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Research Article

Nuclear Exothermic Reactions in Lattices Pd: A Theoretical Study of d–d Reaction

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Abstract

The aim of this paper is to demonstrate that the Coulomb barrier has variations in both time and space. Further, in this paper, we have taken the interaction between deuteron-optical photons, we want to clarify this point, of course, these photons have a vibrational frequency of interest because it was discovered that the interaction between photons and deuterons causes the Coulomb barrier is not static, that has of oscillations in different directions within the lattice. So we can conclude that this phenomenon of cold fusion that breaks new ground in modern nuclear physics. In recent years, over 20 years, have seen thousands of experiments and theoretical models to explain the phenomenon of fusion at low energy (LENR) in specialized heavy hydrogen systems. We can say that a new possible way to obtain nuclear energy without waste is emerging. Nevertheless in spite of experimental contributions, the theoretical framework is not known. In this work, we try to explain the deuteron–deuteron reactions within palladium lattice by means of the coherence theory of nuclear and condensed matter. The coherence model of condensed matter affirms that within a deuteron-loaded palladium lattice there are three different plasmas: electrons, ions and deuterons plasma. Then, according to the loading percentage $x = \mathrm{D/Pd}$, the ions deuterium can take place on the octahedrical sites or in the tetrahedral in the (1,0,0)-plane. In the coherence theory it is called β-plasma the deuterons plasma in the octahedral site and γ-plasma which in tetrahedral. We propose a general model of effective local time-dependent deuteron–deuteron potential, that takes into account the electrons and ions plasma oscillations. The main features of this potential are extracted by means of many-body theory considering the interaction deuteron–phonon–deuteron. In fact the phonon exchange produces a attractive component between two deuteron within the D_2 molecular. This attractive force is able to reduce the inter-nuclear distance from about 0.7 to 0.16 Å. It means that the lattice strongly modifies the nuclear environment with respect to free space. In this way according to deuterons energy, loading percentage and plasma frequency we are able to predict high o low tunneling probability. The fusion rates (s^{-1}) computed vary from 10^{-70} to 10^{-17} and also a set of other mechanism, which could be enhanced these values, are proposed. In this way we hope that by means of this approach in the future will be possible to realize and control the nuclear exothermic reactions that take place in the condensed matter in order to obtain clean energy.

Keywords: Cold fusion, Coulomb barrier, d–d Reactions, Many body

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1. Introduction

In this model of lattice takes place within the Coherence Theory of Condensed Matter and represents a general theoretical framework accepted from most of scientists that work on cold fusion phenomena. In the coherence theory of condensed matter [5], it is assumed that the electromagnetic (e.m.) field due to elementary constituents of matter (i.e. ions and electrons) plays a very important role on system dynamics. In fact considering the coupling between (e.m.) equations, due to charged matter, and the Scrödinger equation of field matter operator, it is possible demonstrate that in proximity of e.m. frequency, ω_0, the matter system shows a coherence dynamics. For this reason, it is possible to speak about coherence domains whose length is about $\lambda_{CD} = 2\pi/\omega_0$. Of course, the simplest model of matter with coherence domain is the plasma system. In the usual plasma theory, we must consider the plasma frequency ω_p and the Debey length that measures the Coulomb force extension, i.e. the coherence domain length. For a system with N charge Q of m mass within a volume, V, the plasma frequency can be written as

$$\omega_p = \frac{Q}{\sqrt{m}}\sqrt{\frac{N}{V}}, \tag{1}$$

$$\omega_p \approx 10 \text{ eV}/\hbar.$$

In this work, we study the "nuclear environment" that it is supposed existent within the palladium lattice D_2-loaded and at room temperature as predicted by Coherence Theory. In fact when the palladium lattice is loaded with deuterium gas, some peoples declared that it is possible observe traces of nuclear reactions [1–3]. For this reason, many physicist speak about Low-energy Nuclear Reaction (LENR). The more robust experiments tell us that in the D_2-loaded palladium case the nuclear reactions more frequent are [3,4]:

$$\mathrm{D+D} \to {}^3\mathrm{H} + \mathrm{p} + 4.03 \text{ MeV}, \quad \mathrm{D+D} \to {}^4\mathrm{He} + 23.85 \text{ MeV}. \tag{2}$$

Thus, an experimental analysis of this phenomenon requires neutron, proton and gamma rays detectors. A brief list follows of detectors that are most frequently quoted in the literature. Further (n = neutron, p = proton, in parenthesis the probabilities of the three final branches). The first step in the reaction is the creation of a ^{4}He nucleus with an excess energy of 24 MeV.

