LIGHT ION REFLECTION STUDIED BY MONTE CARLO SIMULATION AND TRANSPORT THEORY*

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ABSTRACT

The reflection of light ions, such as H^+, $^3He^+$ and $^4He^+$, with energies of 0.1- 10 keV, from Cu and Ni surface has been studied by Monte Carlo simulation and transport theory. The Monte Carlo simulation gives the detail energy spectra for the reflected particles and their angular distribution for different incident angles. It shows that the reflected particle energy spectra can be approximately described by an analytical formula for the whole energy range, all the incident angles and different ion- target combination studied here. The reflected particle energy vs its average reflection angle to the surface normal can almost be expressed by a universal curve for all cases studied here. The reflection energy spectra are used for the calculation of the reflection coefficient by transport theory including the realistic surface correction. The present work is compared with both experimental measurement and other simulation codes.

Keywords: Particle reflection Monte Carlo simulation Transport theory

I . INTRODUCTION

Reflection of low energy light ions from solid surfaces is of great interest to the controlled fusion research. A great number of research works on this topic have been published since 1970s. Only some of these publications will be mentioned[1- 15] here. Since in the fusion research, one may expect that the fluxes from plasma to first wall have broad energy and angular distributions, with the energies of the particles, such as hydrogen, deuterium, tritium and helium, ranging from several eV to a hundred keV and energy distribution peaking within the range from a hundred eV to 1 keV[16], the research of the light ion reflection is important in the energy range of 0.1- 10 keV at different incident angle to the surface normal. Up to now, most of the experimental studies of the reflection coefficients were carried out for normal ion incidence onto the target, but for grazing incidence experimental data are very scarce [13,14,17]. Most successful theoretical treatments of reflection from solid surfaces have used Monte Carlo codes. On the other hand, this important problem has not yet been thoroughly solved by transport theory although some efforts have been made in this direction[1,2]. A common difficulty in the transport treatment is to take proper account of the discontinuity at the surface especially for the cases of grazing incidence. In the present work a method of realistic surface correction is presented in the transport

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calculation of particle reflection coefficients for different incident angles, based on the energy spectra provided by the Monte Carlo simulation. The results are compared with recent experimental data and some other computer simulation results and shown in satisfactory agreement.

II. MONTE CARLO SIMULATION

A computer simulation code has been set in our group, by use of which the information of surface reflection, among other information on ion transport in solids,can be obtained. The interatomic potential used in the program is BZ potential[18]. The electronic stopping data used can be changed, according to the different cases, in different types, such as Lindhard- Scharff electronic stopping formula[19], Ziegler's data table[20], Andersen and Ziegler's table[21] and four-parameter formulae[22]. For the case of surface reflection for low energy light ions, at grazing incidence, a reasonable selection of impact parameters for the atomic collision on the first atomic layer is very important. Since total reflection will happen at a certain critical angle for the case of grazing incidence, it seems that, as a complement to the binary collision approximation at the surface, it is necessary to use an analogue of the critical angle for a particle penetrating an atomic plane that is used in the estimation of channeling angles. This is equivalent to the use of a surface barrier. Our simulation result shows that the energy spectra of reflected ions, $G(E)$, for different ion species, H^+, $^3He^+$ and $^4He^+$ and for different incidence angle in the whole energy range studied here can be approximately described by the following formula,

$$G(E)= A\{[C+D(E/E_0)^2]\,(B-E/E_0) + \exp[-(E/E_0-B)^2/2\sigma^2]\} \qquad (1)$$

where E is the energy of the reflected ion, E_0 is the energy of the incidence ion, C, D, B and σ are adjustable parameters to fit the different ion- target combination, incidence energy and incidence angle to the surface normal. A is a constant to be determined by the normalization condition

$$\int_0^{E_0} G(E)\,dE = NR_N \qquad (2)$$

Where N is the total incidence particles, R_N is the particle reflection coefficient. As an

Table 1

The parameters used in Eq. (1) for 1 keV and 8 keV $^3He^+$ ion with incidence angle of 0°, 40°, 60°, 70° and 8 from the normal of surface

Energy E_0	1 keV					8 keV				
Incidence angle α	0°	40°	60°	70°	80°	0°	40°	60°	70°	80°
B	0.55	0.88	0.92	0.95	0.97	0.40	0.55	0.75	0.80	0.95
σ	0.31	0.175	0.166	0.110	0.055	0.52	0.50	0.45	0.35	0.14
C	0.355	0.68	0.27	0.055	0.008	0.29	0.55	0.61	0.41	0.134
D	0.973	5.77	3.50	2.00	0.21	1.5	1.2	4.0	1.5	1.8

