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HEATING OF D_2 GAS TARGETS BY INTENSE TRITIUM ION BEAMS

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ABSTRACT

This study examines the problem of heating due to bombarding a D_2 gas with a T^+ beam to produce 14-MeV neutrons. Such a neutron source is proposed for testing the effects of neutrons on materials to be used in a fusion reactor. Ionization and electronic state excitation by the beam and ionization, electronic and vibrational excitation, dissociation, momentum transfer, and dissociative recombination by secondary electrons are considered. For most beam energies of interest, ionization will play the dominant role in transferring energy from the beam to the target gas. Dissociative electron recombination is particularly important because it allows the energy involved in overcoming the ionization threshold to be released very rapidly as kinetic energy. The results of our study are applied to a specific Intense Neutron Source design in which ~60% of the energy deposited by the beam will emerge as heat while the supersonic D_2 gas remains in the target interaction region. Less than 10% of the energy is given off as radiation.

I. INTRODUCTION

Materials damage caused by 14-MeV neutrons is anticipated to be one of the most critical problems associated with fusion powered reactors. To investigate this problem, the Los Alamos Scientific Laboratory (LASL) is developing an Intense Neutron Source (INS) facility that will provide a fusion-reactor-type neutron environment.[1] Because the probability of producing a 14-MeV fusion neutron is quite low compared with other competing processes, the fundamental design limitation of all proposed INS facilities is the amount of heat that must be dissipated in the neutron producing target. To minimize this problem several proposed INS designs use a supersonic, flowing D_2 gas target. In this study we examine the various paths followed by the energy deposited by a T^+ beam in such a target gas and have estimated the time it takes for this energy to emerge in the form of heat.

In Secs. II-IV we discuss the various energy pathways and the appropriate rates considered in this study. In Sec. V we apply our results to the design proposed for the LASL INS facility.

II. INITIAL ENERGY DEPOSITON

To determine the modes into which the energy of the T^+ beam will initially be deposited, we have relied on the work of Dalgarno and Griffing[2] who considered the fate of a proton impinging onto H_2.

Basically, the T^+ ions can ionize or excite the D_2 molecules, or they can capture an electron from a molecule and proceed as a neutral tritium atom. In turn, the neutral T atoms can also ionize or excite D_2 molecules.

III. D_2 RELAXATION

The fate of the energy introduced into the electronic states of D_2 is somewhat uncertain because the collisional self-quenching rates for D_2^* are unknown (our literature search also failed to provide self-quenching rates for H_2^*). We expect these rates to be slow because of the large difference in energy between the levels of the electronic states and the average thermal energy of the molecules. However, Hiskes and Freis[3] and Cahill[4] report that energy placed in certain electronic states can escape as radiation on a submicrosecond time scale. Radiation from the singlet states will arise from cascading transitions down to the ground state. This radiation can, therefore, be multiply scattered and will be absorbed eventually by the chamber walls. Alternatively, the radiation from the triplet states arises from transitions that will lead eventually to the $b^3\Sigma_u^+$ dissociative state. Therefore, the energy of the triplet states must be broken down into three categories: energy carried away by radiation, translational energy of the dissociated atoms, and energy required to overcome the molecular bond. The radiation energy will be absorbed by the chamber walls. The energy required to overcome the molecular bond will emerge as thermal energy on a time scale that will depend on the density of D atoms and the extent to which this energy subsequently hangs up in vibrational states.

In Sec. IV we show that a significant fraction of the energy deposited into the gas by ionization can subsequently appear as vibrational excitation in the D_2 molecules owing to electron collisions. The self-quenching rates of H_2 vibrational states are well known,[5] and we have no reason to believe that D_2 rates will be markedly different. These rates are, of course, dependent on the temperature of the gas. However, for the temperature range of interest in this study (< 1500 K), these rates are comparatively slow, requiring several microseconds for the states to relax.

IV. ELECTRONS

We know from Ref. 2 that for most initial T^+ beam energies much of the energy deposited will go into ionization of D_2. We must therefore examine, in detail, the energy distribution of the electrons, the final disposition of this energy, and the time scale for electron-molecule recombination. In our examination of the electron energy distribution we used a computer program that was developed by Elliott and Greene[6] for calculating the time behavior of electron energy spectra in e-beam generated, unsustained, laser systems. The unique feature of this program is its ability to model the initial secondary electron spectrum. For this modeling, we used a formalism suggested by Green and Sawada[7] to model the Opal et al.[8] data.

