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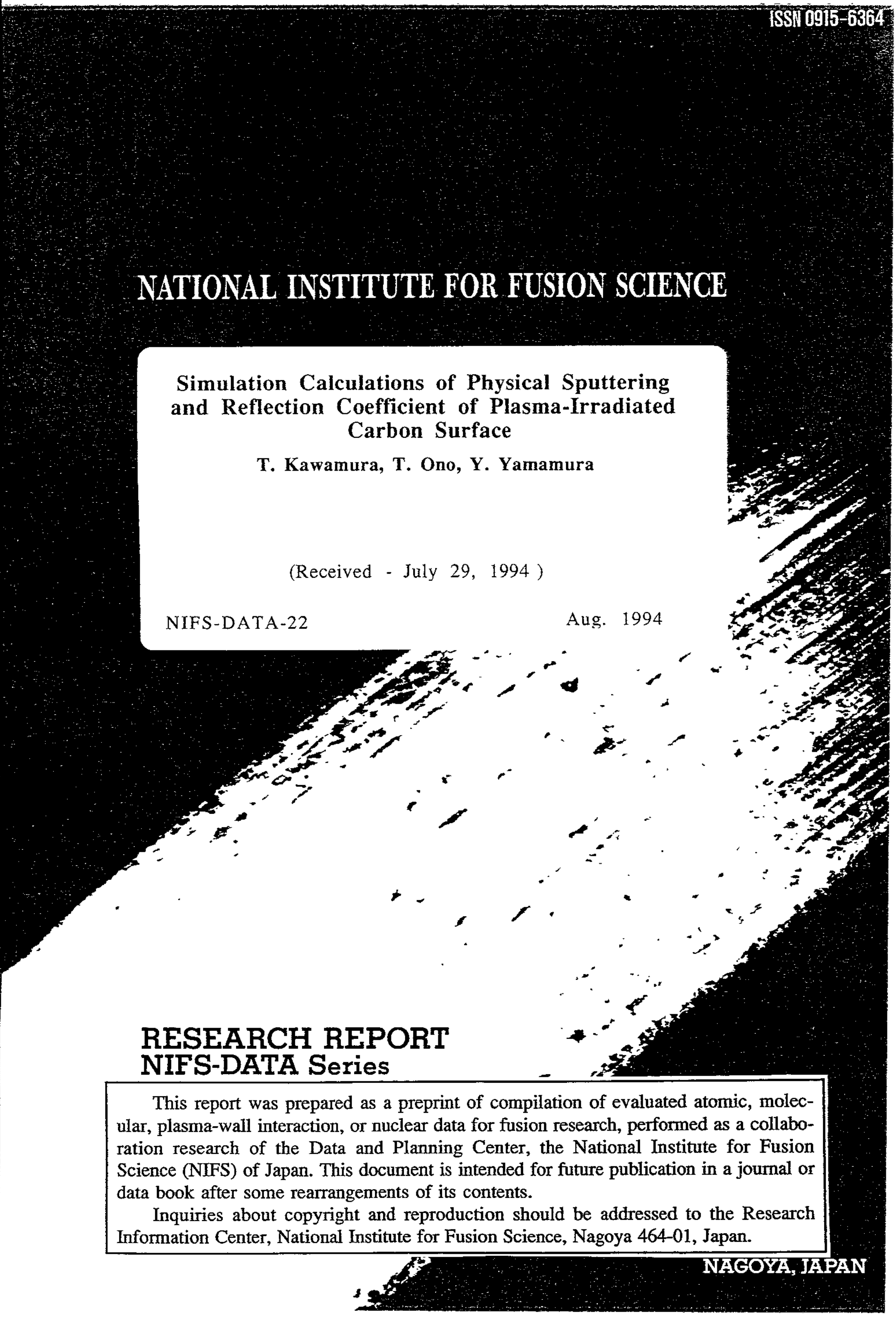

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Simulation Calculations of Physical Sputtering and Reflection Coefficient of Plasma-Irradiated Carbon Surface

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Simulation Calculations of Physical Sputtering and Reflection Coefficient of Plasma-Irradiated Carbon Surface

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Abstract

Physical sputtering yields from the carbon surface irradiated by the boundary plasma are obtained with the use of a Monte Carlo simulation code ACAT. The yields are calculated for many random initial energy and angle values of incident protons or deuterons with a Maxwellian velocity distribution, and then averaged. Here the temperature of the boundary plasma, the sheath potential and the angle δ between the magnetic field line and the surface normal are taken into account.

