Study of the lattices with CFC with varying temperature

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***Abstract*—** In this theoretical study, it is underlined that the presence of micro-cracks in the lattice structure increases the probability of tunneling effect between two deuterons by some orders of magnitude with respect to non-deformed lattices. We have derived an expression to compute the tunneling probability within a micro-crack, and hypothesized a D^+_2-D^+_2 binding mechanism Finally, the overall indications provided by these theoretical simulations appear to suggest that the deformation of the crystalline lattice, at varying temperature, seems able to influence the process of tunneling between the deuterons in the metal, while the forced loading with D_2 has, in general, no evident positive effects in pure metals, but in some cases could, on the contrary, condition the phenomenon negatively.

***Keywords*—** Condensed Matter, Dislocation, Micro-crack.

I. INTRODUCTION

IN reference[1] the author has shown that the thickness of the Coulomb barrier varies according to parameters such as the density of impurities within the lattice, the temperature of the system and the vibrational energy of the deuterons.

As showed in previous papers[2,3] we have computed the tunneling probability for the three-dimensional isotropic lattice using the following potential for deuterons:

$$V(r) = k\frac{q^2}{r}\cdot\left[V(r)_M - J\frac{\xi kT\,R}{r}\right] \qquad (1)$$

Here $k = \frac{1}{4\pi\varepsilon_0}$ is the Coulomb constant, q the deuteron charge, R the nuclear radius, ξ a parameter depending on the structural characteristics of the lattice (number of "d" band electrons) varies between $1.5\cdot10^{-3}$ and $2.5\cdot10^{-3}$, T the absolute temperature, J the concentration of impurities in the crystalline lattice, and $V(r)_M$ is the intermolecular Morse potential which, in this case, has the expression[1,2,3]:

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

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$\left(J/\varsigma\right)$ the depth of the barrier, the parameters ς and φ depend on the dynamic conditions of the system, while r_0 is the classic point of inversion.

This expression takes into account the interaction between deuterons and the variations in temperature, but not of deuteron-phonon coupling, using an appropriate correction to the Morse potential.

In this case the tunneling probability increases according the reduction of coulomb barrier (see fig 1).

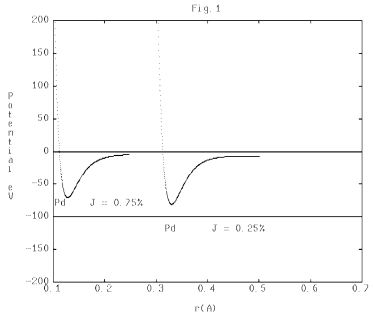

Fig. 1 The trends of the potential, containing the Morse contribution (2), for two different values of impurity concentration computed in palladium lattice. Note how the minimum distance between two deuterons decreases according to the impurities concentration.

The aim of this paper is to study the role of micro-crack on the tunneling probability. More exactly, we selected the main parameters that affect the micro-crack[4,5] and derived an expression for the tunneling probability that depends on these quantities. For these purposes we used two potential kinds: a nuclear potential independent on the lattice parameters and the potential (1) that varies according to the lattice parameters. Moreover we discuss the possibility of a contrary effect due to the forced loaded D_2 in the lattice. This work can be considered the next step of a more general study regarding the enhancement of tunnel probability between two deuterons. In fact in the previous papers[1,2,3] we have investigated how the potential between two deuterons is modified by means of lattice parameters; whilst now we discuss the influence of micro-crack on the tunnel probability. Finally we analyze the synergy between micro-crack formation and lattice parameters that affect the potential.

The calculations were performed supposing that the interaction between deuterons takes place within a lattice of Palladium, which has a cubic crystalline structure, 10 "d" band electrons and at variable temperature. The lattice parameters values have been taken from literature regarding the Palladium[5,8].

To summarize, the objective of this study is to confirm the hypothesis regarding the micro-cracks through quantitative estimation of the time-dependent coefficient of structural deformation of the perturbed crystalline lattice[1], obtained for different energy values in the range 150-250 eV.