This reaction has been extensively studied, mostly, through experiments performed with the help of particle accelerators, which means in quasi-vacuum and with energetic particles (>105 eV). This is quite different from the CF experiments, which take place in condensed matter at room temperature (energies of the order of a small fraction of an eV).

In this work, we also propose a 'coherence' model by means of which we can explain the occurrence of nuclear reactions and their probability according to the more reliable experiments. First, we will start from the analyze of environment, i.e., of plasmas present within palladium (d-electron, s-electron, Pd-ions and D-ions) using the coherence theory of matter; finally, we will use the effective potential reported in [7,8] adding the role of lattice perturbations by means of which we compute the d–d tunneling probability.

2. The Plasmas Present within No Loaded Palladium

According to Coherence Theory of Condensed Matter, in a Pd crystal at room temperature the electron shells are in a coherent regime within coherent domain. In fact, they oscillate in tune with a coherent e.m. field trapped in the coherent domains. For this reason, in order to describe the lattice environment, we must take into account the plasma of s-electron and d-electron.

2.1. The plasma of the d-electrons

They are formed by electrons of palladium d-shell. We can start computing:

$$\omega_{\mathrm{d}} = \frac{e}{\sqrt{m}}\sqrt{\frac{n_{\mathrm{d}}N}{V}} \tag{3}$$

as d-electrons plasma frequency. As already seen in the chapter about plasmas, this value must be increased by a 1.38 factor in the case of a real plasma, due to distribution of neutralizing charges (Pd ions, in this case).

We can understand this correction observing that formula (**??**) is obtained assuming a uniform d-electron charge distribution. But of course the d-electron plasma is localized in a shell of radius R (that is about 1 Å), so the geometrical contribution is

$$\sqrt{\frac{6}{\pi R}} = 1.38. \tag{4}$$

Labeled with ω_{de} the *renormalized* d-electron plasma frequency, we have [5]:

$$\omega_{\mathrm{de}} = 41.5\ \mathrm{eV}/\hbar \tag{5}$$

and the maximum oscillation amplitude ξ_{d} is about 0.5 Å.

2.2. The plasma of delocalized s-electrons

The s-electrons are those which in the lattice neutralize the adsorbed deuterons ions. They are delocalized and their plasma frequency depends on loading ratio (D/Pd percentage) by means of the following formula [5]:

$$\omega_{\mathrm{se}} = \frac{e}{\sqrt{m}}\sqrt{\frac{N}{V}}\sqrt{\frac{x}{\lambda_{\mathrm{a}}}}, \tag{6}$$

where

$$\lambda_{\mathrm{a}} = \left[1 - \frac{N}{V}V_{\mathrm{pd}}\right] \tag{7}$$

and V_{pd} is the volume effectively occupied by the Pd-atom. As reported in [5], we have

$$\omega_{\mathrm{se}} \approx x^{1/2} 15.2\ \mathrm{eV}/\hbar. \tag{8}$$

For example for $x = 0.5$, we have $\omega_{\mathrm{se}} \sim 10.7$ eV/$\hbar$.

2.3. The plasma of Pd-ions

Finally, we must consider the plasma due to palladium ions that form the lattice structure. In this case, it is possible to demonstrate that the frequency is [5]

$$\omega_{\mathrm{pd}} = 0.1\ \mathrm{eV}/\hbar. \tag{9}$$

3. The Plasmas Present within D_2-loaded Palladium

We know that the deuterium is adsorbed when is placed near to palladium surface. This loading can be enhanced using electrolytic cells or vacuum chambers working at opportune pressure [9,10]. By means theory of Condensed Matter, we are assumed that according to the ratio x = D/Pd, three phases concerning the D_2–Pd system exist:

(1) phase α for $x < 0.1$,
(2) phase β for $0.1 < x < 0.7$,
(3) phase γ for $x > 0.7$.