A new fitting formula for an arrangement of the numerical data of sputtering yield is introduced, in which six fitting parameters are determined from the numerical results and listed. These results provide a way to estimate the erosion of carbon materials irradiated by boundary plasma.

The particle reflection coefficients for deuterons and their neutrals from a carbon surface are also calculated by the same code and presented together with, for comparison, that for the case of monoenergetic normal incidence.

[Keywords: physical sputtering, reflection coefficient, carbon surface, plasma irradiation, fitting formula, sheath effect]

§ 1 Introduction

In the development of fusion devices it becomes important to estimate the erosion rate of the first wall and the divertor plate under irradiation by the boundary plasma. Physical sputtering by ions and charge-exchanged neutrals from the boundary plasma is a basic process contributing to the erosion rate of plasma - facing materials and to the generation of impurities. Physical sputtering yields depend on the initial energy as well as on the incident angle of the primary particles. Therefore the average sputtering yields for primary particles with a Maxwellian velocity distribution are needed for more realistic estimation of the erosion rate. Several studies to do this have already been reported [1-5]. For example the authors reported self-sputtering yields of a carbon material irradiated by plasma particles with a Maxwellian velocity distribution using a Monte Carlo simulation code ACAT [4].

In this paper the physical sputtering yields of a carbon surface irradiated by protons and deuterons with a Maxwellian velocity distribution are calculated with ACAT [6] to complete the database for carbon irradiated by boundary plasmas. A fitting formula for the sputtering yield is introduced with six coefficients determined from the numerical results. This formula provides a way to estimate the erosion of carbon materials irradiated by boundary plasmas. The particle reflection coefficients of deuterons from the boundary plasma are also calculated with the same code.

§ 2 Model and Numerical Results

In this calculation the velocity distributions of plasma ions and charge - exchanged neutrals are assumed to be Maxwellian in the boundary plasma that is far from the surface. In a sheath region in front of the solid surface plasma ions are accelerated. The angle δ between the magnetic field line and the surface normal is related to the sheath effect on the gyration of ions. Therefore, the electron temperature T_e, the ratio of ion temperature to electron temperature, and the angle δ are chosen as the parameters to calculate sputtering yields for plasma ions. In boundary plasma electron temperature measurements are made quite often, but ion temperature measurements are scarcely done. Thus ion temperature T_i is introduced through a parameterized ratio of T_i/T_e in the present calculations. In the following plasma temperature is meant to be electron temperature for incident plasma ions. However, ion temperature is adopted as plasma temperature only for incident neutrals with a Maxwellian distribution. The detailed procedure of the calculation with ACAT is given in a previous paper [4] .

In Fig.1 the sputtering yields are plotted for three cases : for monoenergetic normal incidence, charge-exchanged neutral deuterons and plasma ions with a Maxwellian velocity distribution . The abscissa is the energy at normal incidence or the temperature in eV .The average yields for charge-exchanged neutrals are much greater than for the case of monoenergetic normal incidence as a result of the major contribution of neutrals with glancing angles of incidence. The average yields for plasma ions, where $\delta = 0^\circ$ and $T_i/T_e=1$, are reduced due to the sheath acceleration as compared to the case of neutrals. It is also to be noted that the average yields for plasma ions are shifted towards lower energies (temperatures) compared to those at monoenergetic normal incidence because of the same reason as mentioned above. Then the sputtering threshold energies are a few eV, which are about an order of magnitude smaller than those at monoenergetic normal incidence. This tendency should be taken into consideration in the selection of a material of the first wall.

The sputtering yields for deuterium ions from the boundary plasma with two different T_i/T_e values, where the magnetic field lines obliquely intersect the solid surface, are given in Fig.2. The fact that the yields become larger for larger δ is attributed to the increase in the number of ions with glancing angles of incidence. The tendency about sputtering threshould energy pointed out above is seen to be more pronounced for $T_i/T_e = 5$ than for $T_i/T_e =1$.

