DEUTERON INTERACTIONS WITHIN MICROCRACKS OF A D2 LOADED LATTICE AT ROOM TEMPERATURE

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Abstract - This paper describes the results obtained analysing the process of deuteron fusion, catalysed by the plasmons (quasi-particle due to collective excitation on metallic lattice) of a metallic lattice with CFC (Cubic Face Centred) structure, on varying the temperature. The increased probability of fusion, a consequence of raising the temperature, promotes the hypothesis that a sort of chain reaction, catalysed by microcracks formed in the structure as a result of D2 loading, may favour the process. In fact evaluating the fusion probability of deuteron-plasmon system within microcrack, it has been computed a increasing of fusion probability respect with fusion probability on lattice surface .

Keywords - Microcracks, deuteron-plasmon ,chain reaction.

I. INTRODUCTION

This study has the aim of analysing the possible influence, which variations in temperature and energy could have on the phenomenon of deuterium fusion because of micro-deformations or micro-cracks produced in the lattice. Working on cubic lattice, let us to better handle any topology change as lattice stress or deformation. Moreover working on palladium it is very interesting since many experiments has been performed regarding the fusion of D_2 system within the palladium lattice[1]. These could in fact be able to concentrate in their vicinity a significant fraction of the deuterons present in the metal. In particular[2], the author has suggested that deuteron-plasmon coupling could increase the rate of fusion by acting as an effective interaction attractive to deuterium nuclei, reducing the distance at which Coulomb repulsion becomes dominant. With this in mind, a study was made of crystalline lattices with certain structural characteristics: in particular, the analysis focused on lattices with ten or more electrons in the "d" band. The present work will concentrate on Palladium because, when subjected to thermodynamic stress, this metal has been seen to give results which are interesting from both the theoretical and experimental points of view.
Further, it is assumed that the phenomenon of fusion is not only conditioned by structural characteristics and the thermodynamic conditions of the system, but also by the concentration of impurities present in the metal, correlated with the deuterium loading within the lattice itself.
The analysis has attempted to determine whether, in the case of the three-dimensional isotrope, D_2 loading can lead to the formation of micro-cracks in an analogous manner to that suggested for temperature variation in reference[3]. This would constitute an ulterior verification of the hypotheses proposed.

II. THREE DIMENSIONAL MODEL

The aim is to determine whether, and within what limits, deuterium loading can condition the rate of fusion within a generic cubic lattice, trying to isolate the D_2 contribution from any other possible effects caused by lattice defects, or by other characteristics or thermodynamic conditions, or even by any "micro-deformations" of the crystalline lattice caused by temperature variations. This type of phenomenon can be considered as a perturbation "external" to the system and should be distinguished from "internal" perturbations.
In the case of external perturbations, the interaction between the impurities present and the dislocation[4]

produced in the metal during micro-deformation can distinctly modify the electrical properties of the material. Because of the different arrangement of the atoms with respect to the unperturbed lattice, some particular reactions can then occur so that the impurities become incorporated in the nucleus of the dislocations.

The results presented here were obtained using a numerical simulation to determine the trend of the barrier penetration factor, *K*, as a function of the temperature and the concentration of impurities present in the metal under examination.

In a precedent paper we have showed some results regarding a one-dimensional model[1] but in this model we didn't take into account the reduction of coulomb barrier due to impurities concentration. Now we want treat this topic, but to easily execute the calculation it is better use an isotropic tree-dimensional model.

In a three-dimensional model, the probability of fusion between not-free deuterium nuclei, i.e. deuterium nuclei on metal surface no inside of metal bulk[5], within the crystalline lattice is equal to the probability of penetrating a Coulomb potential barrier $V(r)$, given by:

$$|P|^2_{\text{int}} = \exp\left(-2\int_0^{\alpha} K(r)_{\text{int}}\, dr \right) \qquad (1)$$

$\alpha \cong 0.11$ Å and $K(r)_{\text{int}}$ is given by:

$$\mathrm{K}(r)_{\text{int}} = \sqrt{2\mu[\mathrm{E} - V(r)]/\hbar^2} \qquad (2)$$

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

The interaction potential can then be further extended to the three-dimensional isotropic case.

