Theoretical Model Of The Probability of Fusion Between Deuterons within Deformed Crystalline Lattices with Micro-Cracks at Room Temperature

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Abstract. In this paper, we wish to demonstrate that the deformation of the crystalline lattice, at room temperature, can influence the process of fusion of the deuterons introduced into the lattice by deuterium loading. In fact, calculating the probability of deuteron-plasmon fusion within a micro-crack, showed, together with the enhancement of the tunnelling effect, an increase of at least 1-3 orders of magnitude compared to the probability of fusion on the surface of the lattice. These phenomena open the way to the theoretical hypothesis that a kind of chain reaction, catalysed by the micro-cracks produced in the structure as a result of deuterium loading, can favour the process.

1. Introduction

As a result of the numerical calculation performed for different metals, varying the temperature, the total energy and the concentration of impurities, it was possible to conclude that the probability of fusion was in effect substantially enhanced by increasing these parameters. In this paper, we wish to confirm the hypothesis regarding micro-cracks, by means of quantitative theoretical estimates of the coefficient of structural deformation of the perturbed[2] crystalline lattice independent of time, obtained for different temperature values in the range 100-300 K. In particular, we calculated the probability of fusion within a micro-crack, comparing it with that calculated on the surface, to evidence a possible enhancing effect.

Further, we also wish to observe, theoretically, any influence on the phenomenon produced by variation in temperature, which could favour the fusion of the deuterium nuclei as a consequence of the deformations and micro-cracks produced in the lattice. In fact these may be able to concentrate in their vicinity a relevant fraction of the deuterons present in the metal.

The phenomenon hypothesised above could possess characteristics analogous to the formation of the Cottrell atmosphere in metals[2], known for some time in solid state physics, which essentially consists of a redistribution of the impurities present in the metal around a dislocation of the ions making up the lattice.

In these cases, the interaction between the dislocation and the impurities present can significantly modify the electrical properties of the material; further, some particular reactions can occur, incorporating the impurities in the nucleus of the dislocations, as a result of the different arrangement of the atoms with respect to that of the unperturbed lattice. This type of process has been extensively studied in the literature for the case of crystalline semiconductors at high temperature[2] and for metals[2]. In the latter, for example, it is found that the concentration of interstitial impurities around a linear dislocation, with a point component, depends on the temperature according to a law of the type:

$$c = c_0 \exp\left[\frac{\beta}{bkT}\right] \tag{1}$$

where c_0 is the concentration of impurities in the zone with zero internal pressure, $b^3 \simeq v_i$ the volume of the ions constituting the lattice, while β is proportional to the difference

v_d - v_i between the volume of the atoms of the impurities and that of the lattice ions.

Our conjecture is that in a metal, such as Pd, a similar phenomena could occur between the atoms of deuterium penetrating the lattice as a result of deuterium loading and the micro-cracks produced by variations in temperature.

In this case, the parameter β of the previous expression would be *negative*, determining an increase in the concentration of deuterons in the vicinity of the micro-crack, which would then catalyse the phenomenon of fusion.

The procedures, such as deuterium loading within lattices[3].

In effect, it is found that with the appearance of micro-cracks, in agreement with the "chain reaction" hypothesis proposed in reference[1], there is an increase in the rate of deuteron fusion within the lattice, obtained by evaluating the number of events per minute with a numerical simulation programme which employs the "WKB" method for the approximate solution of the wave equation. This calculation, which takes account of all the physical parameters, provides theoretical information, which we consider interesting, for "impure" metals at room temperature and for average deuteron energies.

2. Three-dimensional model of spherical symmetry

The numerical calculation, performed for three typical metals (Pd, Ti and Pt) on varying the temperature and total energy, in turn dependent within certain limits on the temperature, made it possible to conclude that the probability of fusion is in effect enhanced by increasing *P, T* and *E*.