The particle reflection coefficient of a carbon surface for plasma deuterons with a Maxwellian velocity distribution is given in Fig.3 together with that for monoenergetic deuterons at normal incidence. The coefficient for neutral deuterons becomes larger due to the increased contribution of neutrals at glancing incidence.

§ 3 Fitting Formula for Sputtering Yields

As a formula to fit the numerical sputtering data for incident particles with a velocity distribution, we have used a function $Y(T)$ of the plasma temperature T [eV] of the form

$$Y(T) = Q_1 T^{1/2} \left(1 - (Q_2 / T)^{Q_3} \right)^{Q_4} / \left(1 + Q_5 T^{Q_6} \right), \qquad (1)$$

where Q_i are unknown parameters to be determined. Q_1 is an adjusting factor for the whole function. Q_2 is an effective threshold temperature for sputtering. Both Q_3 and Q_4 represent the rising characteristics of the data in the low temperature range, while both Q_5 and Q_6 fit the decreasing trend at high temperature. As mentioned above, temperature T is meant to be electron temperature for incident ions. However ion temperature is adopted as temperature only for incident neutrals with a Maxwellian distribution. The method of determining Q_i is as follows : First the values of both Q_5 and Q_6 are determined from the high temperature data by the least squares method. Secondly, the rest are estimated from the low temperature data by the same method as in the high temperature region. Then a parameter run is made for Q_i to get good agreement between the formula and data . To make Q_i of different data sets correlative, the ratio of the Q_1 values, for incident ions other than protons or for protons at the δ values other than 0°, to the Q_1 value for protons at $\delta = 0°$, is set equal to the ratio of the maximum yields obtained by the least squares polynomial approximation applied to the corresponding data. In addition Q_3, Q_5 and Q_6 are fixed respectively at the same values for the different δ values. Under these conditions, the Q_i values are calculated again through the process mentioned above.

The values of Q_i derived with the above method are listed in Table 1. The data sets of Q_i correspond to incident particles of hydrogen, deuterium and helium neutrals with the velocity distribution and to incident proton and deuteron plasma ions for the different δ values, respectively. The solid curves shown in Figures 1 and 2 are drawn using the fitting formula with the Q_1 values given in Table 1. It is clear, from these figures, that the fitting formula agrees well with the numerical data. In fact, accuracy of the fittings done here is 4.6 % on the average.

§ 4 Summary

In order to estimate the effective erosion of carbon materials irradiated by a boundary plasma the average sputtering yields by incident particles of hydrogen, deuterium and helium with Maxwellian distributions are calculated using the simulation code ACAT. The particle reflection coefficients of the carbon surface by deuterons with the velocity distribution are also calculated with the same code.

A fitting formula is introduced and its parameters are determined by the numerical results. The formula is shown to be very accurate.These data could be useful for estimating erosion and for impurity modelling of the scrape-off plasma. Calculations on the other materials are proceeding and will be published in a forthcoming report.

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Figure Captions

Fig.1 : Sputtering yields of a carbon material irradiated by deuterons for the cases of monoenergetic normal incidence, charge-exchanged neutrals and ions with a Maxwellian velocity distribution. The abscissa is the energy at normal incidence or ion temperature in eV. The solid curves are drawn using a fitting formula (1) with the Q_i values listed in Table 1.

Fig.2 : Sputtering yields of a carbon material irradiated by deuterium plasma ions with a Maxwellian velocity distribution ; (a) for $\delta = 0^\circ$, 30° , 60° and 80° with $T_i/T_e = 1$. The solid curves are obtained from a fitting formula (1) with the Q_i values listed in Table 1; (b) for $\delta = 0^\circ$, 30° , 60° and 80° with $T_i/T_e = 5$. The solid curves are obtained with a fitting formula with the Q_i values listed in Table 1. The abscissa is the electron temperature in eV.

Fig.3 : Reflection coefficients of deuterons from a carbon material for neutrals and ions with a Maxwellian velocity distribution with $T_i/T_e=1$ and for monoenergetic deuterons at normal incidence. The abscissa is the energy at normal incidence or ion temperature in eV.