The potential $V(r)_{\text{int}}$ will then be expressed in the following way:

$$V(r)_{\text{int}} = k\,\frac{q^2}{r}\cdot\left[\, V(r)_M - J\frac{\xi\ kT\ R}{r}\,\right] \qquad (3)$$

where $k = 1/4\,\pi\,\varepsilon_0$, q is the deuton charge, R the nuclear radius, ξ a parameter which depends on the structural characteristics of the lattice (number of "d" band electrons and type of lattice symmetry), varying between *0.015 - 0.025*, T the absolute temperature of the metal under experimental conditions and

$$J = J_0 \exp\left[\frac{\beta}{bkT}\right] \qquad (4)$$

where J_o is the concentration of impurities in the zone with a null internal pressure, $b^3 \simeq v_i$ the volume of the ions making up the lattice, while β is proportional to the difference v_d - v_i between the volume of the atoms of impurities and the volume of the lattice ions.

III. THE PRESENCE OF IMPURITIES IN THE CRYSTALLINE LATTICE

In this case the Morse potential will be:

$$V(r)_M = \left(J/\varsigma \right)\exp\left(-2\varphi\left(r - r_0 \right)\right) - 2\exp\left(-\varphi\left(r - r_0 \right)\right) \qquad (5)$$

In this equation, the parameters ς and φ depend on the dynamic conditions of the system, while r_0 is the classic point of inversion.

Equations (1) and (2) refer to the process of "not free" fusion, i.e. fusion within the crystalline lattice.

The "catalysing" effect of the lattice has been studied from the theoretical point of view: in particular, it was showed[2] that, considering the interaction between deuterium nuclei and collective plasmonic excitation in the metal, rate fusion λ_f in a gas consisting of λ deuterons with density ρ is given by:

$$\lambda_f = \lambda\,\frac{4\pi\rho\hbar}{\mu_d}\left\langle\frac{1}{p}\right\rangle \qquad (6)$$

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

The aim of this work is to demonstrate the possibility of a further effect enhancing the probability of fusion, principally due to the presence of impurities in the metal.

The effect of vibrational energy, which is typically of the order of some eV for the quantum states under consideration, will be ignored here.

Electronic screening, a result of the metallic lattice, represents an important effect on the fusion reaction. Already studied by Rabinowitz et al[6], this effect can be taken into account using a model in which the negative charge is distributed over a thin shell of radius R.

Because of the interaction potential within the metal, the "shifted" Coulomb potential can be written as:

$$V = (kq^2)\left[(1/r) - (1/R)\right], \qquad r_1 \le r \le R \tag{7}$$

where q is the charge of the deuteron, r_1 is the nuclear radius and $k=1/4\pi\varepsilon_0$.
This gives $V = 0$ per $r > R$.
The solution for the semi-classic tunneling factor Λ is[6]:

$$\Lambda = D \exp\left\{-2\gamma(r_1)\right\} \tag{8}$$

$$\gamma(r_1) = (\pi / 2\hbar)\left[(2q^2 / 4\pi\varepsilon_0)\,\mu r_2\right]^{1/2} \tag{9}$$

In (8), D is a numerical constant of the order of unity, μ is the effective reduced mass of the deuton, r_2 is the classic point of inversion and $\hbar$ is Plank's constant.
To take into account the effect of the impurities present, the product $J\eta$ is substituted for D in (8), where J represents the concentration of impurities and η is a numerical constant.
It is now possible to consider a cubic lattice structure subjected to micro-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:

$$D_L = \iiint_{\omega} J \frac{\rho l^2 \nu b^2}{\alpha 2hR} \exp\left(-\frac{U_0}{kT}\right) d\omega \tag{10}$$

ρ is the density of the mobile dislocation within the lattice at a non-constant lattice temperature, l^2 is the area between the lines of separation between two adjacent dislocations, caused by a curving of the lattice[7] R is a coefficient whose value depends on the stress within the lattice, α is proportional to the thermal increment and represents the effect of the sudden variations in temperature to which the lattice is subjected and which lead to the formation of microcracks, ν^2 is the vibration frequency of the deuterons in the metal, considered constant here, b^2 the stress line which dampens the transformation of the crystalline lattice and

$$U_0 = 2U_j - Dbd\left(\sigma - \sigma_i\right)_{\varepsilon_0} \tag{11}$$

is the activation energy.

