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Research Article

Calculation of Deuteron Interactions within Microcracks of a D_2 Loaded Crystalline Lattice at Room Temperature

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Abstract

We have analysed the possibility that the coefficient of lattice deformation, linked to the formation of microcracks at room temperature and low energies, could influence the process of fusion. The calculated probability of fusion within a microcrack, in the presence of D_2 loading at room temperature and for impure metals, shows moderately elevated values compared with the probability of fusion on the surface. For all the temperatures in the 150–350 K range and for all the energies between 150 and 250 eV, the formation of microcracks increases the probability of fusion compared to non-deformed lattices, and also reduces the thickness of the Coulomb barrier. Using the trend of the curve of potential to evaluate the influence of the concentration of impurities, a very high barrier is found within the pure lattice ($J \approx 0.25\%$). However, under the same thermodynamic conditions, the probability of fusion in the impure metal ($J \approx 0.75\%$) could be higher, with a total energy less than the potential so that the tunneling effect is amplified. Finally, we analysed the influence of *forced* D_2 loading on the process.

Keywords: Collective plasmonic excitation, Dislocations, Fusion within a microcrack, Tunneling effect

1. Introduction

This study has the aim of analyzing the possible influence, which variations in temperature and energy could have on the phenomenon of deuterium fusion because of microdeformations or microcracks produced in the lattice. These could in fact be able to concentrate in their vicinity a significant fraction of the deuterons present in the metal. In particular, the author has suggested [1] 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.

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Further, it is hypothesized 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 will attempt to determine whether, in the case of the three-dimensional isotrope, D_2 loading can lead to the formation of microcracks in an analogous manner to that suggested for temperature variation in [1]. This would constitute an ulterior verification of the hypotheses proposed.

2. 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 "microdeformations" of the crystalline lattice caused by temperature variations. This type of phenomenon can be considered as a perturbation "external" to the system [2] and should be distinguished from "internal" perturbations.

In the case of external perturbations, the interaction between the impurities present and the dislocations [4] produced in the metal during microdeformation 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 three-dimensional model, the probability of fusion between not-free deuterium nuclei within the crystalline lattice is equal to the probability of penetrating a Coulomb potential barrier $V(r)$, given by

$$|P|^2_{\text{int}} = \exp\left(2\int_0^{\alpha} K\,(r)_{\text{int}}\,\mathrm{d}r\right), \tag{1}$$

where α is 0.11 Å and $K(r)_{\text{int}}$ is given by

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

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

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

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

$$V\,(r)_{\text{int}} = k\frac{q^2}{r}\left[V\,(r)_{\text{M}} - J\frac{\xi k T R}{r}\right], \tag{3}$$

where $k = 1/4\pi\varepsilon_0$, q is the deuteron 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 and 0.025, T the absolute temperature of the metal under experimental conditions and J is the percentage of impurities in the crystalline lattice.

In this case the Morse potential will be:

$$V(r)_{\text{M}} = (J/\varsigma)\ \exp\left(-2\varphi\,(r - r_0)\right) - 2\exp\left(-\varphi\,(r - r_0)\right). \tag{4}$$

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 "catalyzing" effect of the lattice has been studied from the theoretical point of view: in particular, it was shown [1] that, considering the interaction between deuterium nuclei and collective plasmonic excitation in the metal, fusion rate λ_f in a gas consisting of λ deuterons with densityρ is given by

$$\lambda_f = \lambda \frac{4\pi\rho\hbar}{\mu_d} \langle 1/p \rangle , \tag{5}$$

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. [3], 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:

$$V = kq^2 [(1/r) - (1/R)] , \quad r_1 \leq r \leq R, \tag{6}$$

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 $r > R$.