Table Caption

Table 1 : Parameter values of Q_i of a fitting formula (1) for the projectiles indicated. In case of ions, each data set of Q_i corresponds to one of the four δ values indicated, respectively. Temperature T of the formula is expressed in units of eV.

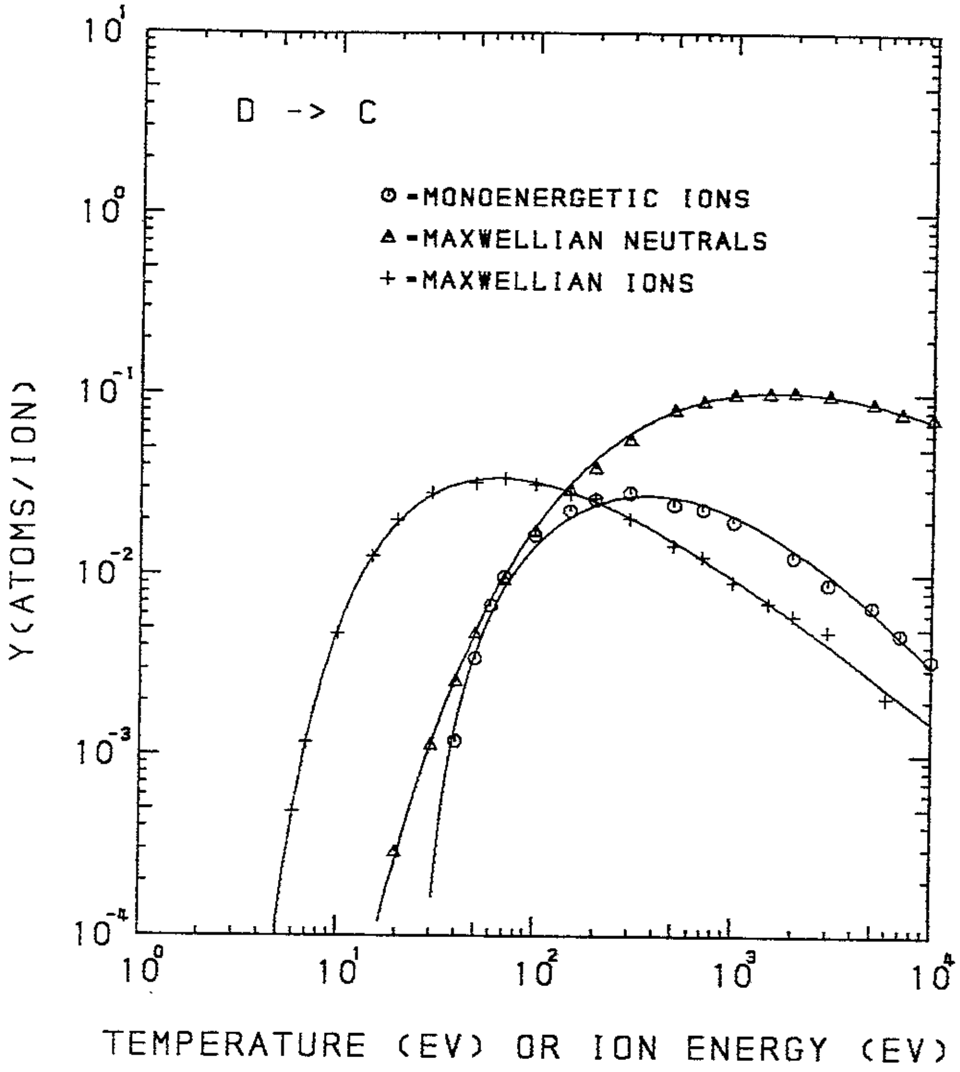
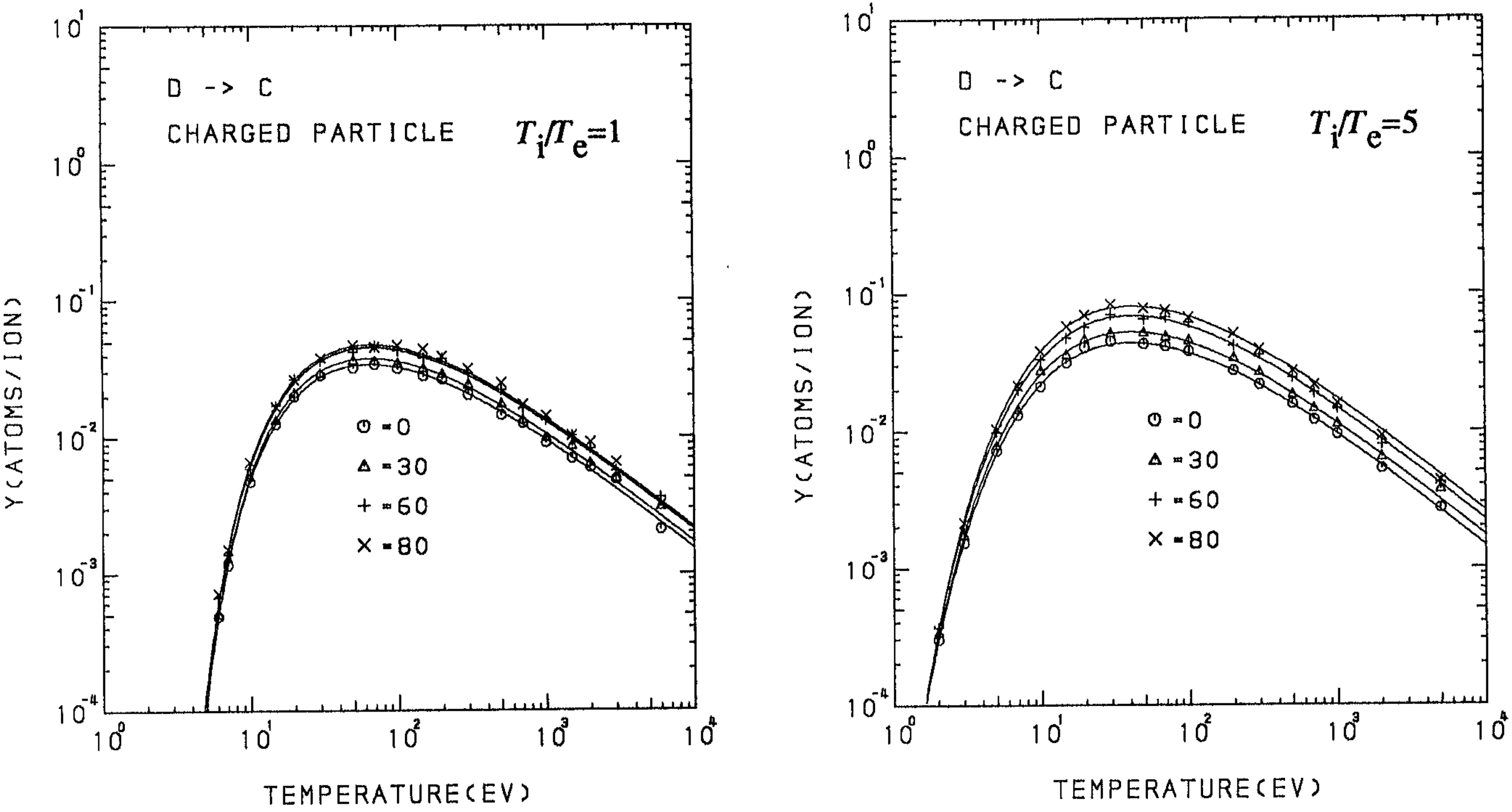