In this last expression, σ - σ_i is the stress applied to the small dislocations to a good approximation

$$\sigma_i \simeq \frac{\mu b}{2\pi \ell} \tag{12}$$

and ℓ has the dimensions of a wavelength, while μ is an elastic constant which depends on the characteristics of the lattice. In the equation (11) we have

$$\varepsilon_0 = \varepsilon_\beta - \beta t^m \tag{13}$$

β depends on the temperature and m is a variable which depends on the lattice (in this case it is equal to 1/3).

$$2U_j \simeq kT_c \ln(X / \dot{\varepsilon}) \tag{14}$$

is obtained from the comparison of two curves with deformation velocity $\dot{\varepsilon}$, T_c is the "critical temperature" for the formation of the microcracks and $X \simeq 10^5$ in the CGS system. d indicates the distance between dislocations which have not undergone internal splitting, b can be associated with the inter-atomic distance and D depends on the time of movement of the dislocations. The aim here is to determine the probability of fusion within a deuterium loaded metal.
Further, the same problem will be treated from the aspect of the concentration of impurities contained in the metal.
If (1) is divided by (6) and multiplied by (10), it follows that:

$$\Gamma \approx \frac{\exp\left(-2\int_0^{\alpha} K(r)_{int}\, dr\right)}{\lambda \cdot \frac{4\pi\rho\hbar}{\mu_d} \cdot \left\langle \frac{1}{p} \right\rangle} \cdot D_L \tag{15}$$

Equation (15) represents the probability of deuteron fusion within a micro-crack: it is inversely proportional to the number of nuclei absorbed by the metal.
Using (15) and adopting the Morse potential to calculate $K(r)_{int}$, the probability of fusion, normalized

to the number of events per minute, was obtained by means of a numerical simulation program which utilizes the "WKB" method. The results are reported in Table 1. Within the metal, the probability of fusion given by (1) was evaluated numerically, making use of (3) and (5) and taking the center of mass system as the reference system[1]. In the particular case of impure Palladium with:

$\alpha \simeq 0.15$ Å, $E \approx 237.2$ eV
$J = 0.75\%$, $T = 250.2$ K

The result is $\Gamma_{pd} \approx 10^{-41}$, $P_{int} \approx 10^{-46}$.
For this result, and also for those obtained using the WKB method incorporated in numerical simulation programs, a range of temperatures between 100 and 300 Kelvin were considered. The potential (3), for Pd pure to 0.25%, was substituted by the "shell" potential, as follows:

$$V = \left(k \ q^2 \right) \left((1/r) - \frac{\mathrm{K\,T}}{J\varepsilon \ R} \right), \qquad r_1 \le r \le R \qquad (16)$$

Where $\mathrm{K\,T}$ is the mean kinetic energy of the gas, ε is the vibrational energy (typically of the order of some eV for the quantum states considered) and q is the deuton charge. Under these particular dynamic conditions, the probability of fusion normalized to a number of events per minute was obtained for Palladium.

IV - RESULTS AND DISCUSSION

The probability of fusion within "pure" Palladium, under the same dynamic conditions as the previous example, is then given by:

$\alpha \simeq 0.15$ Å $\quad E \approx 237.2$ eV
$J = 0.25\%$ $\quad T = 250.2$ K.

The result is $\Gamma_{Pd} \approx 10^{-45}$, $P_{int} \approx 0^{-48}$.

Other values of T , Γ and P are reported in Tables 1 and 2.

Palladium $J \approx 0.75\%$, T-range ≈ 100-300 K, $\alpha \approx 0.34$ Å, $\lambda = 10^{-3}$ eV / min, M_{Pd} /μg

