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Energy loss of low energy ion N^{+q} grazing on the Al(111) surface*

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The total energy loss of N^{+q} ions (for $v <$ Bohr velocity) grazing on the Al(111) has been simulated without any 'fit' parameter and compared with the experimental data. The energy loss due to the charge exchange, happening before the N^{+q} hits the Al(111) surface, is studied. The present simulation shows that the energy loss strongly depends on the charge state of the projectile and the lattice orientation of Al(111) surface. The calculated total energy loss agrees with experimental data very well.

Keywords: energy loss, charge exchange, grazing
PACC: 3000, 3120, 3440, 3450B

1. Introduction

The recent availability of the sources for the slow highly charged ions (SHCI) has led to a flurry of research activities. One is faced with the interesting problem, how the processes, including electron capture and loss, x-ray emission,[1−3] plasma excitation of electron gas above the solid surface,[4] collision with lattice atoms and the hollow ions (atoms) formation,[5] cause the electronic, nuclear and charge exchange energy loss, when the slow ($v < v_0 =$ Bohr velocity) multicharged ions graze on the solid surface. Several experiments on the energy loss of SHCI in solid targets have been devoted to the study of the effect caused by the projectile charge state. Different conclusions have been extracted from the experiments via transmission through thin foil[6,7] or scattering on the solid surface.[8−13] A remarkable enhancement of energy loss with the initial charge state has been observed in Refs.[7,11] and is differently explained with the pre-equilibrium charge state effect[7] and the presence of inner-shell vacancies.[11] Very recently, Tökési *et al*[14] presented a theoretical study of the dissipative components of the force acting on the SHCI moving in front of a solid surface at a large distance and used it to calculate the energy loss of charged particles at a large distant collisions under various grazing incidence angles. However, the energy loss due to the distant collision is too small as compared with those from transmission and scattering. None of the previous energy loss studies included the energy loss caused by charge exchange, which becomes more effective for highly charged ions because of the complex neutralization process when the multi-charged ions approaching the solid surface. In this paper, based on the experimental results of Ref.[11], we focus our study on the charge exchange and the total energy loss of N^{+q} ions grazing on the Al(111) surface with different incident charge state and azimuthal angle.

2. Interactions of multicharged ions with surfaces

In the present simulation, the target is an ideal single crystal aluminium (Al) with a clean and flat Al (111) surface. The coordinate system is set at a lattice point on the top layer of the solid, with the x-axis parallel to the lattice row orientation ($[10\bar{1}]$) and the z-axis perpendicular to the surface. The azimuthal angle is measured relative to the x-axis. In the vicinity of the surface, at every trajectory point the projectile multicharged ion experiences the forces from two sources: One is from the interaction between

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projectile and the target atom, whose interaction potential can be treated as Coulomb term multiplied by a screening function.[15] This Coulomb force is well approximated by summing all the forces of over 45 lattice atoms lying nearest to the scattering ion. The other is from the interaction between projectile and its image charge caused in the metal, whose potential is described by Echenique's quantum-mechanical self-image potential.[16] By using these forces Newton's equations of motion are solved numerically. Thermal vibrations of the target atoms are taken into account by using random displacements based on Debye model. In the first step, the bulk temperature of 240 K is taken for all crystal atoms.

The interaction of a multicharged ion with the surface is a true many-body problem. The charge transfer occurs mainly through resonant and Auger processes. A theoretical analysis of the neutralization dynamics above the surface has been presented on the basis of the classical over-the-barrier[17,18] in which resonant multi-electron capture of conduction electrons, resonant loss into the unoccupied states of the conduction band, and the intra-atomic Auger de-excitation were considered and the transient formation of hallow atoms was described. In addition, in the close vicinity of the target surface, the outer shell electrons in the projectile can be peeled off by scattering of target surface electrons. In the present simulation we use the same approach in terms of coupled rate equations in which enter the cross sections and rates for capture, loss, peeling off and de-excitation to simplify this fairly complex array of process as in Refs.[18, 19] and references therein:

$$v_\perp(R)\frac{\mathrm{d}}{\mathrm{d}z}P_n(R) = I_{\mathrm{n}}^{\mathrm{c}}(R) - I_{\mathrm{n}}^{\mathrm{l}}(R)P_n(R) - I_{\mathrm{n}}^{\mathrm{p}}(R)P_n(R) + \frac{1}{2}\sum_{n'>n} A_{n,n'}P_{n'}^2(R) - P_n^2(R)\sum_{n'<n} A_{n',n}, \qquad (1)$$

where R is the projectile-surface distance, $v_\perp$ the projectile velocity in the direction normal to target surface, P_n the electron population in the nth shell of the projectile, $I_{\mathrm{n}}^{\mathrm{c}}$ the current of captured electrons, $I_{\mathrm{n}}^{\mathrm{l}}$ the current of electron lost, $A_{nn'}$ the Auger rate of a projectile, and $I_{\mathrm{n}}^{\mathrm{p}}$ the decay constant due to the 'peeling-off' (PO) process.

Accompanying the charge exchange of projectile with the metallic surface, the energy loss takes place. The energy loss caused by an electron exchange can be described as a 'soft' collision, in which momentum conservation only in the direction of incident beam need be imposed.[20] The charge-exchange energy loss is calculated in the same way as in Ref.[20],

$$\Delta E_{\mathrm{cap}} = B_{\mathrm{T}} - B_{\mathrm{P}} + E_{\mathrm{P}}\frac{m_{\mathrm{p}}}{4m_{\mathrm{T}}}\Big(\frac{m_{\mathrm{P}}+m}{m_{\mathrm{P}}} - \frac{B_{\mathrm{T}}-B_{\mathrm{P}}}{E_{\mathrm{P}}} - \frac{m}{m_{\mathrm{P}}}\Big)^2, \qquad (2)$$

$$\Delta E_{\mathrm{loss}} = \frac{1}{2}mv^2 + \frac{m_{\mathrm{P}}}{m_{\mathrm{P}}+m}(B_{\mathrm{P}}+E_{\mathrm{C}}) + E_{\mathrm{P}}\frac{m_{\mathrm{P}}}{4m_{\mathrm{T}}}\left(\frac{B_{\mathrm{P}}+E_{\mathrm{C}}}{E_{\mathrm{P}}}\right)^2, \qquad (3)$$

where ΔE_{cap} and ΔE_{loss} denote the energy losses resulting from the electron capture and loss respectively; m_{P}, m_{T} and m denote the mass of the projectile, target atom and electron respectively; B_{T} and B_{P} the binding energy of the electron to the target and the projectile cores; E_{P} is the projectile energy, v the laboratory-frame velocity of the projectile, E_{C} the mean kinetic energy of electron separated from the projectile.

According to our simulation, the N^{5+} ions become atoms with L-subshell vacancy at about 6 a.u. away from the surface. When the projectile is close enough to reach electron gas of the solid surface (<6 a.u.) and the rate equation (1) does not work any more, we assume the projectile enters the electron gas in the bulk of the solid and adopt an empirical model based on the velocity-dependent electron-stripping criterion in which the ionization degree is in good agreement with experimental values for heavy ions in solid.[21] When the projectile velocity is less than the Fermi velocity of the electron gas, the local-field corrected (LFC) dielectric function can provide a more accurate description of the excitations of the surface electron gas by including the exchange–correlation interaction among the electrons. Based on the low-velocity approximation of the excitations along with the LFC bulk dielectric function, an analytical expression for the position-dependent electronic stopping power has been developed in Refs.[22,23] and can be expressed

as[22]

$$S_e(r_z) = 2k_F^2 \frac{v}{v_F} \int_0^1 \kappa d\kappa [\tilde{\sigma}_n(\kappa)]^2 H(\kappa, r'_z), \qquad (4)$$

where $r'_z = R - r_d$, and r_d is the average atomic radius of the target, R the projectile-surface distance, the term $\tilde{\sigma}_n(\kappa)$ the surface electronic density, and $H(\kappa, r'_z)$ the dielectric character of the target.

