DOE/ET-53088-369 IFSR #369

Influence of Attractive Interaction between Deuterons in Pd on Nuclear Fusion

T. Tajima, H. Iyetomi [b,c] and *S. Ichimaru* [c]
Department of Physics and Institute for Fusion Studies
The University of Texas at Austin
Austin, Texas 78712

April 1989

[b] *Materials Science Division, Argonne National Lab.*
[c] *Department of Physics, University of Tokyo, JAPAN*

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T. Tajima [a], H. Iyetomi [b,c], and S. Ichimaru [c]

(a) Department of Physics and Institute for Fusion Studies
University of Texas
Austin, TX 78712

(b) Materials Science Division
Argonne National Laboratory
Argonne, IL 60439

(c) Department of Physics
University of Tokyo
Bunkyo-ku, Tokyo 113
Japan

Submitted 14 April 1989; revised 20 April 1989

It is shown that in a heavily deuterated palladium metal a pair of deuterons exhibit attractive interaction at short distance (≈ 0.1 Å - 0.7 Å) due to strong Coulomb correlations in the ion-sphere model and due to the screening action of localized 4d electrons. This mechanism leads to enhanced thermonuclear reactions at room temperatures some 50 orders of magnitude faster than that in a D_2 molecule. Characteristic signatures of predicted nuclear reactions are described.

Reports [1,2] on evidence of nuclear fusion of isotopic hydrogen nuclei and possible generation of heat in a laboratory condensed matter through electrolysis provide us much excitement and bewilderment. One of the most challenging questions with fusion research in general and the above two experiments using Pd electrodes in particular is how two positively charged nuclei come to fuse. Rafelski et al. [3] suggested a mechanism of a bound d-d molecule squeezed by a heavy electron.

In heavily deuterated palladium ($\approx$ PdD) Pd atoms form a fcc lattice, while deuterium atoms sit in the octahedral positions to form a tight overall NaCl-type lattice (β-phase) with the lattice constant $d \approx 4.08$ Å [4,5]. Deuteriums would migrate itinerantly from a cell to a cell under electrolysis driven by the applied voltage or the chemical potential in a fashion similar to superionic conductors. A palladium atom has ten d-shell electrons. We shall show that a deuterium atom in the Pd lattice exerts in effect an *attractive* electric potential in short distances (0.1 Å - 0.7 Å) to another deuterium due to strong Coulomb correlation effects [6,7]. Such an attractive electric potential between a pair of deuterons gives rise to a bound state for deuterons in equilibrium and to a substantial reduction of the Coulomb barrier turning point for itinerant deuterons. We shall show that such itinerant deuterons fuse with other deuteron nuclei in the dense electron system at a rate many tens of order of magnitude faster than that expected from a gaseous deuterium molecule.

In the present article our physical model consists of: (i) ten (per atom) Pd 4d-shell electrons and a deuterium electron forming screening cloud of electrons (density n_e) with an effective mass m^*; (ii) the Pd core electrons and nuclei as a dielectric medium with a dielectric constant ε_c; (iii) strong short-range correlation between dense deuterons represented by the ion-sphere model [6,8]. It is noted here that in Pd a deuteron is unlikely to form an atomic (de^-) or molecular (dde^-) bound state, as inferred from mobility and other evidences [1,4].

The effective interaction potential between deuterons are expressed as

$$\phi_{dd}(r) = \phi_{IS}(r) + \phi_{sc}(r). \tag{1}$$

In the short-range regime ($r < a = (3/4\pi n_d)^{1/3}$) where n_d is the deuteron density the ion-sphere potential $\phi_{IS}(r)$ is given [6] by

$$\phi_{IS}(r) = -\frac{9}{10}(2^{5/3} - 2)\frac{e^2}{a_e\varepsilon_c} + \frac{e^2}{4a_e\varepsilon_c}\left(\frac{r}{a_e}\right)^2, \tag{2}$$

with $a_e = (3/4\pi n_e)^{1/3}$. This model has been shown valid in the strong coupling regime [6] characterized by $\Gamma = e^2/(a_e T) >> 1$. The screened potential $\phi_{SC}(r)$ is written in the wave number (q) space as

$$\phi_{SC}(q) = \frac{4\pi e^2}{q^2\varepsilon_c\varepsilon(q,0)} . \tag{3}$$

The dielectric function $\varepsilon(q,\omega=0)$ for degenerate electrons has been evaluated with the local field correction due to Ichimaru and Utsumi [9]. An effective mass m^* in Eq. (3) takes into account the strong correlation in the d-shell electrons. Degenerate electron liquids are characterized by