T ≈	100 K		140 K		180 K		220 K		260 K		300 K	
E (eV)	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈	Γ ≈	P ≈
150	10^{-80}	10^{-89}	10^{-67}	10^{-69}	10^{-77}	10^{-86}	10^{-63}	10^{-65}	10^{-65}	10^{-66}	10^{-60}	10^{-68}
160	10^{-73}	10^{-86}	10^{-65}	10^{-68}	10^{-73}	10^{-83}	10^{-61}	10^{-63}	10^{-63}	10^{-63}	10^{-58}	10^{-65}
170	10^{-72}	10^{-85}	10^{-63}	10^{-65}	10^{-73}	10^{-85}	10^{-60}	10^{-62}	10^{-60}	10^{-64}	10^{-56}	10^{-62}
180	10^{-69}	10^{-83}	10^{-60}	10^{-62}	10^{-72}	10^{-84}	10^{-59}	10^{-61}	10^{-58}	10^{-63}	10^{-55}	10^{-60}
190	10^{-67}	10^{-81}	10^{-57}	10^{-60}	10^{-71}	10^{-83}	10^{-57}	10^{-60}	10^{-56}	10^{-62}	10^{-50}	10^{-58}
200	10^{-66}	10^{-79}	10^{-55}	10^{-59}	10^{-70}	10^{-82}	10^{-55}	10^{-59}	10^{-54}	10^{-61}	10^{-40}	10^{-54}
210	10^{-65}	10^{-76}	10^{-54}	10^{-58}	10^{-69}	10^{-78}	10^{-53}	10^{-57}	10^{-53}	10^{-60}	10^{-47}	10^{-52}
220	10^{-64}	10^{-75}	10^{-52}	10^{-57}	10^{-64}	10^{-77}	10^{-52}	10^{-56}	10^{-52}	10^{-59}	10^{-46}	10^{-51}
230	10^{-60}	10^{-72}	10^{-51}	10^{-56}	10^{-63}	10^{-76}	10^{-51}	10^{-55}	10^{-50}	10^{-58}	10^{-45}	10^{-50}
240	10^{-59}	10^{-67}	10^{-50}	10^{-55}	10^{-62}	10^{-74}	10^{-49}	10^{-54}	10^{-49}	10^{-57}	10^{-43}	10^{-48}
250	10^{-58}	10^{-65}	10^{-49}	10^{-53}	10^{-61}	10^{-73}	10^{-48}	10^{-52}	10^{-48}	10^{-53}	10^{-41}	10^{-46}

Table 1 *- For "impure" Pd ($J \approx 0.75\%$), using the Morse potential, the probability of fusion Γ within a micro-crack in the presence of D_2 loading, normalized to the number of events per minute, was calculated for different values of temperature (varying from 100 K to 300 K) and energy (varying from 150 eV to 250 eV). It should be noted that the probability generally increases with T and E, and is systematically several orders greater than the probability of surface fusion* ***P****.*

Palladium $J \approx 0.25\%$, T-range ≈ 100-300 K, $\alpha \approx 0.34$ Å, $\lambda = 10^{-3}$ eV / min, M_{Pd} /μg

T ≈	100 K		140 K		180 K		220 K		260 K		300 K	
E (eV)	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^{-73}	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^{-60}	10^{-66}
180	10^{-71}	10^{-75}	10^{-75}	10^{-80}	10^{-69}	10^{-75}	10^{-65}	10^{-72}	10^{-62}	10^{-73}	10^{-50}	10^{-65}
190	10^{-69}	10^{-73}	10^{-73}	10^{-78}	10^{-67}	10^{-74}	10^{-64}	10^{-70}	10^{-60}	10^{-72}	10^{-57}	10^{-64}
200	10^{-67}	10^{-72}	10^{-72}	10^{-75}	10^{-65}	10^{-73}	10^{-62}	10^{-69}	10^{-58}	10^{-71}	10^{-56}	10^{-62}
210	10^{-65}	10^{-70}	10^{-67}	10^{-74}	10^{-64}	10^{-72}	10^{-60}	10^{-68}	10^{-56}	10^{-68}	10^{-55}	10^{-59}
220	10^{-64}	10^{-67}	10^{-68}	10^{-73}	10^{-63}	10^{-70}	10^{-59}	10^{-67}	10^{-54}	10^{-67}	10^{-54}	10^{-57}
230	10^{-63}	10^{-65}	10^{-66}	10^{-71}	10^{-61}	10^{-69}	10^{-57}	10^{-66}	10^{-52}	10^{-63}	10^{-50}	10^{-54}
240	10^{-61}	10^{-63}	10^{-64}	10^{-70}	10^{-60}	10^{-68}	10^{-55}	10^{-64}	10^{-51}	10^{-61}	10^{-49}	10^{-51}
250	10^{-60}	10^{-61}	10^{-63}	10^{-69}	10^{-50}	10^{-64}	10^{-54}	10^{-62}	10^{-49}	10^{-59}	10^{-45}	10^{-40}