II.TUNNELING MODEL WITHIN A MICRO-CRACK

The aim is to establish whether, and within what limits, the tunneling probability within a micro-crack in a generic cubic lattice subjected to deuterium loading, can be conditioned or influenced not only by extensive lattice defects[9,10] and by other characteristics and thermodynamic conditions, but also by any deformations Ψ undergone by the crystalline lattice on varying the temperature. If this indeed occurs, it is not difficult to hypothesize the following path reaction: deformation induces dislocation; dislocation induces micro-crack; within micro-crack deuterium-deuterium binding provide energy[9] and, this energy can induce another deformation. Therefore, the energy produced by "micro-explosions" within the micro-cracks (due to the deuteron-deuteron binding) could favor the creation of new micro-cracks, which by the same mechanism would, in turn, capture other deuterons. This could result in a kind of chain reaction.

The quantum tunneling of interacting deuterons is described[1,11] (in a "free-space") by the factor Λ:

$$\Lambda(\hat{\alpha}) = -2\int_{\hat{\alpha}}^{\hat{\beta}} \sqrt{\{2M[E - V(r)]\}}\,dr \qquad (3)$$

where *V(r)* is the repulsive Coulomb potential, $\hat{\alpha}$ is the distance between two deuterons where *V(r) = E* and $\hat{\beta}$ is the typical nuclear distance (~ *0.1 10*$^{-13}$ *m*).

Of course, the region of greater interest is that where $E \le V(r)$, giving a tunneling effect.

Considering, for the sake of simplicity, a cubic lattice structure subjected to deformations, the probability of tunneling within a micro-crack, Γ, upon varying the temperature can now be calculated. The present paper focuses on the cubic structure of the lattice, specifically on Palladium, because it has a readily observable geometry.

Indicating the volume of a single lattice cell by $d\Omega$, the deformation of the entire lattice is given by[5]:

$$\Psi \cong \left\{ \iiint_{\Omega} \eta \left(J \frac{\rho L^2 \nu b^2}{\alpha 2hR} \left(\frac{1}{\Lambda} \int_0^{\Lambda} c(r, J)\,dr \right) \exp\left(-\frac{U_0}{kT} \right) \xi_{(r)} \right) d\Omega \right\} \qquad (4)$$

In (4), $J = J_0 \exp\left[\frac{\beta}{bkT} \right]$, J_0 is the concentration of impurities in the zone with zero 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 impurity atoms and that of the lattice ions; η is a parameter which depends on the electronic and lattice structure of the metal considered. Furthermore, the density of the mobile dislocation within the lattice at variable lattice temperature is indicated by ρ, so that the thermodynamic stress of the deuterium nuclei is not rendered negligible per unit volume, with L^2 the area between the lines of separation between two adjacent electrons, determined during a deformation of the lattice at variable temperature, R is the curvature assumed by the dislocation during deformation, α the proportional thermal increase, representing the effect of the abrupt variations in temperature to which the crystalline lattice is subjected and as consequence of which micro-deformations are formed; ν is the vibration frequency of deuterons in the metal[7], which is considered "negligible" here and will be treated with medium temperatures, b^2 the stress line producing the transformation of the crystalline lattice for small variations of stress within the lattice;

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

the activation energy, which is always less than a couple of jogs since $\sigma - \sigma_i$ is the stress applied to the small dislocations and, with good approximation, it is found that $\sigma_i \simeq \frac{\mu b}{2\pi \ell}$ where ℓ has dimensions of one length, while μ is an elastic constant depending on the characteristics of the lattice; $\varepsilon_0 = \varepsilon_\beta - \hat{\beta} t^m$, where $\hat{\beta}$ depends on the temperature for the "deformations"; m is a variable which depends on the lattice and, in this case, is equal to $\frac{1}{3}$; $2U_j \simeq kT_c \ln(X/\dot{\varepsilon})$ is obtained by the comparison of two curves with deformation velocity $\dot{\varepsilon}$; T_c is the "critical temperature" for the formation of micro-cracks which can be evaluated for cubic metals as within the range of temperatures[5,7,8] between 200 - 300 K, $X \simeq 10^5$ in the CGS system, d indicates the distance between dislocations which have not sustained an internal split, *b* can be associated with the inter-atomic distance and