$r_s = a_e/(a_B\ \varepsilon_c) > 1$ where a_B is the Bohr radius of an electron with m*.

Figure 1 shows an example of $\phi_{dd}(r)$ calculated with $m^*/m = 10$ and $\varepsilon_c = 1.0$. Note that at room temperatures two deuterons can approach each other up to the WKB turning point $r_t = 0.14$ Å, as compared with 0.74 Å (the distance of a gaseous deuterium molecule). Both of the two terms in Eq. (1) are important to yield the significant attractive behavior of $\phi_{dd}(r)$ at short distances (0.1 Å - 0.7 Å).

The nuclear reaction rate per a pair of deuterons with the rest mass M reads according to the standard formula,

$$\lambda = \frac{2n_d}{(\pi M)^{1/2}\, T^{3/2}} \int_0^{\infty} E\sigma(E)\exp(-E/T)\, dE \,. \tag{4}$$

The cross section $\sigma(E)$ is related to the Gamow penetration factor p(E) through $\sigma(E)=S(E)p(E)/E$, where S(E) is intrinsically determined by the nuclear reaction. We can approximately calculate p(E) as

$$p(E) = \exp\left[-\pi\sqrt{\frac{Me^2 r_t}{\hbar^2 \varepsilon_c}}\right] = \exp\left[-261.6\sqrt{\frac{r_t(\text{Å})}{\varepsilon_c}}\right]. \tag{5}$$

Equation (5) exhibits an extremely sensitive dependence of p(E) on the parameters: r_t, ε_c, and M; r_t and M will change when nuclear reactions other than between deuterons are considered.

The nuclear reactions we consider are:

primary reactions

$$d + d \rightarrow p + t \ (4.03\ \text{MeV}): \qquad S \approx 53\ \text{keVb} \tag{6}$$

$$d + d \rightarrow n + {}^3He \ (3.27\ \text{MeV}): \qquad S = 53\ \text{keVb}^{[3]} \tag{7}$$

secondary reactions

$$t + d \rightarrow n + {}^4He \ (17.6\ \text{MeV}): \qquad S = 1.7 \times 10^4\ \text{keVb}^{[10]} \tag{8}$$

$$n + d \rightarrow t + \gamma \ (6.3\ \text{MeV}): \qquad \sigma = 0.5 \times 10^{-3}\text{b}^{[11]} \tag{9}$$

$$p + d \rightarrow {}^3He + \gamma \ (5.5\ \text{MeV}): \qquad S = 2.5 \times 10^{-4}\ \text{keVb}^{[12]} \tag{10}$$

$$p + p \rightarrow d + e^+ + \nu_e \ (1.4\ \text{MeV}): \qquad S = 4 \times 10^{-22}\ \text{keVb}^{[12]} \tag{11}$$

The results of the nuclear reaction rates for the above processes are shown in Fig. 2 and Table 1. In the stellar interior thermonuclear reaction rates are drastically enhanced by the strong Coulomb screening effects among ions [6,8].

