A Possible Mechanism for Bulk Cold Fusion in Transition Metals Hydrides.

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Abstract. – A simple phenomenological model for the high fusion rate recently observed in transition metal deuterides is presented. It is shown that the existence of localized vibrational modes of deuterium atoms, like those actually found in NbD and TaD, can account for the experimental fusion rates.

Considerable interest has been aroused by the recent suggestion that nonnegligible rates of deuteron-deuteron fusion processes can be achieved in deuterium-rich Pd and Ti samples under several experimental conditions [1]. Although the dynamics of the process is not established and several hypotheses can be proposed, it is clear that, due to the very low kinetic energy available in solid state at near room temperature, the only way to get over the barrier between the nuclei is a tunnelling process. It is also clear that the conditions giving rise to such a relatively high rate of tunnelling through the barrier are not very common and that some peculiar process or condition affecting the effective thickness of the barrier is necessary.

Although presently available experimental data do not allow to distinguish between surface and bulk contributions, we believe that both the possibilities should be investigated.

The aim of this letter is to show that a possible mechanism contributing to the observed phenomenon can be ascribed to the dynamics of the hydride lattice and that phonon modes actually detected in transition metal-hydrogen systems, have energies of the right order of magnitude to yield the observed fusion rates. First of all we note that in ordinary conditions the deuterons behave as relatively localized atoms as one can realize from the phonon dispersion relations [2] by neutron diffraction experiments. Because of the localized character of deuterium atoms, their root-mean-square fluctuation can be obtained by
assuming the following approximate relationship:

\[ \langle u^2 \rangle = \hbar^2 / 2M \ \text{ctgh} \left( 0.5E_v \beta \right) f_v / E_v, \]

so that in a f.c.c. lattice where deuterium occupies two octahedral holes the fusion rate is approximatively given by [3]

\[ \Phi = 6 \cdot 10^{-16} \left[ 3 / (4\pi \langle u^2 \rangle) \right]^{3/2} \exp \left[ -3/8 \left( R^2 / \langle u^2 \rangle \right) \right] \text{ (fusions/s/2 deuterons)}, \]

under the hypothesis that the deuterons move independently (localized states) and all the octahedral sites are occupied. In eqs. (1) and (2) \( E_v \) is the deuterium vibrational energy, \( f_v \) the oscillator strength of the mode, \( \beta = 1/k_B T \) and \( M \) the deuteron mass. It is important to note that eq. (1) suitably adapted can be used to describe the stretching modes of a molecule. Using for \( E_v \) the experimental value of 364 meV one obtains for \( \Phi \) at room temperature the vanishingly small value of \( 10^{-52} \) fusions/s/molecule. From eqs. (1) and (2) it is apparent that \( \Phi \) is strongly dependent on the vibrational energy and in fact in fig. 1 we report \( \Phi \) as a function of \( E_v \) at \( T = 300 \text{ K} \) assuming \( f_v = 1 \). Looking at this figure, we realize that a vibrational energy of the order of 40 meV is sufficiently low to enhance the fusion rate to the observed level \( (10^{-28} + 10^{-21}) \). The effect of a variation of \( f_v \) is shown in fig. 2 where the fusion rate at room temperature is plotted as a function of \( f_v \) at an energy of 18 meV. The reason for this choice will be explained in the final considerations.

In order to reproduce the observed enhancement of the fusion rate at the \( \alpha - \beta \) transition temperature (413 K in the case of Pd) we have adopted for \( f_v \) the following expression:

\[ f_v = f_{v0} \exp \left[ - (T - T_0) / W_T + 1 \right], \]

where \( f_{v0} \) is a constant to be determined, \( T_0 \) is the transition temperature and \( W_T \) is a
Fig. 2. – Fusion rate per deuteron pair as a function of the oscillator strength at a vibrational energy of 18 meV.

measure of the width of the transition. The quantity \( f_{v0} \) has been fixed by the requirement that the maximum fusion rate should be of the order of \( 10^{-21} \). The calculated variation of \( f_v \) and \( \log \Phi \) as a function of \( T \) are shown in fig. 3 for an energy of 18 meV.

Fig. 3. – Fusion rate per deuteron pair as a function of temperature (dashed line) when a simple behaviour of the oscillator strength vs. temperature (full line) is assumed.

The hypothesis that systems close to diffusionless transitions (like those exhibited by the metal lattice in the case of hydrides) develop complex vibrational features is supported by experimental evidence [4, 5]. Such features are due to local fluctuations of the crystal structure [5] and apparently are rather common. Though no information about palladium and titanium hydrides is available when the systems are close to the structural transition, nonetheless the presence of a relatively low-energy dispersionless mode has been observed in both NbD and TaD [6]. The energy of such a mode is about 18 meV in these systems. As a consequence we have adopted this value of the energy in the above calculations, even though
this choice is essentially irrelevant since all foregoing calculations can be repeated for other suitable values of the vibrational energy. Moreover such a mode will contribute to the hydrogen motion so that it can be directly responsible for the increase of the fusion rate in the bulk. If this is the case, it is apparent that the crossing of the transition region is important in developing such an effect.

REFERENCES