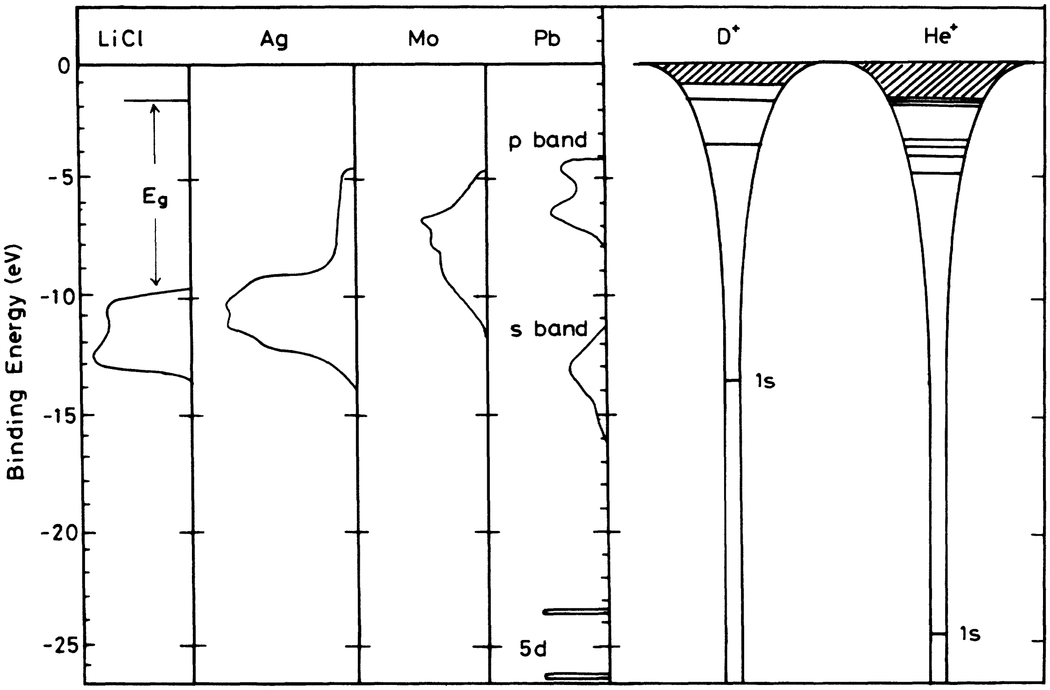

FIG. 6. Density of states of the targets used in this study and the energy level diagram of D^+ and He^+ ions.

Mo(111) and Ta(111) surfaces causes no surface peaks corresponding to the metal atoms. The oxide formed on these metal surfaces may be a metallic compound with low oxidation numbers (MoO_2, TaO), so that the metal *d* electrons relevant to the neutralization of D^+ are not perfectly transferred to the O 2*p* state.

In the case of the He^+ scattering, the following two local electronic transition processes have been described: (1) If an inner-shell *d* level of the target atom is located within 5 eV of the ground-state He 1*s* level, the He^+ ion is neutralized due to the quasiresonant neutralization process (QRN).[40] If the QRN occurs, pronounced oscillations in the scattered ion yield are observed as a function of the kinetic energy. (2) If the 1*s* orbital of He^+ ($1s\sigma$ orbital) is promoted in the molecular state due to antibonding interaction with a target core orbital, the energy-level crossing (ELC) of the $1s\sigma$ orbital with a surface valence band results in neutralization of He^+ ions or excitation of the valence electrons.[20,21] The promotion of the $1s\sigma$ orbital is strongly dependent on the species of the target elements and is suppressed in case an almost-filled *d* orbital of the target is located at a shallower energy position than the vacant −24.6-eV level of He^+ and no QRN process takes place. With respect to D^+ scattering, since the vacant 1*s* orbital (−13.6 eV) is located at a fairly shallow energy position compared to that of He^+, the interaction of the D 1*s* level with the valence band is more likely to occur. As D^+ approaches the surface, its 1*s* orbital may shift due to the image force effect or the interaction with the target core orbitals and can readily cross with a broad valence band. If ELC takes place during scattering, a large decrease in intensity of ions surviving neutralization occurs simultaneously with the appearance of a loss peak due to surface electronic excitation.[19–21] The energy dependence of the D^+ intensities shown in Fig. 5, indeed, is the evidence of the ELC process in which the D 1*s* orbital crosses with the closed Cl 3*p* band above a threshold energy of about 20 eV. Similar effects on the electronic transition can be seen in D^+ scattering from oxygen or fluorine atoms shown in Fig. 2. As regards D^+ scattering from Ba^{2+} and Cs^+ shown in Figs. 2 and 3, the ion can capture or excite an electron localized at the adjacent anion site due to the long-range interaction via the ELC process.[19–21] Consequently, the spectral features resulting from the interaction between the D 1*s* level and the anion *p* orbital are quite similar to those of He^+ scattering.[41]