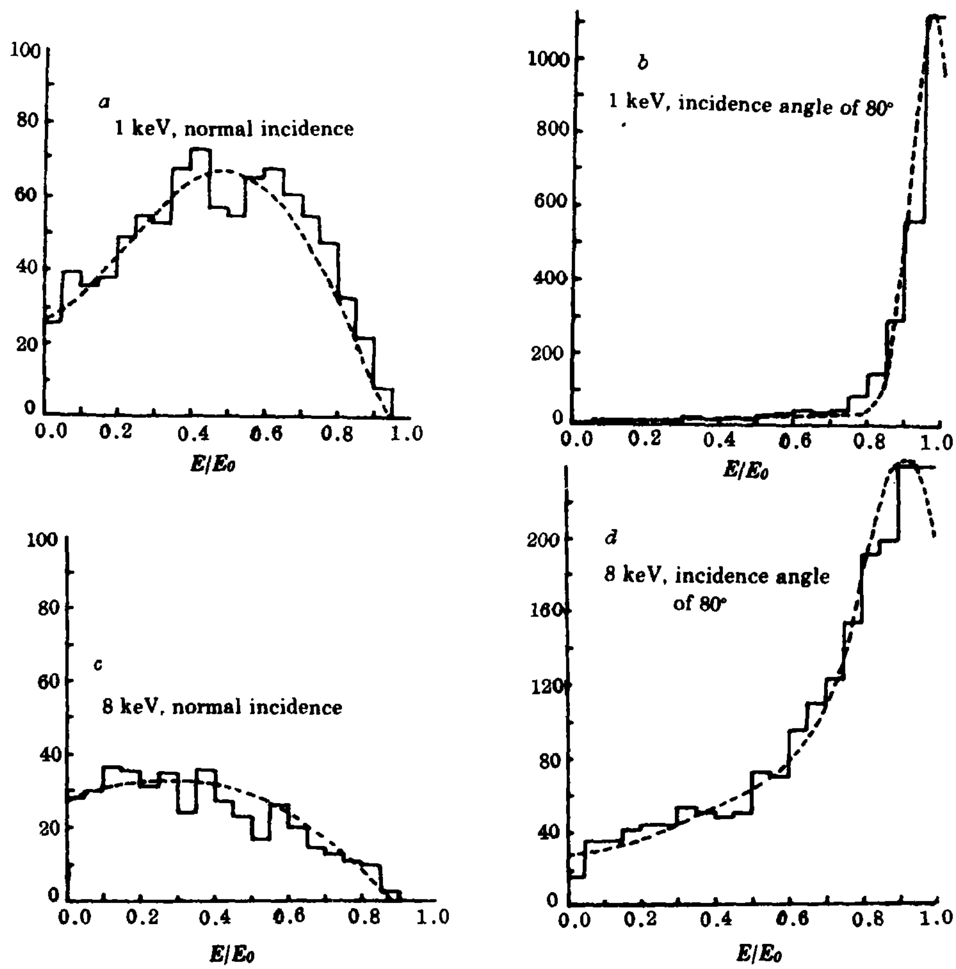

Fig. 1 The energy spectra of reflected $^3He^+$ from amorphous Ni surface

example, in Table 1 the parameters for 1 keV and 8 keV $^3He^+$ with different incidence angle, reflected from Ni surface are listed. The reflected energy spectra for 1 keV $^3He^+$ with incidence angle 0° and 80° are shown in Fig. 1(*a*) and (*b*) respectively, and that for 8 keV $^3He^+$ with incidence angle of 0° and 80° are shown in Fig. 1(*c*) and (*d*) respectively. The dashed curves in Fig.1 are the energy spectra obtained byuse of Eq. (1) to compare with the Monte Carlo simulation. Another remarkable result of our simulation is that the reflected particle energy, E, against its average reflected angle, $\bar{\theta}$, to the surface normal can almost be expressed by an universal curve independent of the incidence energy and incidence angle. This feature is shown in Fig.2.