The following table refers to the probability of fusion calculated on the surface of Palladium[1]). It shows the trend of the probability of deuteron fusion in impure Pd (J = 0.75%) on varying T and E (Tab.1 in reference[1]). Palladium, which has CFC symmetry, shows higher values for the probability of fusion than Pt and Ti, for temperatures between 36.7 K and 63.7 K and energies between 140 eV and 240 eV.

T ≈	**36.7 K**	**45.7 K**	**54.7 K**	**63.7 K**
E ≈	**P ≈**	**P ≈**	**P ≈**	**P ≈**
140	10^{-60}	10^{-55}	10^{-59}	10^{-54}
160	10^{-52}	10^{-47}	10^{-50}	10^{-44}
180	10^{-45}	10^{-43}	10^{-42}	10^{-40}
200	10^{-42}	10^{-41}	10^{-39}	10^{-38}
220	10^{-40}	10^{-39}	10^{-37}	10^{-36}
240	10^{-37}	10^{-35}	10^{-35}	10^{-33}

An important effect on the reaction, due to the metal lattice, is represented by electronic screening. This effect, already studied by Rabinowitz et al.[4], can be taken into account using a model in which the negative charge is distributed around the nucleon in a thin shell and can be schematised supposing the electric charge to be uniformly distributed with a thin spherical shell, with a radius $R \geq r_1$ equal to the effective range of the interaction between the nucleons, describable in terms of a "shifted[4]" Coulomb potential.

$$V = \left(kq^2\right)\left[1/r - 1/R\right] \qquad r_1 \leq r \leq R \qquad (2)$$

where q is the charge of the deuton, r_1 is the nuclear radius, $k = 1 / 4\pi\varepsilon_0$. Then $V = 0$ for $r > R$. The solution for the semi-classic tunnelling factor Λ is[4]:

$$\Lambda = D \exp\left[-2\gamma(r_2)\right] \tag{3}$$

$$\gamma(r_2) = (\pi/2\hbar)\left[\left(2q^2/4\pi\varepsilon_0\right)\mu r_2\right]^{1/2} \tag{4}$$

In equations (3) and (4), D is a numerical constant of the order of unity, μ the effective reduced mass of the deuton, r_2 the classic point of inversion, and $\hbar$ is the reduced Planck constant. To take account of the effect of the impurities present in the metal, we modify the constant D in (3) substituting the product $J\eta$, where J is the concentration of impurities and η a numerical constant, $\eta \cong 1$.

The function γ is proportional to the electrical charge of the nucleons and to the square root of the product μr_2, where μ is the reduced mass of the mass centre system for an interaction of two bodies, and r_2 is the classic point of inversion.

Of the three metals considered, Palladium seems to be the most effective in catalysing fusion, as a result of its structural characteristics: This can be understood from a qualitative point of view, observing that the curve of interaction potential, within the metal, has a trend which requires a lower quantity of total energy.

The numerical calculation d-d in this case can be expressed as follows[1]:

$$V(r) = k_0 \frac{q^2}{r} \cdot M_d \left(V(r)_M - \frac{J k T R}{r} \right) \tag{5}$$

where $V(r)_M$ is the Morse potential, $k_0 = 1/4\pi\varepsilon_0$, q is the charge of the deuton and therefore q^2/r is a potential, M_d the reduced mass of the deuterium nuclei, T the absolute temperature at which the metal is experimentally placed, J the concentration of impurities in the crystalline lattice and R is the nuclear radius.

3. Deformation in cubic lattices

In this section we wish to establish whether, and within what limits, the rate of fusion within a micro-crack in a generic cubic lattice subjected to deuterium loading can be conditioned or influenced, as well as by extensive lattice defects and by the other characteristics and thermodynamic conditions, also by any "deformations" produced in the crystalline lattice by variations in the temperature.

If this effectively occurs, it is not difficult to hypothesise that the energy produced by the micro-explosions within the micro-cracks present, could favour the creation of new fractures, which in turn would, by the same mechanism, capture other deuterons, and so on.

On the other hand, the formation of micro-cracks in Palladium electrodes produced by the energy released during long periods of electrolysis[5] has already been observed experimentally for some time, but has until now been considered only a consequence of nuclear fusion. In fact, Heui Kyeong An, et al.[6] an energy peak within micro-cracks during electrolysis.