3. Results and discussion

In the present work, the electronic and charge-exchange energy losses are included. In addition, nuclear energy loss resulting from the collision of projectile with the target atoms is also automatically switched on in our simulation.

In Fig.1 we plot the charge exchange number and charge exchange energy loss as functions of the initial charge state of projectile N grazing on the Al(111) surface at an incident angle $\theta = 0.7°$. Here the charge exchange works mainly through resonant and Auger processes and happens before the projectile hits the Al(111) surface. So the charge exchange energy loss is completed in front of the surface. As shown in Fig.1, the charge exchange number and charge exchange energy loss increase exponentially with projectile initial charges, and the charge exchange energy loss contributes a lot to the total energy loss for highly charged projectile grazing on the Al(111) surface.

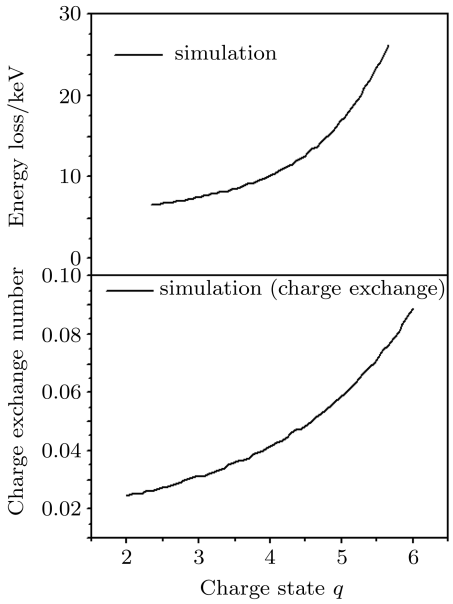


Fig.1. The charge exchange energy loss and the charge exchange number as functions of initial charge state of 140 keV projectile N grazing on the Al(111) under incident angle $\theta = 0.7°$.

As shown in Fig.2, the present calculated total energy loss increases faster and agrees better with the experimental data than that obtained in Ref.[23], in which the same model was used but without charge exchange and elastic energy loss (it is also called nuclear energy loss) switching on.

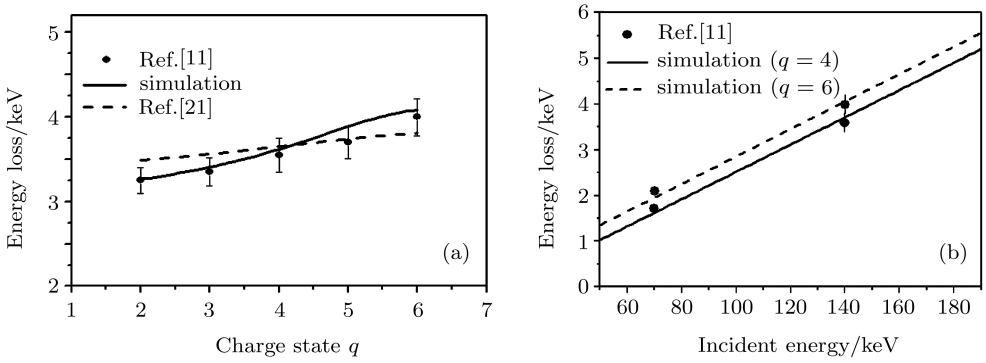


Fig.2. The energy loss as a function of initial charge state and energy of the projectile N grazing on the Al(111) under incident angle $\theta = 0.7°$. (a) the energy loss as a function of initial charge state of projectile with energy 140 keV; (b) the energy loss as a function of incident energy of projectile with charge state $q = 4$ and $q = 6$.