D depends on the time of movement of the dislocations. Furthermore, integrating[7] $\frac{1}{\Delta}\int_0^{\Delta} c(r,J)\,dr$ on the upper limit Δ, which is the length of the Pd specimen, we obtain the ratio of mean loading; $c(r,J)$ is the local concentration of D_2^+ ions in the Palladium lattice matrix, at constant time t, along the three dimensions. Finally, $\xi_{(r)}$ is the number of dislocations.

Considering the deformations occurring in cubic-type lattices of metals such as Pd at room temperature, the aim is to evaluate the dislocation of atoms induced in the crystalline lattice by the lattice deformation. This is in order to determine the influence of this phenomenon on deuteron-deuteron binding.

It was considered above that within a micro-crack, the possible consequence of a dislocation[1] under opportune conditions would be that a greater number of events might take place than on the lattice surface. Some micro-cracks could in fact be able to concentrate in their vicinity a relevant fraction of the deuterons present in the metal. To demonstrate this, approximate calculations were performed, taking into account of lattice deformation and of micro-crack depth.

The depth of the micro-crack $L_D(T)$, a function of the lattice temperature, is given by[5]:

$$L_D(T) = \frac{F_{(out)}\, r}{J\xi_{(r)}[(l/2)^2 - r^2]^{1/2}} \qquad (5)$$

The quantity[5]

$$\left(\frac{F_{(out)}}{L_D(T)J}\right)\delta r \qquad (6)$$

is the change in the elastic and potential energies of the external mechanisms per unit length of the lattice, due above all to variations in the thermodynamic conditions produced by thermal exchange with the external system; r the distance between the centre of the dislocation and the centre of mass of the lattice, and δr a small variation of this distance.

The final expression for the probability of tunneling within the lattice must contain the term $L_D(T)$.

The phenomenon hypothesized above would possess characteristics analogous to the formation of a Cottrell[5] atmosphere in metals, 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. It can happen that, in these cases, the interaction between the impurities present and the dislocations significantly alters the electrical properties of the material. Furthermore, particular reactions can take place, incorporating the impurities in the core of the dislocation as a result of the different arrangement of the atoms with respect to that of the unperturbed lattice. These types of processes are been extensively studied for high temperature crystalline semiconductors [12] and for metals.

In fact if this occurs, it is not difficult to hypothesize that the energy produced by micro-explosions within the micro-cracks could favor the creation of new micro-cracks, which, in turn, would capture other deuterons through the same mechanism. The interaction between the impurities present and the dislocations produced in the metal during deformation could, therefore, notably modify the electric properties of the material.

With regards to the role of D_2 loading, our opinion is that an adequate theoretical description of loading can, therefore, be obtained only by treating it as a time independent[2] perturbation. But in this case it should be necessary to consider the fact that the rate of tunneling within the metal depends, under conditions far from those of saturation, on the number of deuterium nuclei absorbed in unit time, which could also be a function of the coefficient of lattice deformation. As to avoid these theoretical difficulties we deduce to perform our calculations under condition of saturation.

In this condition, we suppose that when a lattice undergoes a thermodynamic solicitation, the Ψ deformation induces a local variation in the deuterium atoms loaded in the lattice. Of course, it is obvious that higher the deformation is, higher the density variation is. More precisely, within micro-cracks it is reasonable to attend an accumulation of atoms; thus in first approximation we can write regarding the deuterium concentration ρ_M (within a micro-crack)