Our hypothesis is that deuterons are injected into the micro-crack with force during loading and are therefore more likely to emit energy in micro-explosions, which in turn produce further micro-cracks. In this way the phenomenon observed could favour the process, enhancing the probability of fusion of the deutons absorbed by the metal lattice.

We wish to study the internal perturbations which can take place in the lattice following D_2 loading and the consequent modifications in the properties of the metal. The loading does not, in fact, simply provide an increase in the percentage of deuterium present, with a resulting disequilibrium of the "d" band; rather this type of procedure also determines, according to our hypothesis, lattice deformations followed by dislocations which cause micro-cracks in the structure.

It can happen then that the interaction between the impurities present and the dislocations produced in the metal during deformation, significantly modify the electrical properties of the material. Some particular reactions can then take place which incorporate the impurities in the nucleus of the dislocations[7], as a result of the different arrangement of the atoms with respect to that of the unperturbed lattice. An adequate theoretical description of the loading can therefore be obtained, in our opinion, only by treating it as a

perturbation independent of time.

We must also consider the fact that, under conditions far from those of saturation, the rate of fusion, within the metal depends on the number of deuterium nuclei absorbed in unit time, which could also depend on the deformation of the lattice. It is necessary therefore to study both phenomena.

It is known that in the presence of interaction between deuterium nuclei and collective plasmonic excitation in the metal, the number of fusions λ_f in a gas consisting of λ deuterons with density ρ is given by[11]:

$$\lambda_f = \lambda \cdot \frac{4\pi\rho\hbar}{\mu_d} \cdot \langle \frac{1}{p} \rangle \tag{6}$$

where μ_d is the reduced mass of the deuterium nuclei, p is their impulse, and where the parentheses $\langle\ \rangle$ represent the thermal mean.

For simplicity we can now consider a cubic lattice structure subjected to deformations and calculate the probability of fusion within a micro-crack, Γ, on varying the temperature.

Indicating the volume of a single cell by $d\Omega$, the deformation of the entire lattice is given by:

$$\Psi \cong \left\{ \iiint_{\Omega} \eta \left(J \frac{\rho L^2 \nu \mathrm{b}^2}{\alpha 2hR} \chi \exp\left(-\frac{U_0}{kT} \right) \xi_{(r)} \right) d\Omega \right\} \tag{7}$$

where J is the concentration of impurities and η is a parameter which depends on the lattice and electronic structure of the metal under consideration.

In this study we have concentrated on the cubic structure of the lattice, in the specific case of Palladium, because it has an easily observable geometry and we have indicated by ρ the density of the mobile dislocation[8] within the lattice at non constant lattice temperature, so that the thermodynamic stress of the deuterium nuclei per unit volume must be taken into consideration.

Further, demonstrate this, approximate calculations were made in which the lattice[7,8,9] deformation and the micro-crack depth were taken into account.

Taking the centre of mass system as that of reference, the probability of fusion in a zone of the metal in which there is no micro-crack (e.g. on the surface) can be written[1] as:

$$\left|P\right|^2_{\mathrm{int}} = \exp\left(-2 \int_0^{\alpha} \mathrm{K}(r)_{\mathrm{int}}\, dr \right) \tag{8}$$

(12)

α is 0.15Å , $\mathrm{K}(r)_{\mathrm{int}}$ is given by:

$$\mathrm{K}(r)_{\mathrm{int}} = \sqrt{2\mu\left[\mathrm{E} - V(r)\right]/\hbar^2} \tag{9}$$

(13)

E is the total initial energy, principally thermal in nature; μ is reduced mass of the deuteron ; $\hbar$ is Plank's constant.

Equations (8) and (9) refer to the process of fusion within the crystalline lattice.