Also of interest is the neutralization of D^+ by Ag^+ and Pb^{2+} ions shown in Figs. 3(a) and 3(b), for which no threshold energy for the appearance of the surface peak is observed in the energy range from 10 to 300 eV. This implies that the neutralization of D^+ on these elements is not due to ELC but due to (Q)RN. As for the resonant tunneling process, it has been pointed out that the charge-transfer probability is dependent strongly on the bandwidth *W*;[38,42] thus at small *W*, the neutralization probability oscillates as a function of the kinetic energy due to the quantum-mechanical interference effects. But since the electron once transferred to the band escapes away from the target within a finite lifetime ($\sim\hbar/W$), the interference effects fade away with increasing *W*. Then the averaged neutralization probability increases from 0.5 at the narrow-band limit to unity at the wide-band extreme. As has been indicated,[43] moreover, an excitation energy of a few eV required for D 1*s* to overlap with the valence band can be supplied only by the image charge effects for ordinary solid surfaces. Since the metallic surface has an extended *sp* band, resonant neutralization can occur with a probability close to unity. In the case of ionic compounds, the valence-band width is far smaller than that of metallic surfaces since the cation *s* and *p* bands become an empty conduction band which is separated from the valence band by the band gap. Specifically, the valence band of AgCl is characterized by a strong mixing of the Ag 4*d* state and the Cl 3*p* state and the bandwidth has been reported to be 6 eV.[31,44] Since the lifetime of a hole in this band (1×10^{-16} s) is about one order of magnitude smaller than the collision time of 100-eV D^+ on Ag or Cl, D^+ can be neutralized completely due to resonant neutralization (RN). The case for D^+ on Pb^{2+} due to the Pb 6*s* band is similar. It should be emphasized here that although RN due to the Ag 4*d* or Pb 6*s* band is quite specific, RN due to the anion *p* band seems less pronounced despite the resonant condition being met satisfactorily in energy. This effect is not quite clear at present but may be due to the orbital symmetry effects: the orbital symmetry of the target atomic level and the vacant ionic level are of essential importance for description of the molecular state. For example, in He^+ scattering the pronounced oscillation due to QRN occurs for *d* levels of the target, while even if the target *p* level satisfies the resonant condition in energy, the electronic transition is due mainly to ELC and the oscillation is not clearly observed.[18,40] The promotion of the $1s\sigma$ orbital formed in collision with He is suppressed only by the target *d* orbital, but *p* and *f* orbitals of the target have no pronounced effects on the promotion.[18,20] The D^+ results may also reflect these effects.

The effects of the bandwidth on the probability for (Q)RN can be observed in many other ion-surface combinations: He^+ scattering from Pb yields remarkable oscillations in ion yields due to QRN between He 1*s* and Pb 5*d* levels, whereas D^+ scattering from Pb results in an extremely small ion yield due to RN between the D 1*s* level and the Pb 6*s* and 6*p* bands (see Table I). The surface peak of D^+ from graphite and the diamond (110) surface disappears completely and the background intensity caused by reionization is the main feature of the spectra.

