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NEW RECYCLING MODEL FOR LIGHT IONS AND ATOMS

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NEW RECYCLING MODEL FOR LIGHT IONS AND ATOMS

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ABSTRACT

Recent theoretical studies and experimental results suggest a revision of light-ion reflection models used in simulation codes. Surface impenetrability leads to large reflection coefficients for hydrogen isotopes incident below 5-20 eV. Adsorption below 5-10 eV also depends on saturation of the surfaces. An effective surface roughness is included for all energy regimes. The fraction of nonreflected particles reemitted as molecules depends on the previous exposure of the surface and the incident flux. Simple models of these processes are collected in a form usable in neutral transport codes. The relevance of such models to tokamak design and of interpreting divertor tokamak data is discussed and illustrated by numerical computation.

1. INTRODUCTION

Complete models of high-recycling divertor plasmas in tokamaks and similar plasmas require a comprehensive model of reflection and sticking of light particles (H^+ , H^0 , He^{++} , etc.) incident at low energies and of their subsequent desorption. Here we present such a model. Emphasis is on parameterizing present uncertainties in a calculable model rather than the far more difficult task of estimating the correct model parameters. The effect of

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using different modeling assumptions is illustrated with models of the proposed ASDEX Upgrade experiment and of the PDX divertor.

II. REFLECTION MODEL

The particle reflection coefficient, R_N , is an important component of a comprehensive model. With incident energy around 100 eV, existing experiment and theory¹⁻⁵ give $S \equiv 1 - R_N \sim 0.5$, where S is the sticking coefficient, as illustrated in Fig. 1. At lower incident energies the TRIM¹ and MARLOWE² codes demonstrate the experimental tendency to unity reflection coefficients.³⁻⁵ Unfortunately, this is not necessarily adequate for a comprehensive plasma model, since the neutral particle density is proportional to $S = 1 - R_N$ and not R_N . That such a problem might be significant became clear to us when we found that TRIM¹ results significantly overestimated the sticking of 30 eV K^+ incident on tungsten when compared to very detailed experimental measurements and to a dynamic trajectory model⁶ which had been carefully calibrated against these measurements.⁷

As a heuristic exercise, we therefore applied our dynamic trajectory model to $D^0 + W$. Our results are compared to TRIM calculations in Fig. 1. For our calculations, the potential affecting the incoming deuteron was

$$V = (5.3 \text{ eV}) \exp\{-8z\} + \sum_{j=1}^{50} (27 \text{ eV}) \exp\{-1.74 r_j\} \quad (1)$$

where the distances z above the surface and r_j to fifty nearby target atoms are in Angstroms. The first term in this potential is a scaling of an ad hoc repulsive potential required to reproduce the above-mentioned experimental data. The requirement for this term is thought to result from distortion of the bonding orbitals to fill the surface with electron density, thereby reducing shielding of the nuclear charges.⁷ The second term is a Born-Mayer

potential described in more detail elsewhere.⁸ For the results shown in Fig. 1, the surface atoms were held fixed in their known lattice positions, and projectiles were considered trapped after passing below the fourth subsurface layer. Since a few of these deeply penetrating particles may eventually escape, this procedure gives only an upper limit on the sticking coefficient. However, it is adequate for demonstrating the transition to negligible sticking ($\sim 100\%$ reflection) expected at low incident particle energy ($\lesssim 10$ eV). The solid portion of our computed curve in Fig. 1 may be closest to the actual sticking coefficient in the range 5-15 eV, where inelastic scattering is not important for the first interaction of D^0 incident on the surface but may be significant in preventing return of deuterons traveling downward in the neighborhood of the fourth subsurface layer.

In order to construct useful numerical formulas, the particle reflection coefficient is to be given by $R_N = [R_{ads} \text{Max}(R_{ND}, R_{NS})]^4$. Here R_{ads} is the absorption coefficient defined below (cf. Baskes^{9,10}). R_{ND} is the formula obtained by extrapolating high energy reflection data or calculations (e.g., as presently used in DEGAS code¹¹) with a maximum value $R_{ND} = 1$ and with no correction applied for adsorption, e.g., below $E_{in} = 10$ eV; $R_{NS} = \text{Min}\{1, \exp(b[(E_C/E_I) - 1])\}$, where $E_I = E_{in} \cos^2 \theta$, E_{in} is the incident energy, θ is the angle of incidence from the normal, $E_C = Z_{in} Z_S E_Z$, Z_{in} is the nuclear charge of the projectile, Z_S is the mean nuclear charge of the surface atoms. The scaling with Z_{in} and Z_S represents the dominant term in the Coulomb force. This may slightly underestimate the normalized cutoff energy, E_C , when the effects of denser atomic packing and reduced electronic screening of the repulsive potential for low-Z materials are taken into account. These values therefore lead to an adjustment of previous models in the direction of increased reflection coefficients, but the adjustment may not be strong enough

for low-Z surface materials. The values of E_z and b should be taken as parameters which can be adjusted to match experimental tokamak data or to take account of improved reflection measurements or calculations.