Table 2 *- For "pure" Pd ($J \approx 0.25\%$), adopting the "shell" potential, the probability of fusion Γ within a microcrack, normalized to the number of events per minute, was calculated under the same dynamic conditions as in Table 1. Also here Γ is systematically several orders of magnitude greater than the probability of fusion on the surface* ***P****, but the values are systematically lower than those of the previous case.*

V. CONCLUDING REMARKS

With the theoretical analysis developed it is possible to obtain relatively high values for the probability of fusion for D_2 loaded impure metals at room temperature. On the other hand, results very close to the experimental data have already been obtained without imposing the D_2 loading[5] (for example, for $J \approx 0.75\%$, $E \approx 250$ eV, $T = 300$ K, $\Gamma = 10^{-21}$, $P \approx 10^{-25}$). Judging by the comparison between the two theoretical calculations, it would seem that the experimental procedure reduces the rate of fusion rather than amplifies it. To verify the influence of the concentration of impurities on the process from another point of view, the trend of the potential within the pure lattice ($J \approx 0.25$) was evaluated and a very high curve obtained. Therefore, crossing the

barrier would require a total energy greater than the potential, as shown in Figure 1 for Palladium. If the potential barrier is evaluated for the same metal with a higher level of impurity ($J \approx 0.75\%$), under the same thermodynamic conditions of the system, it is seen that the probability of fusion may be greater than that observed for pure metals, with a total energy lower than the potential so that the tunneling effect is amplified.

The principal aim of the present theoretical analysis was to demonstrate whether and how the coefficient of lattice deformation, linked to the formation of microcracks at room temperature and low energy, could effect the process of fusion.

More precisely, the probability of fusion within a microcrack was calculated numerically and compared with that calculated on the surface to evidence a possible amplification of the tunneling effect. With this aim, we associated the probability of fusion within a microcrack with the coefficient of deformation, Ψ, as a function of deuterium loading, and performed a WKB numerical simulation in the case of a model with CFC structure.

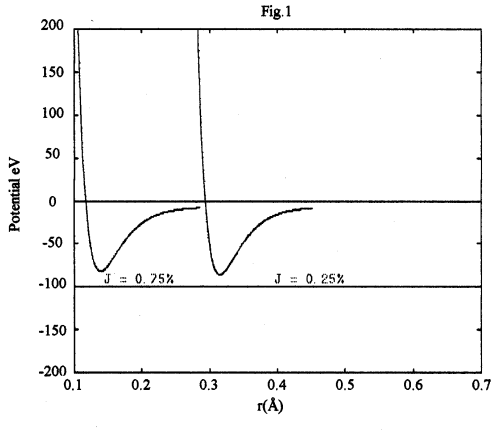

Fig.1. *Semi-classic tunneling appears increased for those metals, which have a concentration of impurity $J \approx 0.75\%$. The Morse potential was calculated at $T = 290$ K. The Coulomb barrier seems very high in the case of pure metals with $J \approx 0.25\%$. The "shell" potential was calculated at $T = 290$ K.*

The results of the research show that, in effect, the values of the probability of fusion with D_2 loading, for impure metals at room temperature, are quite elevated. For all the temperatures over the *150-350 K* range and for all the energies over the *150-250 eV* range, the formation of microcracks increases the probability of fusion compared to the case of non-deformed lattices, and also reduces the thickness of the Coulomb barrier.

To verify the influence of the concentration of impurities on the process, we also evaluated the trend of the potential, within the pure lattice ($J \approx 0.25\%$), obtaining a very high curve (Fig 1).

If the potential barrier is evaluated for the same metal with a higher concentration of impurities ($J \approx 0.75\%$), with the system under the same thermodynamic conditions, it is possible demonstrate that the probability of fusion could be greater than that found for pure metals, with a total energy lower than the potential so amplifying the tunneling effect.

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