The Coulomb potential $V(r)$, containing the temperature contribution, is given by the expression (5) :

The symbols adopted here are the same as those used in (5). In (14), the Morse potential $V(r)_M$ is given by:

$$V(r)_M = (J/\zeta)\left\{ \exp\left(-2\varphi(r - r_0)\right) - 2\exp\left(-\varphi(r - r_0)\right) \right\} \tag{10}$$

(15)

Here, J indicates the concentration of impurities present in the metal, while the parameters φ and r_0 depend on the dynamic conditions of the system.

ζ is a parameter depending on the structural characteristics of the lattice, the number of "d" band electrons

and the type of lattice symmetry, and variable between 0.015 and 0.025.

If we divide (8) by (6) and multiply by (7), it follows that:

$$\Gamma \approx \frac{\exp\left(-2\int_0^{\alpha} \mathrm{K}(r)_{\mathrm{int}}\, dr\right)}{\lambda \cdot \frac{4\pi\rho\hbar}{\mu_d} \cdot \langle \frac{1}{p} \rangle} \cdot \Psi \qquad (11) \quad (16)$$

Expression (11) represents the probability of deuteron fusion within a micro-crack: it is directly proportional to the number of deuterons absorbed by the metal until the target is saturated, thereafter the probability of fusion will be inversely proportional to the number of nuclei absorbed by the metal. In the context of the approximations made, the probability of fusion calculated in this way is equal to the edge deformation coefficient per unit of total deformation of the whole lattice.

From (11), with $K(r)_{int}$ calculated adopting the Morse potential, a numerical simulation programme employing the "WKB" method was used to determine the probability of fusion, normalised to the number of events per minute.

The results of Tab.1 can be compared with those of Tab.2, where the potential (5) was substituted by a "shell" potential of the (2) type, modified as followed:

$$V = \left(k q^2\right)\left((1/r) - \frac{\mathrm{KT}}{J\varepsilon R}\right) \cdot \quad r_1 \le r \le R \qquad (12)$$

where KT is the mean kinetic energy of the gas, ε is the vibrational energy which is typically of the order of some eV for the quantum states under consideration and q is the charge of a deuton.

Table 1. – For "impure" metals ($J \approx 0.75\%$), adopting the Morse potential, the probability of fusion Γ was calculated for Pd within a micro-crack, in the presence of D_2 loading, normalised to number of events per minute, for different values of temperature (100 ÷300 K) and energy (150 ÷ 250 eV). It can be seen that the probability generally increases with T and E, and is systematically greater by some orders of magnitude than the probability of fusion **P** on the surface.

Palladium $J \approx 0.75\%$ T-range ≈ 100 - 300 K $\alpha \approx .34$ Å $\lambda_f = 1.38 \cdot 10^{-3}$ eV / min M_{pd} / μg

T ≈	100 K		140 K		180 K		220 K		260 K		300 K	
E ≈	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈
150	10^{-75}	10^{-77}	10^{-66}	10^{-69}	10^{-67}	10^{-68}	10^{-63}	10^{-64}	10^{-64}	10^{-66}	10^{-60}	10^{-68}
160	10^{-73}	10^{-75}	10^{-65}	10^{-68}	10^{-64}	10^{-67}	10^{-61}	10^{-63}	10^{-63}	10^{-65}	10^{-58}	10^{-65}
170	10^{-70}	10^{-73}	10^{-63}	10^{-65}	10^{-62}	10^{-65}	10^{-59}	10^{-62}	10^{-60}	10^{-64}	10^{-56}	10^{-62}
180	10^{-69}	10^{-72}	10^{-58}	10^{-62}	10^{-60}	10^{-64}	10^{-57}	10^{-61}	10^{-58}	10^{-63}	10^{-55}	10^{-60}
190	10^{-67}	10^{-71}	10^{-56}	10^{-60}	10^{-59}	10^{-63}	10^{-55}	10^{-60}	10^{-56}	10^{-62}	10^{-50}	10^{-58}
200	10^{-65}	10^{-70}	10^{-55}	10^{-59}	10^{-57}	10^{-62}	10^{-54}	10^{-59}	10^{-53}	10^{-61}	10^{-47}	10^{-54}
210	10^{-64}	10^{-69}	10^{-54}	10^{-58}	10^{-56}	10^{-61}	10^{-53}	10^{-57}	10^{-52}	10^{-60}	10^{-44}	10^{-51}
220	10^{-62}	10^{-67}	10^{-52}	10^{-57}	10^{-54}	10^{-60}	10^{-52}	10^{-56}	10^{-51}	10^{-59}	10^{-40}	10^{-47}
230	10^{-60}	10^{-66}	10^{-51}	10^{-56}	10^{-53}	10^{-59}	10^{-50}	10^{-55}	10^{-50}	10^{-58}	10^{-32}	10^{-40}
240	10^{-59}	10^{-65}	10^{-50}	10^{-55}	10^{-52}	10^{-58}	10^{-49}	10^{-54}	10^{-49}	10^{-57}	10^{-27}	10^{-34}
250	10^{-58}	10^{-63}	10^{-49}	10^{-53}	10^{-51}	10^{-56}	10^{-48}	10^{-51}	10^{-48}	10^{-53}	10^{-21}	10^{-25}