The core dielectric constant ε_c and the effective mass m* of the Pd system are determined as follows. The main contribution to ε_c arises from $(4s)^2(4p)^6$ electrons as $\varepsilon_c = 1 + (4\pi\hbar^2 e^2/m)\sum_i n_i/E_i^2$, where n_i and E_i are the i-th shell electron densities and binding energies of Pd: $E_{4p} = -51.1$ eV and $E_{4s} = -86.4$ eV [13]. We thus determine $\varepsilon_c = 1.25$. The experimentally measured plasmon energy is $\hbar\omega_p = 7.4$ eV [14]. Since $\hbar\omega_p^{expt} = \hbar(4\pi n_{4d} e^2/m^*\varepsilon_c)^{1/2}$ and $\hbar\omega_p^{bare} = \hbar(4\pi n_{4d} e^2/m)^{1/2} = 31.0$ eV, we obtain

$m^*/m = \varepsilon_c^{-1}(\omega_p^{bare}/\omega_p^{expt})^2 = 14$. For these values our model predicts the nuclear fusion rates close to the values in the third row in Table 1. The d-d reaction rate for this case is $\lambda_{dd} = 1.1\times10^{-24}$ sec^{-1} at $n_d = 6.25 \times 10^{22}$ cm^{-3}. This value is not too far from the experimental value [2]. On the other hand we may determine m* from the energy band width for 4d-shell electrons. The experiment [15] gives the band width $E_b = 5$ eV. We thus obtain $m^*/m = (E_F/E_b) = 5.7$, where E_F is the Fermi energy of ten ideal electrons per Pd atom. The data closely corresponding to this case is included in row 2 of Table 1. We also considered a different model of treating $(4d)^{2 \text{ or } 4}$ electrons as conduction electrons. In this model the effective mass m* may be determined from the low-temperature measurement [16] of the specific heat c_V.

In summary,

(i) We have shown that the attractive potential between deuterons significantly enhances the rate of thermonuclear fusion reactions in Pd. Enhancement factor varies by many orders (as many as 40 orders) of magnitude, depending on the range of possible parameters (m^*, ε_c). The rate under our preferred parameters for the primary d-d reaction is not inconsistent with the experimental result [2]. The shape of the potential in Fig. 1 may be related to the observation that the reaction stops when the voltage is off: at no voltage state deuterons stay in the equilibrium position, the bottom of the potential well, while with voltage on deuterons begin to move and approach the turning point r_t (see Fig. 1).

(ii) We note that uncertainties in the determination of values for m* and ε_c can sensitively affect the calculation of nuclear reaction rates by many orders of magnitude. Precise knowledge of the screening properties of outer-shell electrons is thus essential. We call for much need for theoretical and experimental studies of this problem in the future.

(iii) We can show that secondary protons and tritiums in Eq. (6) are subject to complete burning. The number of secondary protons N_p is derived as

$$N_p(E) \cong N_p^0 \exp\left[-\frac{S(0)}{\sigma_{max} I_0} \int_E^1 \frac{e^{-A/\sqrt{E+C}}}{E^{3/2}} dE\right], \qquad (12)$$

where A is a constant of order unity, C is a constant of O(m/M), σ_{max} is the maximum collision cross section, and the energy E is normalized by $M(\alpha c)^2/2$ with α being the fine structure constant. It can be shown that as the proton slows down ($E \to 0$), $N_p(E) \to 0$, i. e., it burns out completely, yielding ^{3}He and γ.

(iv) In our domain of parameters (Fig. 2) the p-d reaction rate is comparable with the d-d counterpart in spite of its electromagnetic nature. It is also noted that the rare weak interaction of p-p would be on the verge of detection in some extreme circumstances. The d-t rate per pair, however, is not much faster than the corresponding d-d rate as expected. The d-^{3}He reaction rate is negligible because of doubly charged ^{3}He. These results arise from extremely sensitive dependence of p(E) on the reduced mass and the charges for the interacting particles.

(v) The secondary charged fusion products (p, d, t, ^{3}He, ^{4}He, etc.) suffer collisions, scattered and slowed down, in the Pd system. For fusion product protons, for example, the range is 4 x 10^{-3} cm. Since the mean free path of neutrons in Pd is $(n_d \sigma_n)^{-1} \approx 1$ cm [17], the neutron volumetric effect may come into play when the Pd specimen size exceeds 1 cm.

We appreciate helpful discussions with A. Nakano, T. Udagawa, D. Baldwin, and P. Vashishta. The work was supported by U.S. Department energy and NSF.

