

## COLD FUSION PHENOMENON AND ATOMIC PROCESSES IN TRANSITION-METAL HYDRIDES AND DEUTERIDES

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### ABSTRACT

The cold fusion phenomenon (CFP) is manifest in various events ranging from huge excess energy to various nuclear transmutations in solids containing a high density of hydrogen isotopes (both protium and/or deuterium). Until now there has been no satisfactory explanation. CFP has several characteristics which require explanation consistent with modern physics: the sporadic occurrence of the events, their qualitative reproducibility, localization of nuclear products in small ( $\sim\mu\text{m}$ ) regions at surfaces of samples, occasionally simultaneous occurrence of several events, and so forth. We have tried to provide a consistent explanation of CFP as a whole, using a model (called the TNCF model) with a single adjustable parameter and several premises based on experimental facts. To give physical bases for the premises in the TNCF model, which has shown its ability to give a consistent explanation of CFP, we have worked with neutron bands in solids. In this paper, we show a possibility of neutron bands originating in excited states of neutrons in atomic nuclei on lattice points (in lattice nuclei) mediated by band states of protons (deuterons) occluded in the transition-metal hydrides (deuterides). An indirect nuclear interaction between neutrons in lattice nuclei (the super-nuclear interaction) becomes effective in those crystals when the density of hydrogen isotopes is high and the neutrons are in excited states with widespread wave functions in lattice nuclei. The supernuclear interaction, then, results in the formation of neutron bands which give rise to nuclear reactions observed as anomalous nuclear reactions in solids, the so-called cold fusion phenomenon (CFP). A relation between the physics of transition-metal hydrides (deuterides) and CFP is investigated using the trapped neutron catalized fusion (TNCF) model, which has been successful in the systematic explanation of many phases of CFP.

### 1. INTRODUCTION

The so-called "cold fusion" phenomenon (CFP) [1] which shows anomalous effects in solids with high densities of hydrogen isotopes occurs mainly in transition-metal hydrides and deuterides. The effects include (1) generation of huge amounts of excess heat, inexplicable by ordinary atomic or molecular processes in solids, (2) production of nuclear products only explicable by transmutation of nuclides in the system, (3) emission of neutrons and gamma-photons with several MeV[2 - 4]. It should be emphasized here that the systems where CFP occurs includes both deuterium and hydrogen systems and that CFP has not been observed without ambient neutrons.

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From our present knowledge of CFP, therefore, the description appropriate for it should be "nuclear reactions and accompanying events occurring in solids with high densities of hydrogen isotopes in ambient radiation." The effective systems are notably transition-metal hydrides and deuterides. For brevity, we will use the phrase cold fusion phenomenon (CFP) to describe these events as a whole.

The CFP has several curious characteristics [2 - 5] which have prevented its widespread acceptance. First of all, it has a qualitative but not quantitative reproducibility, i.e. the effect differs very much from null to a maximum for the same experimental conditions defined macroscopically. This means that microscopic variety in a definite macroscopic condition sensitively affects the reproducibility. Second, the phenomenon occurs sporadically, or intermittently without expectation. Third, the distribution of the byproducts in the sample shows localized reactions at surface regions producing the nuclear products. Fourth, there are definite numerical relations between the amounts of products: Describing the amount of a product  $X$  by  $N_x$ , the amount of the excess heat  $Q$  reduced to a number of reactions  $N_Q$ , defined by:

$$N_Q = Q(\text{MeV})/5(\text{MeV}),$$

is comparable with  $N_x$  of other products  $X$ 's ( $X = {}^4\text{He}$ , tritium  $t$ , Nuclear Transmutation (NT) etc.);

$$N_Q \sim N_x.$$

Fifth, it seems that CFP occurs only in the presence of background neutrons. At least to the best of our knowledge, there have been no positive results in any system without them. Sixth, the observed gamma photons are few and predominantly imbalance in their amount with other nuclear products and the excess heat.

Despite many efforts consumed in these more than twelve years, CFP as a whole has not obtained satisfactory explanation based on the firm basis provided by modern physics, i.e. using quantum mechanics, principles governing the physics of atomic and nuclear phenomena.

On the other hand, hydrogen isotopes in transition metals show peculiar characteristics; a large mobility in them [6] and formation of stoichiometric compounds [7]. To explain these characteristics, there are proposed several mechanisms based on the properties of hydrogen isotopes in them. For diffusion of hydrogen (deuterium) atoms, a mechanism is proposed where propagation of hydrogen (deuterium) atoms occurs through ion band states [8].