In the αtphase, the D_2 is in a disordered and not coherent state (D_2 is not charged!). Regarding the other phases, we start remembering that on surface, due to lattice e.m., takes place the following ionization reaction:

$$D_{\text{lattice}} \rightarrow D^{+} + e^{-}. \tag{10}$$

Then, according to the loading percentage $x = \text{D/Pd}$, the ions deuterium can take place on the octahedrical sites or in the tetrahedral in the (1,0,0)-plane. In the coherence theory it is called β-plasma the deuterons plasma in the octahedral site and γ-plasma which in tetrahedral. Regarding to β-plasma it is possible affirms that the plasma frequency is given by [5]:

$$\omega_\beta = \omega_{\beta 0}(x + 0.05)^{1/2}, \tag{11}$$

where

$$\omega_{\beta 0} = \frac{e}{\sqrt{m_\text{D}}}\left(\frac{N}{V}\right)^{1/2}\frac{1}{\lambda_\text{a}^{1/2}} = \frac{0.15}{\lambda_\text{a}^{1/2}}\ \text{eV}/\hbar. \tag{12}$$

For example, if we use λ_a = 0.4 and $x = 0.5$ it is obtained $\omega_{\beta\text{g}}$ 0.168 eV$/\hbar$.

In the tetrahedral sites, the D^+ can occupy the thin disk which encompass two sites.

They present to the D^+ ions a barrier. Note that the electrons of the d-shell oscillate past the equilibrium distance y_0 (about 1.4 Å) thus embedding the ions in a static cloud of negative charge (whose can screen the Coulomb barrier). So, as reported in [5], we have

$$\omega_\gamma = \sqrt{\frac{4Z_\text{eff}\alpha}{m_\text{D}y_0^2}} \approx\ 0.65\ \text{eV}/\hbar. \tag{13}$$

Of course, this frequency depends also on chemical condition of palladium (impurities, temperature, etc.). Due to a large plasma oscillation of d-electrons, in the disk-like tetrahedral region (where the γ-phase D^+'s are located) a high-density negative charge condenses giving rise to a screening potential $W(t)$.

We emphasize that the γ-phase depends on x value and that this new phase has been experimentally observed [11].

4. The d–d Potential

In [7], it was shown that the phenomenon of fusion between many body, i.e. nuclei of deuterium in the lattice of a metal is conditioned by the structural characteristics, by the dynamic conditions of the system, and also by the concentration of impurities present in the metal under examination. In fact, studying the curves of the potential of interaction between deuterons (including the deuteron–plasmon contribution) in this case typical metals Pd, a three-dimensional model showed that the height of the Coulomb barrier decreases on varying the total energy and the concentration of impurities present in the metal itself. The starting potential that links like-Morse attraction and like-Coulomb repulsion can be written in this way [7,8]:

$$V(r) = k_0 \frac{q^2}{r} \left(V(r)_{\mathrm{M}} - \frac{A}{r} \right). \tag{14}$$

In (**??**), $V(r)_{\mathrm{M}}$ is a like-Morse potential and is given by:

$$V(r)_{\mathrm{M}} = D \{\exp(-2\varphi\,(r - r_0))\, 2\, \exp(-\varphi\,(r - r_0))\}, \tag{15}$$

Here, the parameters A, φ and r_0 depend on model. In fact the potential (**??**) is an effective potential whose reliability is demonstrated from its ability to fit the Coulomb potential for $r \to 0$ and the Morse potential in the attractive zone. In this way, following Siclen and Jones [12] define ρ the point where the Coulomb potential is linked by Morse trend, r_0' the equilibrium distance and D' the well. Of course, in the free space for a D_2 molecular ρ is about 0.3 Å , r_0' is about 0.7 Å and D' is – 4.6 eV. But within the lattice the screening effect and the deuteron–deuteron interaction by means of phonon exchange modify very much these parameter values.