D -> C
⊙ -MONOENERGETIC IONS
△ -MAXWELLIAN NEUTRALS
+ -MAXWELLIAN IONS
Y (ATOMS/ION)
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
TEMPERATURE (EV) OR ION ENERGY (EV)

Fig. 1


D -> C
CHARGED PARTICLE
$T_i/T_e=1$
$T_i/T_e=5$
Θ = 0
Δ = 30
+ = 60
× = 80
Y(ATOMS/ION)
TEMPERATURE(EV)
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}

(a)

(b)

Fig.2

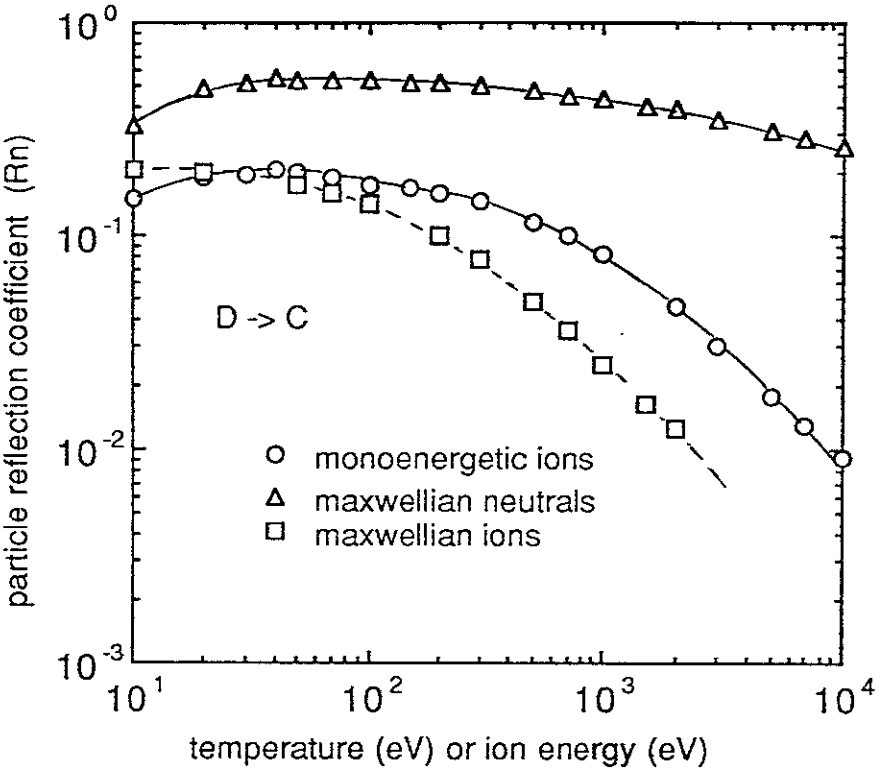

10^0
10^{-1}
10^{-2}
10^{-3}
particle reflection coefficient (Rn)
D -> C
○ monoenergetic ions
△ maxwellian neutrals
□ maxwellian ions
10^1
10^2
10^3
10^4
temperature (eV) or ion energy (eV)

Fig.3

Table 1

projectile	*Ti/Te*	δ	Q_1	Q_2	Q_3	Q_4	Q_5	Q_6
H^0	----	----	2.978	0.1	0.38	84.68	0.0340	1.231
D^0	----	----	6.494	0.1	0.40	80.74	0.0760	1.182
He^0	----	----	20.27	0.1	0.31	54.04	0.0253	1.190
H^+	1	0°	1.141	3.6	0.65	8.284	0.41	1.41
	1	30°	1.295	3.7	0.65	8.083	0.41	1.41
	1	60°	1.496	3.7	0.65	8.116	0.41	1.41
	1	80°	1.593	3.7	0.65	8.129	0.41	1.41
D^+	1	0°	2.330	2.7	0.52	7.158	0.35	1.40
	1	30°	2.591	2.8	0.52	7.015	0.35	1.40
	1	60°	3.186	2.7	0.52	7.268	0.35	1.40
	1	80°	3.323	2.7	0.52	7.256	0.35	1.40
H^+	5	0°	1.093	0.12	0.58	48.09	0.50	1.37
	5	30°	1.236	0.16	0.58	40.50	0.50	1.37
	5	60°	1.627	0.20	0.58	35.56	0.50	1.37
	5	80°	1.869	0.17	0.58	39.46	0.50	1.37
D^+	5	0°	2.950	0.10	0.51	36.21	0.39	1.42
	5	30°	3.518	0.13	0.51	31.54	0.39	1.42
	5	60°	4.564	0.16	0.51	28.27	0.39	1.42
	5	80°	5.346	0.19	0.51	25.84	0.39	1.42

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