Pramāṇa – J. Phys., Vol. 33, No. 2, August 1989, pp. L343–L346. © Printed in India.

The role of combined electron-deuteron screening in *d-d* fusion in metals

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MS received 10 June 1989

Abstract. We propose that the *d-d* fusion rate in palladium can be enhanced by the combined screening of the electrostatic interactions by the itinerant deuterons and the conduction electrons. The model assumes that, under certain conditions, deuterium exists as a D^+ ion in palladium. The combined screening by electrons and the D^+ ions (deuterons) is found to be more effective than that due to electrons alone. The calculated values of the *d-d* fusion rates, considering screening, for composition PdD at 300 K are $10^{-16}\ s^{-1}$ and $10^{-14}\ s^{-1}$ for D_2^+ ion and D_2 molecule respectively. These values lie in the range suggested by the recent electrochemical experiments.

Keywords. Fusion in metals; electron-deuteron screening.

PACS Nos 25·70; 24·10; 21·30

1. Introduction

It is well known that the quantum-mechanical calculation of the fusion rate for D_2 molecule in free space yields a negligibly small value of $\sim 10^{-70}\ s^{-1}$ (Van Siclen and Jones 1986). The recent electrolytic experiments by Fleishmann and Pons (1989) and by Jones *et al* (1989), however, suggest a possibility of a much higher fusion rate of deuterium in palladium at room temperatures. In this communication we propose that if cold fusion is indeed a reality, it may be explained by the combined screening of the Coulomb interactions by itinerant deuterons and the conduction electrons in metals. The chief assumption of our model namely, that deuterium exists as mobile ionized species in palladium under electrolytic conditions, is based on the following facts. It has been established from the electromigration measurements that in palladium, hydrogen exists as a proton with an effective charge $\approx +1$ (Wipf 1978). Likewise, deuterium should also exist as deuteron with an effective charge $\approx +1$. Besides, deuterium is known to be highly mobile in palladium (Volkel and Alefeld 1978). Under these conditions, the deuterons would participate in screening the electrostatic interactions along with the conduction electrons of the metal. The combined screening reduces the Coulomb barrier between the deuterons separated by a distance r by a factor $\exp(-kr)$ (where k is the screening constant), thereby leading to an enhancement in the fusion rate.

For a nominal composition PdD with a substantial fraction of deuterium atoms in an ionized state, the condition of charge neutrality in the bulk can be written as

$$n_P + n_D = n_C \tag{1}$$

where n_P, n_D, n_C, are the bulk densities of the fixed palladium ions, mobile deuterons and the conduction electrons respectively.

For calculating k, one sets up the Poisson's equation for the potential at a radial distance r from a test charge in terms of the net charge densities induced at r. The induced charge densities are obtained using Fermi-Dirac statistics for electrons and Bose-Einstein statistics for deuterons. Upon linearizing the densities as a function of the potential and using the Fourier transform techniques for the Poisson's equation, it can be shown that

$$k^2 = k_C^2 + k_D^2 \tag{2}$$

$$k_C^2 = 6\pi e^2 n_C / E_C \tag{3}$$

$$k_D^2 = [4\pi e^2 n_D / k_B T][z g'_{3/2}(z)/g_{3/2}(z)]. \tag{4}$$

In the above equations $E_C = (2m_C)^{-1}(3\pi^2 \hbar^3 n_C)^{2/3}$ is the Fermi energy of the electron gas, k_B is the Boltzmann constant and T is the temperature. The fugacity z $(0 < z < 1)$ is related to the chemical potential μ via the expression $z = \exp(-\mu/k_B T)$ and the function $g_{3/2}(z) = \sum_{n=1}^{\infty}[n^{-3/2} z^n]$ is well known in connection with Bose condensation (Huang 1963).

Equation (4) is valid for temperatures $T > T_C$ where

$$T_C = [2\pi \hbar^2 / m_D k_B][n_D / 2{\cdot}612]^{2/3}. \tag{5}$$

The Bose condensation temperature of the ideal deuteron gas in PdD calculated from eq. (5) is 6·65 K. From eq. (4) it follows that at high temperatures $k_D \propto T^{-1/2}$. At low temperatures k_D can diverge as $(T - T_C)^{-1/2}$ as $T \to T_C^+$. Thus the contribution to screening from charged bosons is strongly dependent on temperature and exhibits a power-law divergence at T_C^+. However this may not be realizable in PdD due to a sharp drop in the mobile fraction of deuterons at cryogenic temperatures.

The Thomas-Fermi screening by conduction electrons is well known in solid state physics (Kittel 1976). The calculations based on (2)–(4) show that the combined screening by electrons and deuterons is more effective than that due to electrons alone.