Taking into account, the role of coupling between deuteron and plasmons, in [13] the authors have numerically evaluated a d–d potential having the features of potential (**??**) with $D' = -50$ eV and $r_0' = 0.5$ Å and $\rho = 0.2$ Å (in [13] the authors consider only two plasmon excitations at 7.5 and 26.5 eV).

Since the screening effect can be modulated by donor atoms, we have considered in [7,8] the role on impurities and has been demonstrated that we can put:

$$A = JKTR \tag{16}$$

and

$$B = J/\varsigma. \tag{17}$$

Here, J is the impurities concentration, KT the lattice temperature, R the nuclear radius and ζ a parameter to evaluate by fitting.

Finally, we can write the effective d–d potential in this way:

$$V(r) = k_0 \frac{q^2}{r} \left(V(r)_{\mathrm{M}} - \frac{JKTR}{r} \right). \tag{18}$$

In this work, according to coherence theory of condensed matter, we study the role of potential (**??**) in the three different phases: α, β and γ. Whereas regarding the second point, the question is more complicate. In fact, the lattice environment is a mixing of coherent plasmas (ion Pd, electron and deuterons plasma) at different temperature, due to different masses, thus describing a emerging potential is very hard office. The method that in this work we propose is the following: considering the total screening contribution of lattice environment at d–d interaction (i.e. V_{tot}) as random potential $Q(t)$. So in this model we can write

$$V_{\mathrm{tot}}(t) = V(r) + Q(t). \tag{19}$$

Of course, we assume that:

$$\langle Q(t) \rangle_t \neq 0 \tag{20}$$

that is, we suppose that $Q(t)$ (a second-order potential contribution) is a periodic potential (the frequency will be labeled by ω_Q) that oscillates between the maximum value $Q_{\max}$ and 0. More exactly, the charge oscillations of d-shell produce a screening potential having an harmonic features:

$$\mathrm{eV}(r) = -Z_{\mathrm{d}} \frac{ke^2}{2a_0} r^2. \tag{21}$$

In [5], putting Z_{d} = 10/3 and a_0 = 0.7 Å, it is evaluated a screening potential V_0 of about 85 eV. In this way, we can compute ρg V_0/26.9 and at last ρ = 0.165 Å.

To summarize, we can have the following cases in a palladium lattice according to loading ratio.

4.1. α-Phase

In phase αsghe deuterons are in a molecular state and the thermal motion is about:

$$0.02 \text{ eV} < \hbar\omega_\alpha < 0.1 \text{ eV}.$$

This phase takes places when x is less than 0.1, and since $W(t)$ is zero, the d–d potential is

$$V(r) = k\frac{q^2}{r}\left(V_{\mathrm{M}}(r) - \frac{J\,\hbar\omega_\alpha\,R}{r}\right). \tag{22}$$

Expression (**??**) has been partially evaluated in a previous paper [7] but in that case we was interesting only to the dependence of tunneling probability on impurities present within lattice. In this work, we examine the correlation between potential features and loading ratio. In the paragraph 5 we will show some numerical results.

4.2. β-Phase

When x is bigger than 0.1 but less than 0.7, the phase β happens. The interaction takes place between deuteron ions that oscillate by following energy values:

$$0.1 \text{ eV} < \hbar\omega_\beta < 0.2 \text{ eV}.$$

In this case, $W(t)$ is zero, so the potential is given expression (**??**):

$$V(r) = k\frac{q^2}{r}\left(V_{\mathrm{M}}(r)\frac{J\,\hbar\omega_\beta\,R}{r}\right). \tag{23}$$

Comparing expressions (**??**) and (**??**) seems very clear that the weight of impurities is more important in the β-phase. Of course, this conclusion is in according to the previous papers [7,8], where we studied the role of temperature on tunneling effect.

4.3. γ-Phase

Finally, when the loading ratio is higher than 0.7, the deuteron–palladium system is in the phase γ .