$$\rho_M(\Psi) = \rho_0 + a\Psi \qquad (7)$$

where ρ_0 is the average deuterium concentration in the palladium (i.e. not within micro-crack) when the deformation is zero and a is an opportune constant. In this way we increase the concentration of a factor ($1+h\Psi$) with $h=a/\rho_0$. Moreover, the deformation energy, besides contributing to the accumulation of deuterium in the crack, contributes to micro-crack formation. Then, according to the formula (6) we suppose that this variation is inversely proportional to the micro-crack depth. We also assume that these two effects contribute at the same magnitude on the concentration variation, so we can say that the D_2 concentration within a micro-crack is increased of a factor Φ given by the following expression:

$$\Phi \cong 1+\frac{\Psi}{L_D}=1+\frac{\iiint_\Omega \eta\left(J\frac{\rho L^2 v b^2}{\alpha 2hR}\left(\frac{1}{\Delta}\int_0^\Delta c(r,J)\,dr\right)\exp\left(-\frac{U_0}{kT}\right)\xi_{(r)}\right)d\Omega}{\frac{F_{(out)}\,r}{J\xi_{(r)}[(l/2)^2-r^2]^{1/2}}} \qquad (8)$$

At last we suppose that the tunneling probability is increased of a factor that is the same of that relative to the concentration. In this way we can arrive to the final formula regarding the tunneling probability within a micro-crack:

$$\Gamma \approx \Phi \exp\int_{\hat{\alpha}}^{\hat{\beta}} -2\left\{2\mu\left[E-V(r)\right]\frac{1}{\hbar^2}\right\}^{1/2} dr \qquad (9)$$

As a last question, let us understand if we can increase the D_2 concentration within palladium by forced loading. Of course the deuterium quantities for cm^3 that the palladium can contain, at a fixed temperature, has a trend *density versus flow loaded* that finishes in a plateau[6,10]. For this reason we suppose that our calculations are performed for this plateau value. Then, if we suppose to increase the D_2 flow loaded, the tunneling probability should be unchanged. But since the resident time is inversely proportional to the loaded flow, it is reasonable aspects a small diminution of tunneling probability. To summarize, it necessary to be careful to the D_2 loading in the experiments, in fact a very high flow value can condition the tunnel probability negatively.

III. THE NUCLEAR POTENTIAL

In this paper following reference[13] we used a potential that takes into account the three-body problem: two nucleons and an electron.: More exactly we computed the fusion probability between two deuterons hypothesizing that happens a binding like nucleon-electron-nucleon when two deuterons are loaded in a lattice and in particular when they are forced within micro-cracks.

As reported in reference[13], using the radial wave equation for D_2^+, it follows that within the metal there is an effective potential $V(r)$ between two deutons given by:

$$V(r)=\frac{L(L+1)\hbar^2}{M r^2}-\frac{3\alpha}{r}+n4\hbar\sqrt{\frac{\alpha}{m}}\,r^{-3/2} \qquad (10)$$

In (10), M indicates the deuton mass, while m the electron mass.

It can be seen that the effective potential has two minima: the value of the first belongs to the region of the Bohr radius of the electron, and occurs for $L=0$ in $r_1=\frac{4n^2\hbar^2}{\alpha m}$; the second belongs to the region of the Bohr radius for the proton, for $L\neq 0,\ n=0$ in $r_2=\frac{2L(L+1)\hbar^2}{3M\alpha}$ (see fig 2 and 3).

This potential doesn't depend on lattice parameters, but only on distance between deuterons and on quantum numbers. Note the presence of the term $n4\hbar\sqrt{\frac{\alpha}{m}}\,r^{-3/2}$ due to the Electron attraction**.**

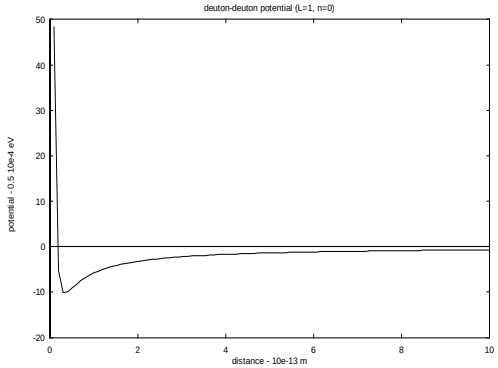

Fig. 2 The trend of the nuclear potential (10), for *L=1* and *n=0* (pure Coulomb barrier). The minimum value occurs for a distance of about 0.3 10^{-13} m. Note in this case we have not any enhancement to the tunnel effect.