Table 2..- For "pure" metals ($J \approx 0.25\%$), adopting the "shell" potential, the probability of fusion Γ was calculated for Pd within a micro-crack, in the presence of D_2 loading, normalised to number of events per second, under the same dynamic conditions as Tab.1. Also here Γ is systematically higher by some orders of magnitude compared to the probability of fusion **P** on the surface, but the values are systematically lower that those of the previous case.

Palladium $J \approx 0.25\%$ T-range $\approx$ 100 - 300 K $\alpha \approx .34$ Å $\lambda_f = 1.38 \cdot 10^{-3}$ eV / min M_{pd} / μg

T ≈	100 K		140 K		180 K		220 K		260 K		300 K	
E ≈	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈
150	10^{-75}	10^{-81}	10^{-76}	10^{-85}	10^{-73}	10^{-78}	10^{-69}	10^{-75}	10^{-66}	10^{-76}	10^{-65}	10^{-71}
160	10^{-74}	10^{-79}	10^{-78}	10^{-83}	10^{-70}	10^{-77}	10^{-68}	10^{-74}	10^{-65}	10^{-75}	10^{-63}	10^{-70}
170	10^{-73}	10^{-76}	10^{-76}	10^{-81}	10^{-69}	10^{-76}	10^{-67}	10^{-73}	10^{-63}	10^{-74}	10^{-59}	10^{-66}
180	10^{-71}	10^{-75}	10^{-75}	10^{-80}	10^{-68}	10^{-75}	10^{-65}	10^{-72}	10^{-62}	10^{-73}	10^{-55}	10^{-65}
190	10^{-69}	10^{-73}	10^{-73}	10^{-78}	10^{-67}	10^{-74}	10^{-64}	10^{-70}	10^{-60}	10^{-72}	10^{-53}	10^{-64}
200	10^{-67}	10^{-72}	10^{-72}	10^{-75}	10^{-65}	10^{-73}	10^{-62}	10^{-69}	10^{-58}	10^{-71}	10^{-49}	10^{-62}
210	10^{-65}	10^{-70}	10^{-67}	10^{-74}	10^{-64}	10^{-72}	10^{-60}	10^{-68}	10^{-56}	10^{-68}	10^{-46}	10^{-59}
220	10^{-64}	10^{-67}	10^{-68}	10^{-73}	10^{-63}	10^{-70}	10^{-59}	10^{-67}	10^{-54}	10^{-67}	10^{-43}	10^{-55}
230	10^{-63}	10^{-65}	10^{-66}	10^{-71}	10^{-61}	10^{-69}	10^{-57}	10^{-66}	10^{-52}	10^{-65}	10^{-41}	10^{-52}
240	10^{-61}	10^{-63}	10^{-64}	10^{-70}	10^{-60}	10^{-68}	10^{-55}	10^{-64}	10^{-51}	10^{-61}	10^{-38}	10^{-50}
250	10^{-60}	10^{-61}	10^{-63}	10^{-68}	10^{-58}	10^{-64}	10^{-54}	10^{-62}	10^{-49}	10^{-56}	10^{-35}	10^{-47}

To confirm qualitatively the effect of enhancing the probability of fusion, the trend of the potential curve was obtained on varying the temperature[12] in the range 100 - 300 K, in the case of Palladium. It can be seen that both the height and the thickness of the potential barrier are less in the impure metal ($J \approx 0.75\%$). Fig.1 shows an example of the potential curves obtained.