$$S(E,T) = A(E) \frac{\Gamma^2}{(T-T_o)^2 + \Gamma^2} U(E-E_i-2T),$$

where E is the energy of the primary electron, T is the energy of the secondary electrons, U is the Heavyside step function,

$$A(E) = \sigma_o KE^{-1} \ln(EJ^{-1}),$$

$$T_o = T_s - 1.0 \times 10^3/(E+2E_i),$$

and

$$\Gamma = \Gamma_s E/(E+\Gamma_b).$$

E_i is the ionization energy and $\sigma_o = 1 \times 10^{-16}$ cm^2. For K, J, T_s, Γ_s, and Γ_b, we used the values given in Ref. 7 for H_2 and treated the T^+ ions as 500-eV primary electrons. The specific energy of the primary is not particularly important because the shapes of these initial secondary electron spectra are relatively independent of E.[8] However, it is important that we normalize S(E,T) to the total electron production rate due to ionization by the beam and subsequent secondary ionization by the electrons. This term provides the source of electrons for the computer program.

The sink for the electrons is, of course, recombination. The recombination time scale is very important because only after recombination will most of the 15.5 eV that went into the ionization threshold return as thermal energy. The possibility that this energy will be available is very real because essentially all of the ions in the gas will exist as molecular ions and, therefore, dissociative recombination can occur. The importance of dissociative recombination cannot be overemphasized. There are several mechanisms for creating molecular ions, such as

$$D^+ + 2D_2 \rightarrow D_3^+ + D_2 \qquad k = 3.0 \times 10^{-29}\ \mathrm{cm^6/s}$$
$$D_3^+ + D_2 \rightarrow D_5^+ + D \qquad k \simeq 1.0 \times 10^{-9}\ \mathrm{cm^3/s}$$

where the rate constants are from Massey et al.[9] Therefore, we expect essentially all of the ions to be molecular: D_2^+, D_3^+, or D_5^+. The rate for dissociative recombination is $\sim 10^{-7}\ \mathrm{cm^3\,s^{-1}}$ for electrons <1 eV (Ref. 10), which can be compared with $10^{-10}\ \mathrm{cm^3\,s^{-1}}$, a typical value for radiative recombination. Finally, dissociative recombination is important because the dissociated partners carry most of the energy of the ionization threshold away as kinetic energy, thus providing an important heat source in the target interaction region. In the computer program we assumed that the ions existed as D_3^+ and we used the dissociative recombination cross sections of Peart and Dolder[10] for H_3^+. Because of their availability, all cross sections used in the program were for H_2. The differences between D_2 and H_2 should not markedly change the electron energy distribution and subsequent electron impact pumping of the various energy modes of the molecules.

The other physical processes included in determining the electron energy distribution are electronic state excitation,[11] dissociation,[12] vibrational excitation,[13] momentum transfer,[14] and electron-electron collisions.[9] For secondary ionization we used the cross sections of Rapp and Englander-Golden.[15]

The computer program integrates forward in time until it achieves a complete steady state, which is defined as one in which the energy distribution is not changing and the number density of the electrons is constant. Once a steady state is achieved in a given element of gas, it will vary only slightly as the element passes through the target interaction region, unless the beam intensity varies or the D_2 achieves such a high temperature that the momentum transfer is reversed and the D_2 begins to heat up the electrons. Our calculations indicate that steady state is generally achieved very rapidly, (a few tens of nanoseconds). These distributions have average energies that are only slightly above thermal values and, hence, they tend to deposit most of the electron energy into the D_2 vibrational states (see Table I).

V. LASL INS DESIGN

The LASL INS design calls for a 1-A, 300-keV tritium ion beam to impinge on a 1-cm^3 interaction region containing 2×10^{19} D_2 molecules flowing at a velocity of 3×10^5 cm/s. The gas will enter the interaction region at 35 K. Under these conditions a tritium ion will deposit ~250 keV of energy in the target gas, and it will take an element of this target gas ~3 μs to cross the interaction region. The fraction of this energy that is converted to heat during the 3 μs will set the upper limit on the T^+ beam intensity.

Taking the values given in Ref. 2 and averaging over the energy range of interest (300 to 50 keV) we estimate that 84.2% of the 250 keV per T^+ ion will go directly into ionization. For this estimate we have placed the energy involved in electron capture into the ionization category. The remaining energy goes directly into collisional excitation or momentum transfer and nearly all of this energy ends up exciting the D_2 electronic states.