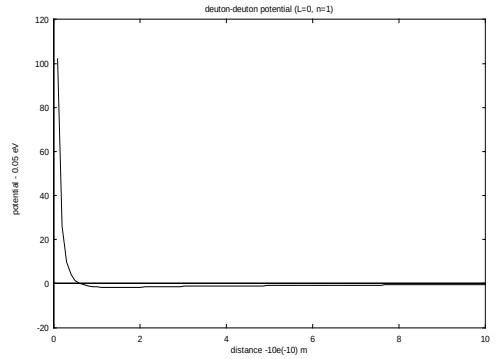

Fig. 3 The trend of the nuclear potential (10), for *L=0* and *n=1*. The minimum value occurs for a distance of about 0.6 10^{-10} m. Note in this case the noteworthy contribution of third term of (10).

Table I
Palladium T(K) ≈ 190 - 350 M_{Pd} /(*μg)*

T ≈	**190 K**	**230 K**	**270 K**	**310 K**	**350 K**
E(eV)	**Γ ≈**	**Γ ≈**	**Γ ≈**	**Γ ≈**	**Γ ≈**
150	10^{-85}	10^{-78}	10^{-75}	10^{-76}	10^{-76}
160	10^{-83}	10^{-77}	10^{-74}	10^{-75}	10^{-74}
170	10^{-81}	10^{-76}	10^{-73}	10^{-74}	10^{-73}
180	10^{-80}	10^{-75}	10^{-72}	10^{-73}	10^{-71}
190	10^{-78}	10^{-74}	10^{-70}	10^{-72}	10^{-69}
200	10^{-75}	10^{-73}	10^{-69}	10^{-71}	10^{-66}
210	10^{-74}	10^{-72}	10^{-68}	10^{-68}	10^{-62}
220	10^{-73}	10^{-70}	10^{-67}	10^{-67}	10^{-60}
230	10^{-71}	10^{-69}	10^{-66}	10^{-65}	10^{-58}
240	10^{-70}	10^{-68}	10^{-64}	10^{-61}	10^{-56}
250	10^{-68}	10^{-66}	10^{-62}	10^{-60}	10^{-55}

in these following three ways. First, we used the formula (3) (tunneling effect in the "free-space") and the potential (10) for *L=0* and *n=1* (table 1). Secondly, we computed the tunneling probability by means of potential (10) (*L=0*, *n=1*) but using the formula (9) (tunneling within micro-crack, table 2). Comparing both cases we can evaluate the effect of micro-crack on tunnel probability. Finally we used the formula (9) again but using the potential (1) that depends on lattice parameters (table 3). In this way we can estimate the synergy effect between micro-crack and the modification of potential due to lattice parameters.

The values of Γ obtained for different values of E (150-250 eV) and T (190-350) are reported in Tables 1, 2 and 3. The values are in agreement by physical considerations. In fact the tunnel probability increases when we consider the micro-crack contribution (see tables 1 and 2), more exactly the tunneling increase of a 10^{-10} magnitude under the same condition in term of potential. Of course, the major increasing of Γ happens when we consider both effects: micro-crack formation and modification of potential due to lattice parameters (see tables 2 and 3). In fact in this case we have an average increasing of 10^{-30}.

Table II
Palladium J ≈ O.75% T(K) ≈ 190 - 350 K M_{Pd} /(*μg)*

The probability of tunneling within a micro-crack was calculated for Pd, using the effective potential (10) and the formula (9). It has been computed for different values of temperature (range 190 - 350 K) and of energy (range 150 - 250 eV). It is seen that the probability generally increases with T and E. Note that, in this case, Γ is higher by about ten orders of magnitude.