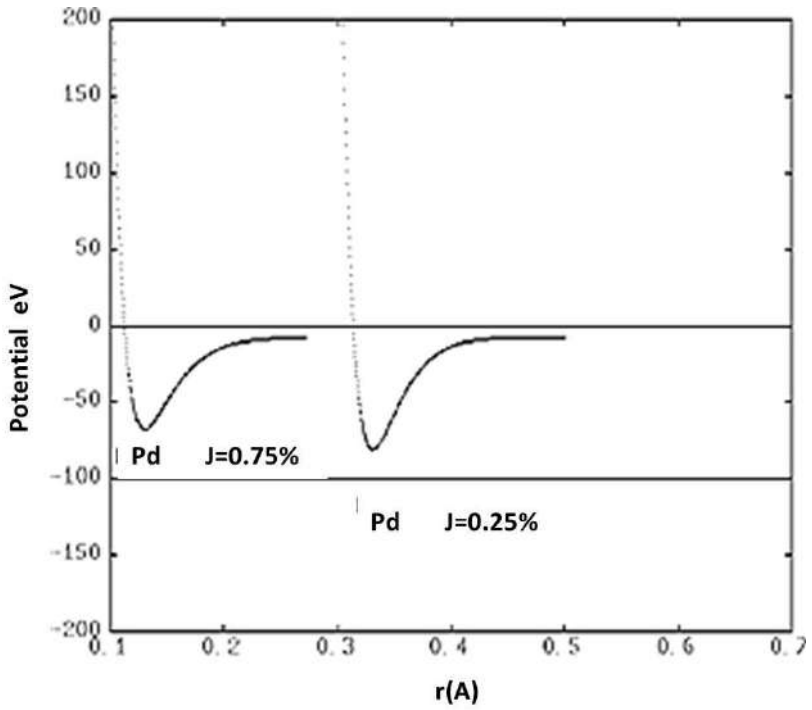

Fig.1. - Comparison between the potentials (14) and (17), in the presence of D_2 for J ≈ 0.75% and J ≈ 0.25%, respectively, at temperature T = 290 K. In the first case, both the height and the thickness of the potential barrier are reduced.

4. Conclusions

The present study was to demonstrate if and how the deformation of the crystalline lattice and the formation of a micro-crack could influence the process of fusion at room temperature. More precisely, we calculated numerically the probability of fusion within a micro-crack, comparing it with that calculated on the surface to evidence a possible enhancement effect. The factors which most catalyse the fusion reactions remain however, in the three-dimensional case, the percentage of impurities *J*, the deformation of the lattice and the consequent formation of micro-cracks, as can be seen by comparing Tab.1 and 2. Further, tunnelling in the presence of deuterium loading was analysed, observing that, from the *theoretical* point of view, the phenomenon can be treated as an internal perturbation of the lattice. As shown in Fig. 1, it was found that in the presence of loading, the tunnelling appears enhanced due to the reduction[1], in both height and thickness, of the barrier "K". The loading seems therefore to be an important factor conditioning the phenomenon of fusion. One of these mechanisms essentially "consists" of a kind of chain reaction between deuterons and plasmons, catalysed by the deformations and micro-cracks which arise in the structure as a result of variations in the thermodynamic conditions and other causes, such as deuterium loading.

This was hypothesised in the present paper and constitutes one of the principal motives of its inspiration. It is however possible to confirm that the initial results obtained so far validate the hypothesis presented here.

5. References

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