This is the more interesting case. The deuterons undergo the screening due to d-electrons shell, so we suppose that the d–d potential must be computed assuming that the well present in potential 14, due to Morse contribution, disappears. In fact if we use a classical plasma model where are the D^+ ions the positive charge and the d-electrons the negative, it is very reasonable suppose that we must use the following potential:

$$V(r,t) = k\ \frac{q^2}{r}\left(V_{\mathrm{M}}(r)\frac{J\,\hbar\omega_\gamma\,R}{r}\right) + Q(t). \tag{24}$$

We emphasize that $Q(t)$ is a not known perturbative potential. About it we can only say that:

$$\langle Q(t)\rangle_{\mathrm{t}} \approx \frac{W_{\max}}{\sqrt{2}}. \tag{25}$$

As said previously, we suppose that it is the screening potential due to d-electrons and its role is that to reduce the repulsive barrier, i.e. ρ and $r'0$.

In next evaluation, we put

$$\langle Q(t)\rangle_{\mathrm{t}} \approx 85 \text{ eV}. \tag{26}$$

5. Results and Discussions

Now we present the d–d fusion probability normalized to number of events per second regarding the d–d interaction in all different phase. More exactly we compare the fusion probability in the phases α, β and γ at varying of energy between –50 and 50 eV. We also consider the role of d-electrons screening as perturbative lattice potential. This treatment, which interests only the case where $Q(t)$ is different from zero, involves that we change the value of point on the x-axes where the Coulomb barrier takes place and, in this case, the final result is that the screening enhances the fusion probability. In order to evaluate the fusion rate (Λ), we applied this formula:

$$\Lambda = A\Gamma. \tag{27}$$

In this case, the Morse potential will be

$$V(r)_{\mathrm{M}} = D\exp\left(-2\,\varphi\,(r-r_0)\right)2\exp\left(\varphi\,(r-r_0)\right),$$

$$E_1 = \text{a few eV},$$

$$E_2 = -D\left(1-\frac{\gamma\,\hbar}{\sqrt{2\mu\,D}}\left(\nu+\frac{1}{2}\right)\right)^2,$$

$$E_3 \sim \left(\frac{m_{\mathrm{e}}}{M_{\mathrm{N}}}\right)E_1 \sim \frac{1}{1000}\text{ eV},$$

$$E_4 = D',$$

where γ is the constant of anharmonicity of the metal and ν is the vibrational constant. Another important quantity is D$'$, which is the depth of the potential well: D this is Morse potential

Now an energy tensor E_{ij}can be built:

$$E_{11} = E_1, \quad E_{22} = E_2, \quad E_{33} = E_3, \quad E_{44} = E_4, \quad E_{ij} = E_i - E_j, \quad E_{ij} = -E_{ji}.$$

Thus, a square quadratic energy value can be determined.

For this case, we assumed a Morse potential as the most realistic.

$$I \approx \frac{e^2\pi\,Z_{\mathrm{a}}Z_X}{4\pi\,\varepsilon_0\,\hbar\,\nu}$$

is the Gamow factor and A is the nuclear reaction constant obtained from measured cross sections (value used was 10^{22} s^{-1}).

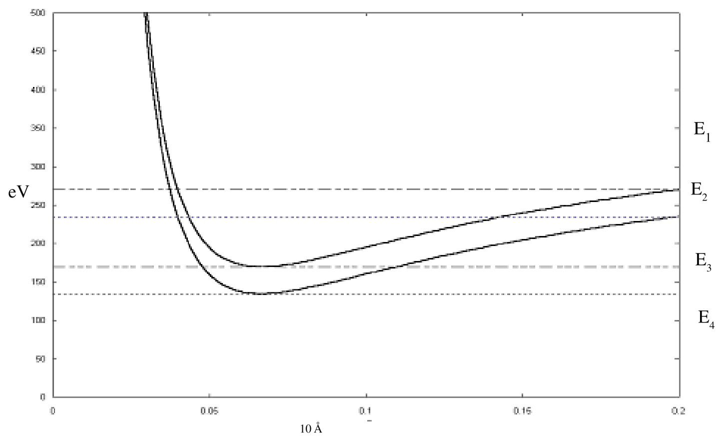


Figure 1. Features of $V(r)$ and $V(r) + W_{\max}/\sqrt{2}$.