T ≈	**190 K**	**230 K**	**270 K**	**310 K**	**350 K**
E(eV)	**Γ ≈**	**Γ ≈**	**Γ ≈**	**Γ ≈**	**Γ ≈**
150	10^{-95}	10^{-88}	10^{-85}	10^{-86}	10^{-81}
160	10^{-93}	10^{-87}	10^{-84}	10^{-85}	10^{-79}
170	10^{-91}	10^{-86}	10^{-83}	10^{-84}	10^{-76}
180	10^{-90}	10^{-85}	10^{-82}	10^{-83}	10^{-78}
190	10^{-88}	10^{-84}	10^{-80}	10^{-82}	10^{-77}
200	10^{-85}	10^{-83}	10^{-79}	10^{-81}	10^{-76}
210	10^{-84}	10^{-82}	10^{-78}	10^{-78}	10^{-74}
220	10^{-83}	10^{-80}	10^{-77}	10^{-77}	10^{-71}
230	10^{-81}	10^{-79}	10^{-76}	10^{-75}	10^{-73}
240	10^{-80}	10^{-78}	10^{-74}	10^{-71}	10^{-71}
250	10^{-78}	10^{-76}	10^{-72}	10^{-70}	10^{-70}

Table III
Palladium J ≈ O.75% T (K) ≈ 190 - 350 M_{Pd}/(*μg)*

The probability of tunneling within a micro-crack was calculated for "impure" Pd (J≈ 0.75%), using the formula (9) and the Morse potential (1), and for different values of temperature (range 190 - 350 K) and of energy (range 150 - 250 eV). It is seen that the probability generally increases with T and E.

Note that in this case we can obtain a 10^{-19} value.

T ≈	**190 K**	**230 K**	**270 K**	**310 K**	**350 K**
E(eV)	**Γ ≈**	**Γ ≈**	**Γ ≈**	**Γ ≈**	**Γ ≈**
150	10^{-66}	10^{-67}	10^{-63}	10^{-64}	10^{-58}
160	10^{-65}	10^{-64}	10^{-61}	10^{-61}	10^{-55}
170	10^{-63}	10^{-62}	10^{-59}	10^{-58}	10^{-53}
180	10^{-58}	10^{-60}	10^{-57}	10^{-56}	10^{-52}
190	10^{-56}	10^{-59}	10^{-55}	10^{-53}	10^{-46}
200	10^{-55}	10^{-57}	10^{-54}	10^{-52}	10^{-43}
210	10^{-54}	10^{-56}	10^{-53}	10^{-50}	10^{-41}
220	10^{-52}	10^{-54}	10^{-52}	10^{-48}	10^{-34}
230	10^{-51}	10^{-53}	10^{-50}	10^{-47}	10^{-25}
240	10^{-50}	10^{-52}	10^{-49}	10^{-42}	10^{-23}
250	10^{-49}	10^{-51}	10^{-48}	10^{-39}	10^{-19}

IV. CONCLUSIONS

By means of a WKB numerical code, we have performed the Γ calculation in these following three ways. First, we used the formula (3) (tunneling effect in the "free-space") and the potential (10) for $L=0$ and $n=1$ (table 1). Second, we computed the tunneling probability by means of potential (10) ($L=0$, $n=1$) but using the formula (9) (tunneling within micro-crack, table 2). Comparing both cases we can evaluate the effect of micro-crack on tunnel probability.

Finally we used the formula (9) again but using the potential (1) that depends on lattice parameters (table 3). In this way we can estimate the synergy effect between micro-crack and the modification of potential due to lattice parameters.

The values of Γ obtained for different values of E (150-250 eV) and T (190-350) are reported in Tables 1, 2 and 3. The values are in agreement by physical considerations. In fact the tunnel probability increases when we consider the micro-crack contribution (see tables 1 and 2), more exactly the tunneling increase of a 10^{-10} magnitude under the same condition in term of potential. Of course, the major increasing of Γ happens when we consider both effects: micro-crack formation and modification of potential due to lattice parameters (see tables 2 and 3). In fact in this case we have an average increase of 10^{-30}.

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