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ε_c	m*/m	r_t(Å)	λ_{dd}	λ_{pp}	λ_{pd}	λ_{dt}
1	1	0.29	2.9e-51	1.9e-56	4.5e-45	2.5e-54
1.5	7	0.18	2.3e-30	1.2e-41	5.3e-28	2.0e-31
1.5	15	0.14	1.1e-24	1.2e-37	2.3e-23	3.3e-25
3	7	0.23	6.5e-22	1.1e-35	4.2e-21	3.6e-22
5	20	0.19	6.5e-13	2.5e-29	9.4e-14	2.7e-12

Table1. The rate λ (in sec^{-1}) of thermonuclear reaction for dd, pp, pd, and dt processes. The density of the projectile and target particles are both 6.25×10^{22} cm^{-3}; r_t is the classical turning point at room temperatures.

Fig. 1. The bare Coulomb potential e^2/r (dotted line), the screened potential $\phi_{sc}(r)$ (dashed line), and the total potential $\phi_{dd}(r)$ (solid line) in Eq. (1) as a function of distance for $m^*/m = 10$ and $\varepsilon_c = 1$.

Fig. 2. The thermonuclear reaction rate λ (in sec^{-1}) for cases with $\varepsilon_c = 1$ (squares), $\varepsilon_c = 1.5$ (circles), $\varepsilon_c = 3.0$ (triangles), and $\varepsilon_c = 5.0$ (crosses) as a function of m^*/m; (a) for the d-d reaction and (b) for p-d.