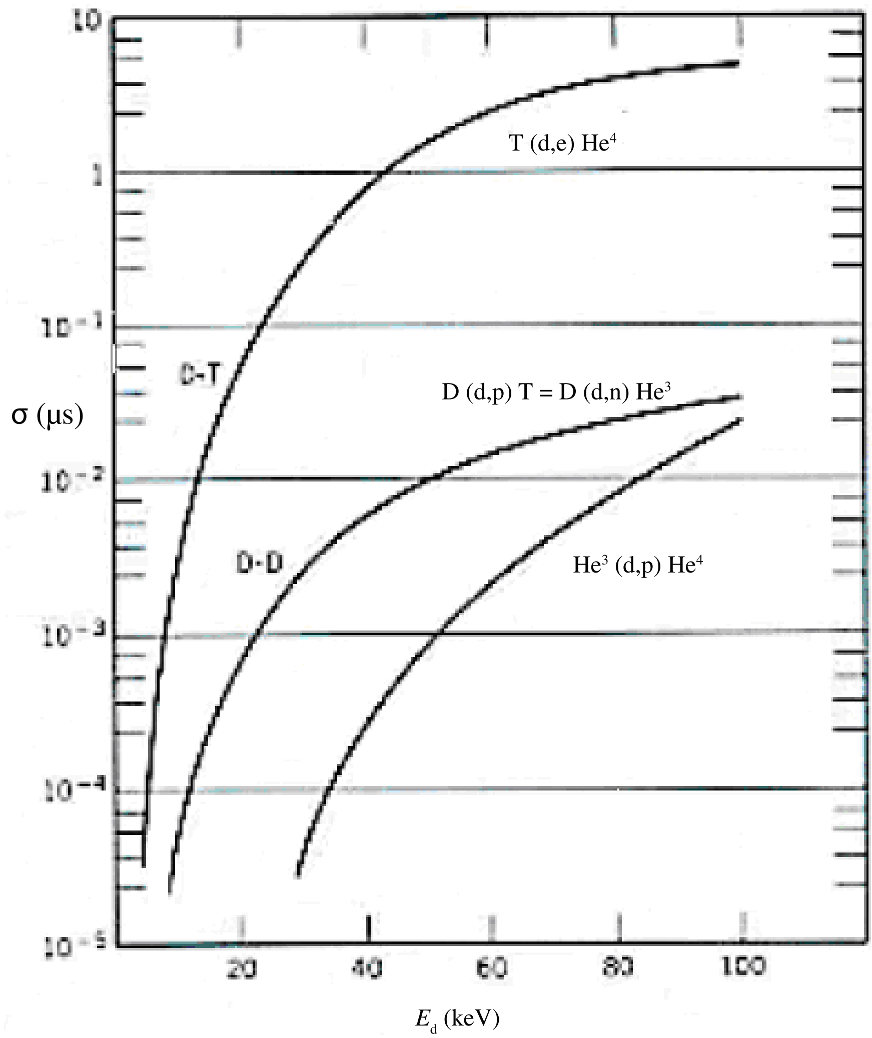
The probability partial reaction that takes into account the factor penetration of the barrier, with Γ Gamow factor. Furthermore, the potential can be considered adiabatic to a very good approximation. In fact, the adiabatic parameter $\hbar(I/V(R))(\mathrm{dV(R)/dt}) < 0.1$ eV, which is much smaller than the plasmon energies (or other typical electron excitation energy).

To have an estimate of the consequence of this result on the d–d fusion rate, let us model the deuterons inside palladium as a classical gas interacting through the total conservative potential depicted in Fig. 1 (full line), at a temperature T'.

From the point of experimental view, in the cold fusion phenomenology, it is possible to affirm that there are three typology of experiments [14]:

(1) those that have given negative results,
(2) those that have given some results (little detection signs with respect to background, fusion probability about 10^{-23} using a very high loading ratio
(3) those that have given clear positive results as Fleischmann and Pons experiments.