As the increase of initial charge state of projectile, the projectile gets deeper into the electron gas, the scattering angle becomes bigger and the stopping length (here it is the path length of the projectile in the electron gas) becomes shorter. For example, according to our simulation, when charge state of the projectile $q = 6$, the stopping length $L \approx 371$, whereas, when $q = 2$, $L \approx 449$. It means the stopping power (energy loss per unit of stopping length) increases faster than the energy loss as the projectile initial charge state increases. Actually, the stopping length is not a good parameter as used to calculate the

energy loss. It is hard to determine where the path in the electron gas starts and stops since the electron density around the solid surface is position-dependent. As shown in Fig.2, the total energy loss increases linearly with the incident energy; and this also agrees reasonably well with the experimental data of Ref.[11] for the N ion with energy 70 keV and charge states $q = 4$ and $q = 6$.

Figure 3 shows the total energy loss and electronic energy loss as functions of incident angle. Since in both cases the energy loss has the same initial charge state $q = 5$ and incident energy 140 keV, the difference between them is due to the elastic energy loss which increases exponentially with the incident angle for grazing scattering.[24] Therefore, the enhancement of the energy loss observed in Ref.[11] is partly from the enhancement of the charge exchange energy loss and partly from the enhancement of the nuclear energy loss.

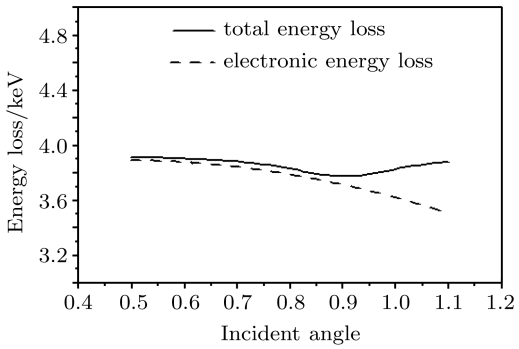


Fig.3. The electronic energy loss and total energy loss as functions of incident angle for 140 keV N^{+5}.

Figure 4 shows the mean energy loss of projectiles N^{+5} with incident energy 140 keV ($0.63v_0$) grazing at different azimuthal angles. It is found that the energy loss depends remarkably on the structure of the crystal surface. This comes from the fact that the stopping length can be prolonged by the surface channelling effect along the axis (e.g. $[10\bar{1}]$,$[11\bar{2}]$) and to what extent the stopping length can be prolonged depends on the line density of the target atoms in the axis.

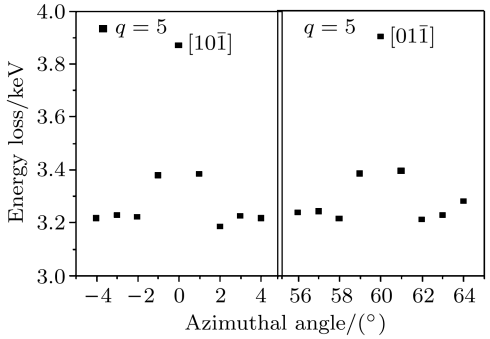


Fig.4. The total energy loss of ion N^{+5} grazing on Al(111) under azimuthal angles around $\Phi \approx 0°$ ($[10\bar{1}]$) and $\Phi \approx 60°$ ($[01\bar{1}]$).

4. Conclusions

Based on the study above, three conclusions can be drawn, although the energy loss of the multicharged ion grazing on metal surface is a complex process, in which both the projectile initial charge state and the structure of the crystal surface can play a role: (1) The charge exchange energy loss increases exponentially with the initial charge state and contributes a lot to the total energy loss for highly charged projectile.(2) The enhancement of the energy loss with initial charge state observed in Ref.[9] can be well explained by taking into account the charge exchange energy loss and the nuclear stopping power. (3) When the projectile grazing on the metal surface, its energy loss depends strongly on the crystal structure.

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