Nominal values of parameters chosen to match computed or experimental reflection data are effective surface roughness $a = 2$, normalized cutoff energy $E_z = 0.1$ eV, and "cutoff sharpness" $b = 2$. The surface roughness should be chosen to be on the order of the average number of bounces a reflected particle makes before escaping back to the plasma region. The nominal values of E_z and b come from scaling the above dynamic trajectory calculations for D^0 incident on tungsten at $\theta = 45^\circ$. Hopefully, these parameters can be calibrated in the future to an expanding experimental data base.

The adjustment to energy reflection coefficients assumes a single elastic scattering event when the particle of mass m_{in} bounces directly backwards off surface atoms of mass m_s . Thus, the energy of a reflected atom is $E = E_{in} [\text{Max}(E_D/E_{in}, R_{NS}E_S/E_{in})]^2$, where $E_S = [(m_s - m_{in})^2 / (m_s + m_{in})^2] E_{in}$ is the maximum energy transfer for elastic scattering, and the factor R_{NS} is included to account for the rapid transition to multiple scatterings at higher energy as the projectile begins to penetrate the first surface layer. E_D is the reflected energy, e.g., as previously used in DEGAS.¹¹ The energy reflection coefficient is $R_E = R_N E/E_{in}$.

The probability of adsorption at low incident energy is taken to be proportional to the fraction $(1 - \theta_S)$ of unoccupied binding sites where θ_S is the surface coverage. Following Bastasz and Haggmark,¹² θ_S is determined by the balance between the influx rate ϕ and thermal and impact-stimulated desorption $\theta_S = 1/4k_{TD} N_a \{[\phi(\sigma_d^2 \phi + 8k_{TD})(1 - R_N)]^{1/2} - \sigma_d \phi\}$, where $k_{TD} = c \exp(-E_d/T_S)$, with $c = 3 \times 10^{-4}$, 0.1, 0.4 for an oxide-covered steel surface, sputter-cleaned steel surface, and clean nickel surface, respectively, $E_d \approx 1$

eV, T_s is the surface temperature in eV, and $\sigma_d = 2 \times 10^{-16} \text{ cm}^2$ is a typical cross section for impact-stimulated desorption, and $N_a = 2 \times 10^{15} \text{ cm}^{-2}$ is a typical concentration of surface binding sites. The incident particle flux, ϕ , can be taken as a rough estimate from previous experience or calculated iteratively for more exact work.

The adsorption coefficient is extrapolated to lower binding energies from the work of Jackson¹³ to obtain $R_{ads} = 1 - (1 - \theta_s) \exp(-E_{in}/E_{ads})$, where $E_{ads} < 2 \text{ eV}$ for hydrogen isotopes on metals. For helium, adsorption can be neglected, and the formula for surface saturation is not required.

In this prescription, we make no distinction between incident ions and atoms because surface neutralization rapidly eliminates the relatively weak image charge attraction of incoming ions, an effect usually small compared to the preacceleration of ions in the electrostatic sheath. (However, the perpendicular energy acquired by ions traversing a sheath potential is $E_{\perp} = 2\gamma_i T_e \cos^2 \theta_{in}$, where $\gamma_i \sim 3$ and $\theta_{in} \sim 60^\circ$ for typical tokamak parameters¹⁴ where we have assumed $T_i \sim T_e$.)

III. REEMISSION MODEL

The above discussion gives a complete prescription for reflection of ions and atoms off material surfaces. This prescription can be applied independently of a detailed knowledge of molecular recycling. However, it is also useful to have an estimate of the fate of adsorbed particles. For the influx rates typical of tokamak experiments, a non-negligible fraction of the adsorbed hydrogen flux is either lost to the walls or may be reemitted as energetic particles by ion impact desorption.

The fraction of the nonreflected particle influx reemitted by impact desorption is given by Eastasz and Hagmark¹² as

$$f_{\text{fast}} = 1/[1 + 2k_{\text{TD}}\theta_S N_a / (\sigma_d \phi)],$$

where $N_a \approx 2 \times 10^{15} \text{cm}^{-2}$ is a typical concentration of surface binding sites, and ϕ is the incident flux. For incident energies well above the hydrogen molecular binding energy, this flux is presumably as fast atoms with the incident energy shared about equally between the reflected and desorbed atoms.