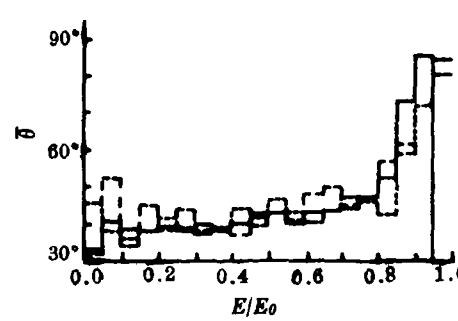

Fig.2 The relationship between the energy of reflected ions, E/E_o, and the average reflection angle, θ , from the surface normal

Ⅲ. THE PARTICLE REFLECTION COEFFICIENT CALCULATED BY TRANSPORT THEORY

Since the usual transport theory treats the ion transport in infinite medium and the reflection from surface is essentially a problem of semi- infinite medium. Surface correction is necessary especially for low energy ion at glancing incidence angle. Bφ ttiger and Winterbon have proposed a method[2] for surface correction in their calculation for reflection coefficient. They assumed an energy spectrum of $\rho\ (E) \propto E^{-\nu}$ with most possible ν value of 3/4, which is certainly not the case for low energy light ion reflection, especially for the case of glancing incidence. Since we can obtain the realistic energy spectra of the reflected particles, the realistic surface correction can be obtained. In fact, the particle reflection coefficient, R_N, can be obtained as follows.

$$R_N = R_N^{(o)} / (1 - R_N^{(2)})$$

$$R_N^{(o)} = \int_{-\infty}^{0} f(x,\alpha)\, dx / \int_{-\infty}^{\infty} f(x,\alpha) \qquad (3)$$

where $f(x,\alpha)$ is the projected range distribution of the incidence ions, α is the incidence angle to the surface normal. The range distribution calculation by transport theory for the case of oblique incidence ions has been given[23,24], and we do not discuss the problem here

$$R_N^{(2)} = \int_0^{E_0} dE \int_{-\infty}^{0} G(E)\, f(x,E,\bar{\theta}(E))\, dx / \int_0^{E_0} dE \int_{-\infty}^{\infty} dx\, G(E)\, f(x,E,\bar{\theta}) \qquad (4)$$

where $f(x,E,\bar{\theta})$ is the projected range distribution with E and $\bar{\theta}$ as parameters. By Eq. (3) and (4) the particle reflection coefficient can be obtained.

Ⅳ. RESULTS AND DISCUSSION

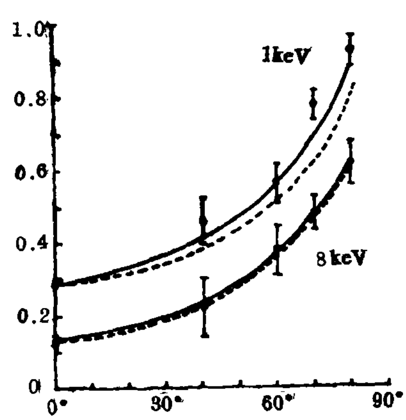

Fig.3 The particle reflection coefficient of 1 keV and 8 keV ⁴He⁺ reflected from Ni, showing the incidence angle dependence of the reflection coefficient

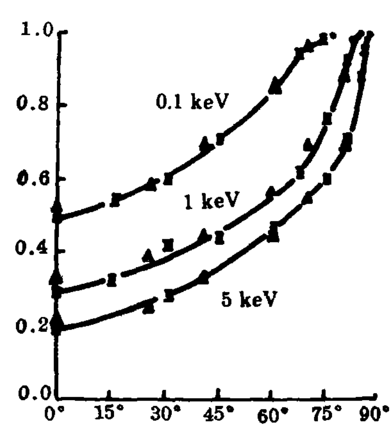

Fig.4 The particle reflection coefficient of 0.1 keV, 1 keV and 5 keV He^+ reflected from Cu, comparing the present work with the work of Oen and Robinson by use of MARLOWE

In Fig.3 the dependence of particle reflection coefficient on incidence angle is shown for 1 keV and 8 keV $^3He^+$ reflected from the surface of Ni. The solid curves are the result of our Monte Carlo simulation. The experimental points are taken from Ref.[14], and the dashed curves are the simulation result by use of the version TRSPR1 of the TRIM programme quoted in Ref.[14], Fig.4 gives R_N v.s. the incidence angle for 0.1keV, 1 keV and 5 keV $^4He^+$ reflected from Cu surface. The marks ▲ are used for the present work, the curves and the points with error bars are the result of Oen and Robinson[5] by use of MARLOWE code. The theoretical calculation result by use of Eq. (3) and (4) agrees with our Monte Carlo simulation very well. For example, the reflection coefficient for 1 keV $^3He^+$ reflected from Ni at incidence angle of 80° obtained by use of Eq.(3) and (4) is 0.869 and that obtained by our simulation is 0.897. This indicates that the events with particles passing the surface more than two times are scare. Thus higher order surface correction besides Eq. (4) is not necessary.

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