We estimate that 17.3% of the energy deposited in the target gas will go into the D_2 electronic states:

TABLE I

FATE OF ENERGY INTRODUCED BY IONIZATION

Pathway	%
Dissociative electron recombination	76
Vibrational excitation	13
Dissociation	5
Momentum transfer	3
Electronic state excitation	2
Electron kinetic energy	1
	100%

4.3% goes into the singlet states and 13% goes into the triplet states. These estimates, which include impact excitation by the T^+ and T atoms and secondary electrons, are necessarily crude because we know very little about the distribution of energy deposition into the electronic states. We have assumed that each state has an equal probability of being excited so that three-fourths of the energy is deposited into the triplet states and one-fourth is deposited into the singlet states. To determine how this energy will then re-emerge as heat, we have assumed that the self-quenching rate of D_2^* is long compared to 3 μs and that the initial distribution is not altered greatly by collisions before radiative decay. That is, the energy placed in the triplet and singlet states will stay in the triplet and singlet manifolds, respectively. The distinction between the two manifolds is important because we expect the radiative decay of the triplet states to result in a dissociation that will immediately place about 5 eV of energy into the translational mode. We believe that another 4.5 eV, which is the energy that went into the molecular bond, will not show up as heat in <3 μs because we expect the recombination to occur onto excited vibrational levels.

Finally, we must be concerned with the energy of the electrons produced by ionization of the D_2. The computer program generated the electron distribution shown in Fig. 1 for H_2 at 300 K. This figure shows a "normalized" distribution $\bar{n}(\epsilon) = n(\epsilon)/[\epsilon^{1/2} \sum_{\epsilon} n(\epsilon)]$. This distribution is achieved in 30 ns and varies only slightly over a wide range in gas temperature. For the distribution shown in Fig. 1, the electron number density is 7.6×10^{14} cm^{-3} and the average electron energy is 0.16 eV.

Because this distribution is established so rapidly, we can assume this distribution for the full 3 μs. This allows us to convolve the cross sections back over the distribution and to determine the energy deposition into each process (Table I). Unfortunately, the rapid equilibration of the electron energy distribution also means that most of the energy that went into overcoming the ionization threshold shows up as thermal energy on a time scale very short compared to 3 μs. The energy that does not emerge as heat is the 4.5 eV that goes into the molecular bond. Although we expect atom-atom recombination in <3 μs, this energy will hang up in the excited vibrational states. This recombination argument also applies to the atoms created by the direct impact dissociation of D_2 by electrons. In such a dissociation an electron will give up ~10 eV but only ~5 eV will emerge as heat in <3 μs.

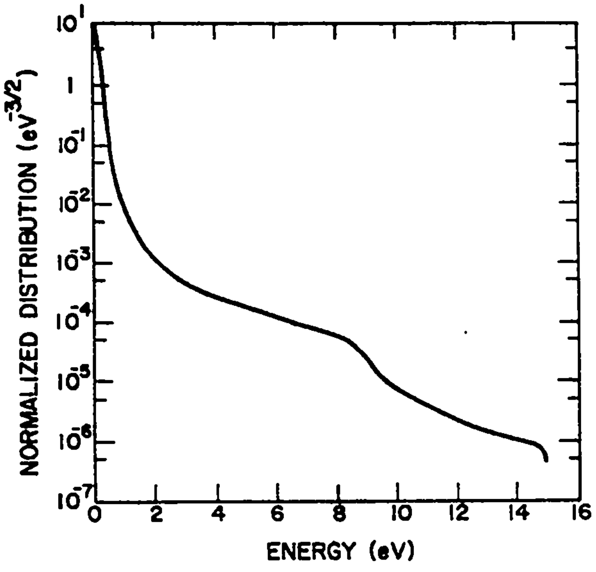

Fig. 1.
Normalized electron distribution for H_2 at 300 K.

All of the previous arguments permit us to show in Table II the fractional breakdown of the energy into the various modes of the D_2 molecule and the fraction of the energy that we expect to appear as thermal energy while the D_2 gas remains in the target interaction region. The numbers for rotational excitation are estimates based on the energy involved in exciting the D_2 rotational levels. We conclude that under these conditions, ~57% of the energy deposited by the T^+ beam will emerge as heat in a time that is short compared to 3 μs. We expect 6% of the energy to be given off as radiation from decaying electronic states. The rest of the energy is hung up in vibrational excitation and will emerge as heat eventually.

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TABLE II

FATE OF ALL ENERGY DEPOSITED IN TARGET GAS

Pathway	%	Rapid Thermal ($T < 3\ \mu s$) %
Dissociation	4	2
Electronic excitation	17	6
Vibrational excitation	11	0
Rotational excitation	< 1	< 1
Dissociative electron recombination	64	46
Momentum transfer	3	3
Electron kinetic energy	< 1	0
	~100 %	~57 %

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