Nevertheless, we think that the experiment like 3-point are few accurate from a point of experimental view. For this reason, we believe that a theoretical model of controversial phenomenon of cold fusion, must explain only the experiments like points 1 and 2. In this case need consider the role of loading ratio on the experimental results. Now, let us begin from α-phase. It is possible affirms that if we load the deuterium with a percentage $x < 0.2$ we do not observe any fusion event! The same absence of nuclear phenomenon is compatible for a loading ratio of about 0.7. Since in this case the predicted fusion probability is less than 10^{-42}. These predictions, of course, are in agreement to the experimental results. But for $x > 0.7$ a set of valid experiments on cold fusion report some background spikes (e.g. see [6]). The remarkable result of our model is that in the γ-phase, as shown in Table 3, we can really observe some background fluctuations, since we predict a fusion probability about 10^{-22} due to a very high loading ratio. This represents a new result with respect to [7,8] since, in those cases, the fusion probability was independent on loading ratio. To conclude we shown that the model proposed in this paper (which unify nuclear physics with condensed matter) can explain some anomaly nuclear traces in the solids. Regarding the experiments at point 3 supposing that they could


10
1
10⁻¹
10⁻²
10⁻³
10⁻⁴
10⁻⁵
σ (μs)
T (d,e) He4
D-T
D (d,p) T = D (d,n) He3
D-D
He3 (d,p) He4
20
40
60
80
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Ed (keV)

Figure 2. xxx.

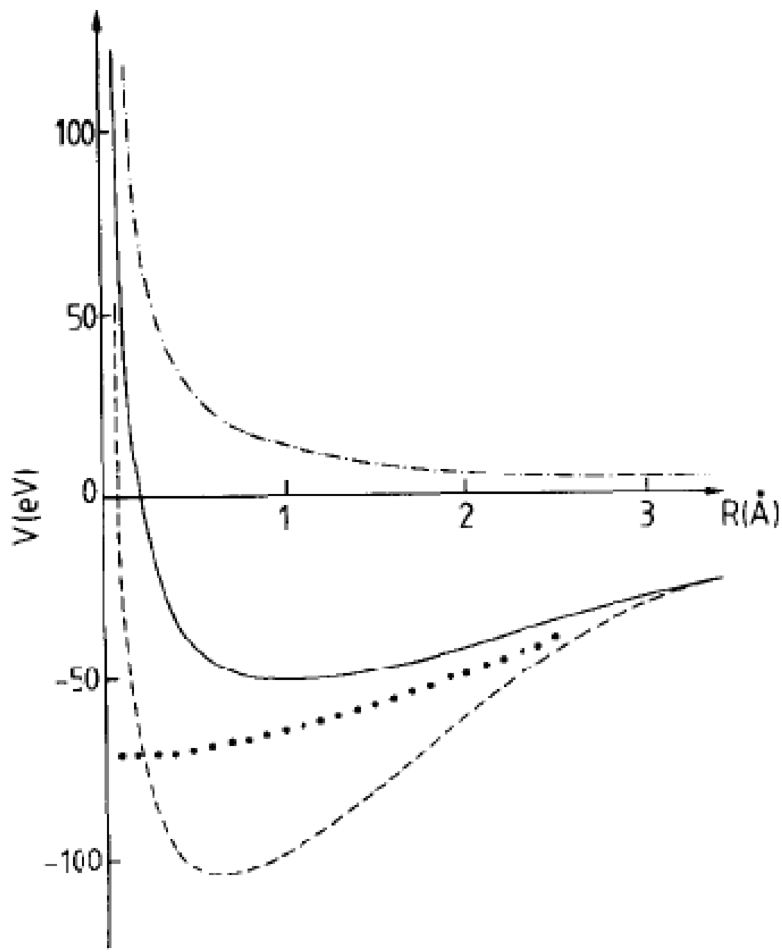

Figure 3. Interaction potentials in eV as a function of d–d distance R in Å.

be real, we would invocate other contribution as micro-deformation occurrence in order to explain the very high fusion rate. The role of micro-crack and of impurities linked by loading ratio will be explored in other speculative works. May be the nuclear physics within condensed matter will be a new very productive scientific topic.

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