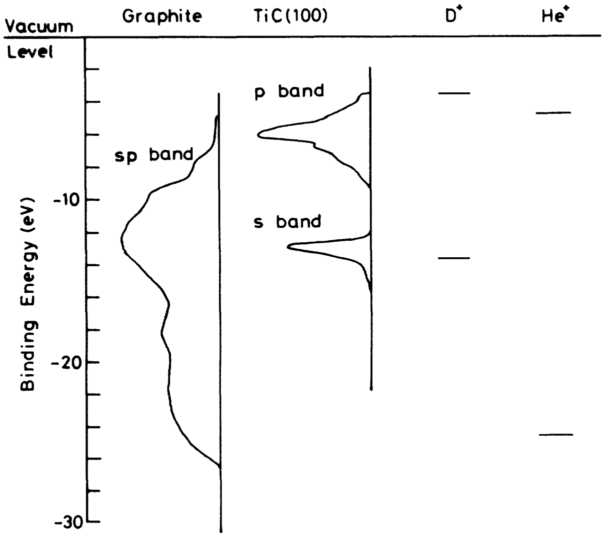

FIG. 7. Density of states of graphite and titanium carbide in the study of the charge exchange of D^+ and He^+ with surfaces.

Figure 7 shows the electronic band structure of the graphite[45,46] as well as titanium carbide.[47] In terms of the sp^2 or sp^3 bonding of carbon, the valence bandwidth is so large (exceeding 20 eV) that RN gives rise to the disappearance of the surface peak of D^+. This is also the case even for the He^+ scattering since, as shown in Fig. 7, the bottom of the valence band of graphite reaches the energy position of the He 1*s* level. Indeed, no surface peak is observed in He^+ scattering from graphite in the energy range below 1 keV. In contrast to this, the surface peak of C has been clearly observed in He^+ scattering from the TiC(100) surface.[48,49] This can be interpreted in terms of the characteristic band structure of TiC shown in Fig. 7: there is a strong covalent mixing between Ti 3*d* and C 2*p* orbitals, and therefore the C 2*s* band is isolated from the C 2*p* band.[47] Because of the small bandwidth and the shallower energy position of the carbon 2*s* or 2*p* band, RN of He^+ scattered from TiC must not be possible. This provides the reason why the surface peak of carbon appears in the He^+ spectra from transition-metal carbides.

V. CONCLUSIONS

From an extensive survey of the charge-exchange behavior in low-energy D^+ scattering, a number of important observations can be made. The most significant is the effect of the electronic band structure on the charge-exchange probability. The surface peak of D^+, missing in scattering from ordinary metal surfaces, appears intensively in scattering from alkali-metal halide or alkaline-earth halide surfaces in which the broad *s* band is empty. The interaction of the D 1*s* orbital with the closed *p* band of chlorides occurs due to the energy-level crossing mechanism with a threshold energy of about 20 eV. The surface peaks of Ag and Pb, however, disappear not only for the elemental surface but also for the chloride surface. This is because the resonant capture of the Ag 4*d* or Pb 6*s* electrons by the vacant D 1*s* level occurs with a probability close to unity. The extremely large probability for the resonant neutralization stems mainly from the band effect; e.g., the hole in the Ag 4*d* or Pb 6*s* band is so ready to diffuse into the band within the collision time that the electron transferred to the D 1*s* level cannot return to the band. Further support for this interpretation can be made in the result for He^+ scattering from graphite and transition-metal carbides, which reveals clearly that the valence-band width and the energy position of the bottom of the valence band relative to the ionic 1*s* level influence the charge-exchange process. The D 1*s* level, usually located very close to the bottom of the valence band, readily overlaps with the band only by the image charge effect and hence the electronic transition easily occurs via the resonant neutralization or the energy-level crossing mechanism. On the other hand, since the He 1*s* level is usually located far from the valence band, the 1*s* level interacts with the band only via the indirect Auger process unless the He 1*s* orbital is promoted sufficiently due to antibonding interaction with the target core orbital. It is thus found that the small ionization energy of deuterium compared to helium provides a main cause for such spectral features as the disappearance of the surface peak.

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