The fraction of the nonreflected flux, $\phi_S = (1 - R_N)\phi$ which is lost by diffusion into the bulk solid can be estimated by an extension of the arguments due to Howe and Langley.^{15,16} Adding impact desorption and surface recombination to the processes they describe gives a pumping fraction $f_{\text{pump}} = [(1 - f_{\text{fast}})\phi_S D / 2k_r t]^{1/2} + d/D^{1/2} t^{1/2}$ in the limit where $f_{\text{pump}} \ll 1$, where $D = \text{Max}(D_0, \phi_S d / C_{\text{max}})$, $D_0 \sim 2 \times 10^{-12} \text{cm}^2/\text{s}$ for hydrogen in unsaturated stainless steel at a bulk temperature $T_B = 300^\circ\text{K} = 0.034 \text{eV}$ (and changes exponentially with inverse temperature), $k_r \sim C_{\text{max}}^{1/3}$, k_{TD} is another measure of the surface recombination rate, $C_{\text{max}} \sim 10^{23} \text{cm}^{-3}$ is the maximum number density of hydrogen in the solid, and $d = 3 \times 10^{-8} E_{\text{in}}$ where d is in cm and E_{in} is in eV. The enhancement of bulk diffusion at high flux as given in the above formula for D is required only for very high fluxes of particles with energies above the reflection cutoff energy, E_c . In the above formula for f_{pump} , t is to be interpreted at an effective time over which the influx has occurred. Most cases of interest have nearly constant particle influxes over an extended time period, so an appropriate choice for t is straightforward.

IV. IMPLICATIONS FOR MODELING TOKAMAKS

1. ASDEX Upgrade: An example of the recycling coefficients predicted by this model is shown in Fig. 2a. The lines labeled "saturated, rough surface" show reflection coefficients from the model for deuterium incident on a transition metal, with an effective surface roughness of $a=2$, and the lines

labeled "unsaturated, smooth surface" show particle reflection coefficients previously used in the DEGAS simulation code for an unsaturated, smooth surface.¹¹ A modest trend towards increased atomic recycling at lower incident energy is clear from Fig. 2a. For data interpretation, it is often assumed that the energy reflection coefficient is about 1/2. In our model, the energy coefficient will be larger than 1/2 (and therefore lead to reduced heating of a divertor plate) at low incident energy. This may help to explain the reduced divertor plate heating observed under reduced divertor plasma temperatures.

The largest impact of using a reflection model for saturated surfaces instead of one assuming unsaturated surfaces should be noticed for very high recycling divertors, where the typical neutral energy can lie below 10 eV. To illustrate this, we show results of simulations of the planned ASDEX Upgrade configuration shown in Fig. 3.¹⁷ The plasma parameters used to support the neutral transport calculation were computed using the SOLID plasma transport code. The energy and particle flows were computed for the outer divertor plate assuming 2.5 MW and 2.5×10^{21} ions H^+ /sec flow along magnetic field lines in the toroidal midplane, with exponential radial scrape-off profile density and temperature widths of 3 cm and 1.5 cm, respectively (cf. Vernickel *et al.*¹⁷). The poloidal projections of the density and electron temperature along the separatrix are shown in Fig. 3. In the region near the divertor plates where the recycling occurs, the ion and electron temperatures were very nearly equal.

Using this configuration, we performed neutral transport simulations using the two reflection models. Charged particles were assumed to be normally incident on the divertor plate passing through a sheath potential of five times the local electron temperature and reflected as for neutrals.¹¹

All nonreflected particles were reemitted as neutral hydrogen molecules in a cosine angular distribution in polar angle, θ , with an energy of 0.03 eV.

The average hydrogen molecule density in front of the pumping ducts is an important physical parameter, which can be obtained with minimal ($\sim 1\%$) Monte Carlo statistical error. We have therefore averaged n_{H_2} over the shaded region indicated in Fig. 3 for several different assumptions about particle reflection (cf. Table I). The first entry in Table I shows the result for an unsaturated, smooth surface model. This model has substantial trapping of particles incident with energy below 10 eV, with instantaneous release of these particles as H_2 . This model therefore gives a relatively large neutral hydrogen density of $1.9 \times 10^{14} \text{ cm}^{-3}$. In the saturated rough surface, we first assumed that all particles incident below 0.5 eV were absorbed, in which case $\langle n_{H_2} \rangle = 1.2 \times 10^{14} \text{ cm}^{-3}$. This substantial reduction in $\langle n_{H_2} \rangle$ from the value obtained with the previous model resulted from the increased reflection.

We note further that when the absorption cutoff was instead 1.0 eV (which is effectively equivalent to reducing the surface saturation in our model), $\langle n_{H_2} \rangle$ decreased to only $1.4 \times 10^{14} \text{ cm}^{-3}$. These results indicate that the role of very low energy particles may be relevant and should be further investigated.

We also changed the parameter E_Z , which controls reflection at higher energies, since the recommended value of this parameter is based on a rather uncertain extrapolation, as described above. For this particular configuration, where the behavior of very low energy particles is dominant, doubling E_Z had no significant effect, as evident from comparing the last two entries in Table I. Thus, the trend towards unit reflection at energies less than ~ 10 eV is the most important difference when changing from an unsaturated surface model to a sawtooth one. However, the exact energy at

which this occurs plays a less significant role.