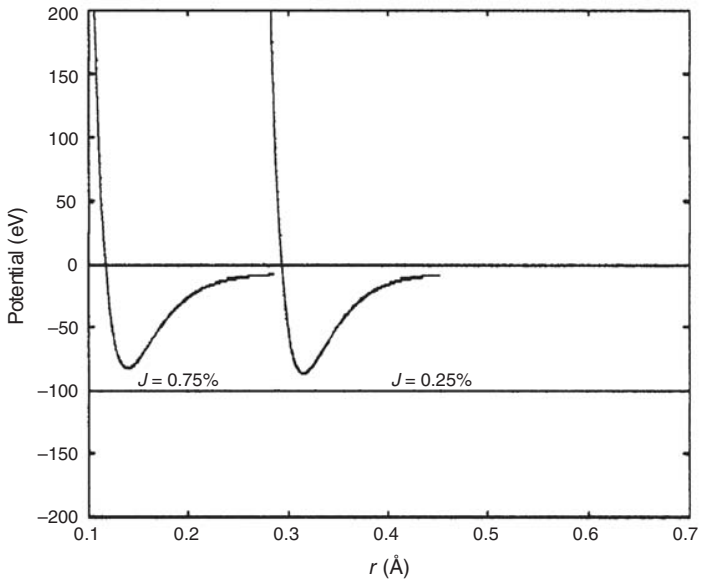

Figure 1. Semi-classic tunneling appears increased for those metals that have a concentration of impurity $J \approx 0.75\%$. The Morse potential was calculated at $T = 290$ K. The Coulomb barrier seems very high in the case of pure metals with $J \approx 0.25\%$. The "shell" potential was calculated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

The solution for the semi-classic tunneling factor Λ is [3]:

$$\Lambda = D \exp\{-2\gamma\,(r_1)\}\,, \tag{7}$$

$$\gamma\,(r_1) = (\pi/2\hbar)\left[(2q^2/4\pi\varepsilon_0)\mu r_2\right]^{1/2}. \tag{8}$$

In Eq. (7), D is a numerical constant of the order of unity, μ the effective reduced mass of the deuteron, r_2 the classical turning point of d–d Coulomb collision process and $\hbar$ is the Plank's constant. To take into account the effect of the impurities present, the product $J\eta$ is substituted for D in Eq. (7), 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 microdeformations and calculate the probability of fusion within a microcrack, Γ, on varying the temperature.

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

$$D_{\mathrm{L}} = \iiint_{\omega} J\frac{\rho l^2 \nu b^2}{\alpha 2hR}\exp\left(-\frac{U_0}{kT}\right)\mathrm{d}\omega, \tag{9}$$

where ρ is the density of the mobile dislocation within the lattice at a non-constant lattice temperature, l^2 the area between the lines of separation between two adjacent dislocations, caused by a curving of the lattice [4], 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 $U_0 = 2U_j - Dbd\,(\sigma - \sigma_i)_{\varepsilon_0}$ is the activation energy.

In this last expression, $\sigma - \sigma_i$ is the stress applied to the small dislocations to a good approximation $\sigma_i \simeq \mu b/2\pi\ell$ and ℓ has the dimensions of a wavelength, while μ is an elastic constant which depends on the characteristics of the lattice. $\varepsilon_0 = \varepsilon_\beta - \beta\, t^m$ where β depends on the temperature and m is a variable which depends on the lattice (in this case it is equal to 1/3). $2U_j \simeq kT_{\mathrm{c}} \ln(X/\dot{\varepsilon})$ is obtained from the comparison of two curves with deformation velocity

Table 1. For "impure" Pd $J \approx 0.75\%$, using the Morse potential, the probability of fusion Γwithin a microcrack 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 to 300 K) and energy (varying from 150 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 $J \approx 0.75\%$, T(range) ≈ 100–300 K, $\alpha \approx 0.34$ Å, $\lambda = 10^{-3}$ eV/min, $M_{\mathrm{Pd}}/\mu\mathrm{g}$)