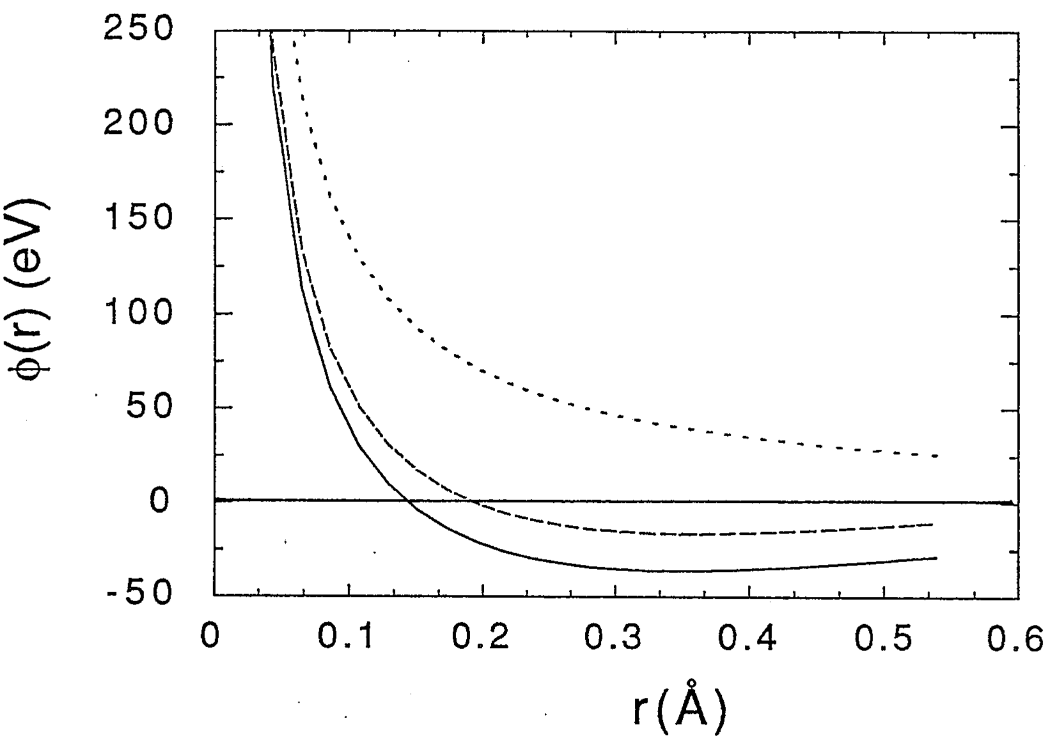
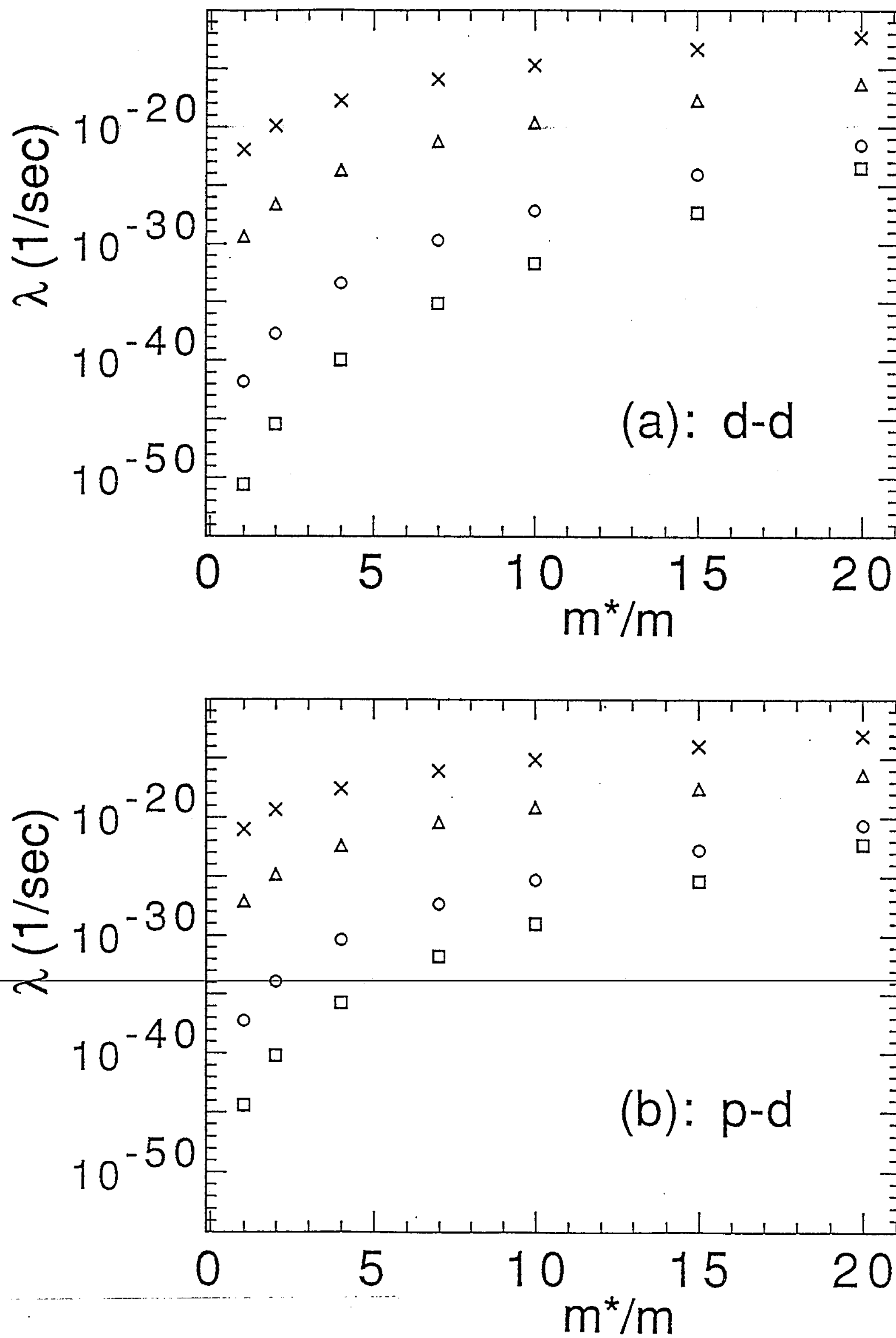


Fig. 1



λ (1/sec)
10^{-20}
10^{-30}
10^{-40}
10^{-50}
(a): d-d
0
5
10
15
20
m*/m
λ (1/sec)
10^{-20}
10^{-30}
10^{-40}
10^{-50}
(b): p-d
0
5
10
15
20
m*/m

Fig. 2