To calculate the fusion rate in the presence of the combined screening, we assume the existence of pairs of deuterons in the interstitial sites of palladium lattice. These form metastable D_2^+ ions or D_2 molecules which undergo spontaneous fusion at a rate

$$R = A[\psi(0)]^2, \quad A = 2 \times 10^{-16}\,\mathrm{cm^3\,s^{-1}} \tag{6}$$

where $\psi(0)$ is the molecular wave function at the origin. At an internuclear separation r

$$\psi^2(r) = [\mu w/(8\pi^{3/2} r_a \hbar)]\exp[-\beta(r)] \tag{7}$$

$$\beta(r) = \int_r^{r_a} [2|2\mu\{E_V - V(x)\} - 1/4x^2|^{1/2} - (1/x)]\,\mathrm{d}x \tag{8}$$

where μ is the effective mass of the d-d system, w is the vibrational frequency, E_V is the ground state energy, $V(r)$ is the interaction potential between the deuterons and r is the inner turning point on the potential energy curve (figure 1). To take the screening into account, we have used the potential

$$V(r) = (1/r)\exp(-kr) - 1{\cdot}5/[1 + 0{\cdot}127r]^4 \tag{9}$$

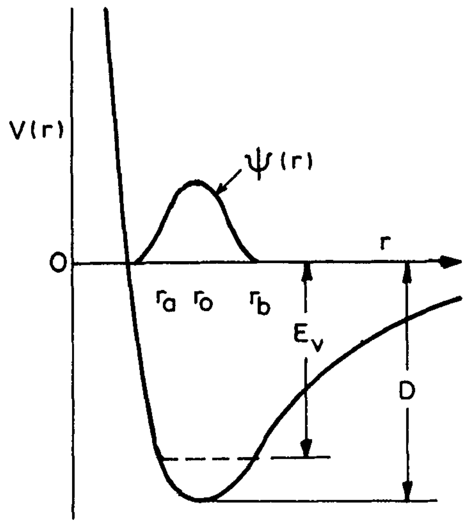

Figure 1. Potential energy curve and ground state wave function for the relative motion of the two nuclei.

which, for $k=0$ is the same as the potential used by Jackson (1957) for an unscreened D_2^+ ion. All the quantities in the above equation are expressed in atomic units. In the present calculations we have assumed that almost all the deuterium atoms are ionized and these can be extended to account the actual fraction of deuterons present by using appropriate values for n_D and n_C.

The calculations using the above equations show that the fusion rate for D_2^+ ions which is 5×10^{-79} s^{-1} in free space increases to 4×10^{-46} s^{-1} in palladium when the screening due to the conduction electrons ($k_C=1{\cdot}0$ au) alone is applied. On the other hand, under the combined screening by deuterons and electrons at 300 K ($k=11{\cdot}6$ au), the fusion rate for D_2^+ ion increases to 5×10^{-16} s^{-1}. Similar calculations were performed for D_2 molecule with the potential $V(r)=(1/r)\exp(-kr)-2{\cdot}18/[1+0{\cdot}18r]^4$. The fusion rates obtained were 1×10^{-63} s^{-1} for $k=0$, 3×10^{-40} s^{-1} for conduction electron screening ($k_C=1{\cdot}0$ au) alone and 1×10^{-14} s^{-1} for the combined screening by deuterons and electrons at 300 K ($k=11{\cdot}6$ au). Thus it is seen that the spontaneous fusion rate increases to 10^{-16} s^{-1} for D_2^+ ion and to 10^{-14} s^{-1} for D_2 molecule at 300 K, which lie in the range of values indicated by the cold fusion experiments.

The fusion rate is a sensitive function of k_D which is proportional to $n_D^{1/2}$. Under electrolytic conditions, the density of deuterons is higher on the palladium surface than in the bulk due to the existence of a large concentration gradient at the surface. Moreover, the mobility of deuterons in the surface layers will also be much higher. As a consequence, the fusion rate will be substantially higher in the surface layers than in its bulk.

Suppose an additional electric field is applied along the length of the deuterium-saturated palladium cathode during electrolysis in the Fleishmann and Pons' type cell. Due to electromigration under the applied field, the fraction of the mobile deuterons will be increased. Further, as pointed out by Wipf (1978), a potential difference of, say, 500 mV can create a deuteron density ratio of 10^8 between the two ends of the cathode. Though this factor is probably an overestimate (due to space-charge effects), under the additional electric field, n_D at one end will nevertheless be enormously higher than that in the absence of the field. As a consequence, we expect that under the application of the additional electric field, the screening will be substantially enhanced which would, in turn, lead to a large increase in the fusion rate. Similarly an increase in the fusion rate can be expected in the Ti-D gas experiment (Ninno *et al* 1989) by the application of the electric field across the titanium metal.

We thank Dr V K Kelkar for computer calculations. We are indebted to Dr J P Mittal and Dr K S V Nambi for their encouragement and support during this work.

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