E (eV)	$T \approx 100$ K		$T \approx 140$ K		$T \approx 180$ K		$T \approx 220$ K		$T \approx 260$ K		$T \approx 300$ K	
	$\Gamma \approx$	$P \approx$	$\Gamma \approx$	$P \approx$	$\Gamma \approx$	$P \approx$	$\Gamma \approx$	$P \approx$	$\Gamma \approx$	$P \approx$	$\Gamma \approx$	$P \approx$
150	10^{-80}	10^{-88}	10^{-67}	10^{-69}	10^{-77}	10^{-86}	10^{-63}	10^{-65}	10^{-65}	10^{-66}	10^{-60}	10^{-68}
160	10^{-75}	10^{-86}	10^{-65}	10^{-68}	10^{-75}	10^{-85}	10^{-61}	10^{-63}	10^{-63}	10^{-65}	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^{-48}	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^{-63}	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^{-63}	10^{-49}	10^{-53}	10^{-61}	10^{-72}	10^{-48}	10^{-52}	10^{-48}	10^{-53}	10^{-41}	10^{-46}

$\dot{\varepsilon}$, 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 Eq. (1) is divided by Eq. (5) and multiplied by Eq. (9), it follows that

$$\Gamma \approx \frac{\exp\left(-2\int_0^{\alpha} K(r)_{\text{int}}\mathrm{d}r\right)}{\lambda\frac{4\pi\rho\hbar}{\mu_d}\langle 1/p\rangle} D_L. \tag{10}$$

Equation (10) represents the probability of deuteron fusion within a microcrack: it is inversely proportional to the number of nuclei absorbed by the metal.

Using Eq. (10) and adopting the Morse potential to calculate $K(r)_{\text{int}}$, 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 Eq. (1) was evaluated numerically, making use of Eqs. (3) and (4) and taking the center of mass system as the reference system [1]. In the particular case of impure palladium with:

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

The result is $\Gamma_{pd} \approx 10^{-41}$, $P_{\text{int}} \approx 10^{-46}$.

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 K were considered.

The potential, Eq. (3), for Pd pure to 0.25%, was substituted by the "shell" potential, as follows:

$$V = kq^2\left((1/r) - \frac{KT}{J\varepsilon R}\right), \quad r_1 \le r \le R, \tag{11}$$

Table 2. For "pure" Pd ($J \approx 0.25\%$), adopting the "shell" potential, the probability of fusion Γwithin a microcrack, normalized to the number of events per minute, was calculated under the same dynamic conditions as in Table 1. Also here Γis 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 (Palladium $J \approx 0.25\%$, T(range) ≈ 100–300 K, $\alpha \approx 0.34$ Å, $\lambda = 10^{-3}$ eV/min, M_{Pd}/μg)

E (eV)	$T \approx 100$ K		$T \approx 140$ K		$T \approx 180$ K		$T \approx 220$ K		$T \approx 260$ K		$T \approx 300$ K	
	$\Gamma \approx$	$P \approx$	$\Gamma \approx$	$P \approx$	$\Gamma \approx$	$P \approx$	$\Gamma \approx$	$P \approx$	$\Gamma \approx$	$P \approx$	$\Gamma \approx$	$P \approx$
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}
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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^{-65}	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^{-68}	10^{-58}	10^{-64}	10^{-54}	10^{-62}	10^{-49}	10^{-59}	10^{-45}	10^{-48}

dove KT 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 deuteron charge. Under these particular dynamic conditions, the probability of fusion normalized to a number of events per minute was obtained for palladium. The probability of fusion within "pure" palladium, under the same dynamic conditions as the previous example, is then given by:

$$\alpha \simeq 0.15\ \text{Å},\ E \approx 237.2\ \text{eV},\ J = 0.25\%,\ T = 250.2\ \text{K}.$$

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

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

3. Conclusions

The present work has shown that microcracks and deuterium loading in the lattice at room temperature have a significant influence on the probability of fusion.

In fact, calculating the probability of interaction within a microcrack, an increase of at least 2–3 orders of magnitude are found compared to the probability of fusion on the surface. Further, 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 (e.g. for $J \approx 0.75\%$, $E \approx 250$ eV, $T = 300$ K, $\Gamma = 10^{-21}$, and $P \approx 10^{-25}$) [5]. Judging by the comparison between the two theoretical calculations, it would seem that the experimental procedure $reduces$ the rate of fusion rather than enhances 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 Fig. 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.

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