2. PDX: To relate recycling models to existing tokamak experiments, we reconsider a previous simulation of the PDX experiment reported earlier.¹⁸ Briefly, the neutrals originate by recycling in the divertor chamber and pass through a plasma of moderate temperature comparable to that used above for ASDEX UPGRADE but with an order of magnitude lower density. We first used the curve for R_N for nearly saturated surfaces expected in the PDX divertor shown in Fig. 2b. As above, all adsorbed atoms were recycled immediately as thermal molecules at 0.04 eV. Fifteen percent of the particles were transmitted, and the average energy of atoms leaving the divertor chamber was 32 eV for this reflection model. When the divertor walls were assumed to be very rough (i.e., "sticky" with $R_N = 0$), then 9% of the particles left the divertor, and the average energy of atoms leaving the divertor dropped to 18 eV. When the particle reflection coefficient was instead doubled (subject to a maximum of unity) to account for the higher reflection expected for low energy particles incident on smooth, saturated surfaces, the average energy of atoms leaving the divertor was again 32 eV, but the fraction of plasma influx escaping from the divertor chamber as neutrals was 27%.

3. Conclusions: Both the energy and number of recycling neutrals can have an important impact on overall plasma particle and energy confinement. Careful consideration of the evolving particle reflectivity of the divertor materials is therefore evidently an important consideration in understanding tokamak experiments. We cannot overemphasize that the specific a priori estimates for numerical values given in this paper are included only to give a feeling for the typical orders of magnitude which may be expected. For example, we quote a surface roughness factor of $a=2$ for use in Eq. (5) because

this may be typical of metal surfaces in some devices. But damaged metal surfaces may have higher surface roughness, and the surface roughness of graphite is often very large. Careful choice of parameters appropriate to a specific simulation using our recycling model should nevertheless allow quantitative simulations relating recycling behavior to quantities more directly relevant to surface conditioning (e.g., k_{TD}), surface roughness, surface temperature, and discharge duration. The model parameters which describe these surface characteristics can then be compared to independent measures or estimates of the surface state, such as discharge cleaning history, microscopy, thermocouple measurements, and ion implantation studies. In the long run, this comparison should facilitate an understanding of recycling behavior which would be impossible with simpler models of particle-surface interaction at low energies.

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TABLE 1

"Pumping Chamber" Hydrogen Molecule Density

Model	E_z (eV)	E_{min} (eV)	$\langle n_{H_2} \rangle$ (10^{13} cm^{-3})
Unsaturated, smooth	—	—	1.9
Saturated, rough	0.1	0.5	1.2
Saturated, rough	0.1	1.0	1.4
Saturated, rough	0.2	1.0	1.4

FIGURE CAPTIONS

FIG. 1. Computed (solid lines) and measured fraction (crosses) of incident particles which stick in solid as summarized by Eckstein and Verbeek for D^+ normally incident on iron (Fe) and tungsten (W), and for stainless steel (SS); and for $D^+ \rightarrow W$ 110 as in Fig. 1b using the model described in this paper, with 45° angle of incidence from the normal and random azimuthal angles of incidence.

FIG. 2 (a) Reflection coefficients with $E_{ads} = 2$ eV for $D \rightarrow Fe$ at incident angle less than 40° from the normal effective surface roughness $a=2$, in Eq. (1), for particles (solid lines) and energy (dashed line), versus a simplistic reflection model for a smooth unsaturated surface (curves labeled "old"). For $\theta \geq 40^\circ$ R_N was replaced by $(R_N + 1)/2$ and the reflection energy was set to $0.9 E_{in}$ rather than using the formula reported in Heifetz et al.¹⁶ (b) Reflection coefficients for PDX Study.

FIG. 3. (a) Poloidal cross section of a toroidally symmetric model of the ASDEX Upgrade tokamak showing the cells used in the DEGAS Monte Carlo neutral transport simulation (dashed lines), and a table of electron temperatures and particle fluxes incident on the outer divertor plate (numbered solid line), and (b) electron temperature and density assumed versus poloidal distance along the magnetic flux surface from segment 1 of the divertor plate. (c) Reflection coefficients for standard PDX case. Circles indicate TRIM calculations from Eckstein and Verbeek⁴ for $D \rightarrow Fe$ at normal incidence.

FIG. 1

FIG. 2

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Temperature and Flux At
Plate Segments

Seg #	T_e (eV)	Γ ($10^{22}/\text{cm}^2\cdot\text{s}$)
1	6.24	2.97
2	4.68	3.55
3	2.90	3.03
4	1.48	2.19
5	0.62	1.42

FIG. 3

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