In the paper by Sussmann et al. [8], they consider that a proton (deuteron) in its ground state is localized due to interaction with the lattice, i.e. by self-trapping. They then assert that there are bands of excited states, which, however, are broadened due to the interaction with the lattice. Since, in this theory, protons (deuterons) propagate in bands of excited states, the energies of excited states forming the bands should coincide with the activation energies for diffusion. There is a fortuitous coincidence of this expectation for Nb-H system above 250 K while there are cases, which do not fit this criterion [6]. Generally speaking, physical processes occurring in the same systems as a whole should be explained from a single point of view, which is reconcilable with modern physics even if the results revolutionize some principles. Thus, it is desirable to explain both the characteristic behavior of hydrogen isotopes and CFP in transition-metal hydrides (deuterides) using quantum mechanics as far as it is possible.

There is a systematic explanation of CFP by a phenomenological model (TNCF model), which assumes the existence of quasi-stable neutrons trapped in solids[2 -5, 9 - 11]. In the development of microscopic verification of propositions assumed in the model, it has been recognized that the neutrons are in band states[12 -15]. One of the remarkable mechanisms of the proposed neutron band formation is that mediated by interstitial protons (deuterons) [14,15]. In the explanation of the mechanism, the excited states of protons (deuterons) in a potential well at interstices were used. The excited states were calculated by assuming a harmonic-oscillator potential at interstices surrounded by nuclei on the lattice points (lattice nuclei).

The excited states of a proton at an interstice are not a localized state but a band state, as suggested by the diffusion rate[8] and, therefore, the neutron band mediated by protons (deuterons) should be extended to include a contribution from hydrogen isotopes in band states. This concept is the subject of this paper.

## 2. Proton (Deuteron) Energy Bands in Transition-Metal Hydrides (Deuterides) Determined by Diffusion Data

The eigenstates of a proton (deuteron) in a translationally periodic potential with minima at the interstices  $\mathbf{b}_m$  are described by Bloch functions  $\phi_k(\mathbf{R})$ [8].

Using the tight-binding approximation, the proton (deuteron) Bloch functions  $\phi_k(\mathbf{R})$  are expressed by localized proton (deuteron) wave functions  $\varphi_p(\mathbf{R}-\mathbf{b}_m)$  at  $\mathbf{b}_m$  with a quantum number  $p$  as follows;

$$\phi_k^{(p)}(\bar{\mathbf{R}}) = N^{1/2} \sum_m \exp(i\bar{k}\bar{\mathbf{b}}_m) \varphi_p(\bar{\mathbf{R}} - \bar{\mathbf{b}}_m) . \quad (1)$$

As the localized wave function  $\varphi_p(\mathbf{R}-\mathbf{b}_m)$ , we can use harmonic oscillator wave functions in a spherically symmetric harmonic oscillator potential at  $\mathbf{b}_m$  ( $(\mathbf{R}-\mathbf{b}_m) \equiv \mathbf{r} = (x, y, z)$ );

$$V_{h.o.}(\bar{\mathbf{r}}) = K\bar{r}^2, \quad (K > 0) \quad (2)$$

Then, the function  $\varphi_p(\mathbf{R}-\mathbf{b}_m)$  are expressed by Hermite polynomials;

$$\varphi_p(\bar{\mathbf{R}} - \bar{\mathbf{b}}_m) = u_{n_x}(x)u_{n_y}(y)u_{n_z}(z), \quad (3)$$

$$u_n(x) = N_n H_n(\alpha x) \exp(-(1/2)\alpha^2 x^2) \quad (4)$$

where  $n_i$  ( $i = x, y$  or  $z$ ) are integers. In this equation,  $H_n(\xi)$  is the  $n$ -th Hermite polynomial, and the constant  $\alpha$  and the normalization constant  $N_n$  are defined by the following equations:

$$\alpha^4 = mK/\hbar^2, \quad (5)$$

$$N_n = \left( \frac{\alpha}{\pi^{1/2} 2^n n!} \right)^{1/2}, \quad (6)$$

where  $m$  is the mass of the proton (deuteron).

The interpretation of experimental diffusion data for the H-Nb (D-Nb) system was successfully given assuming that diffusion of hydrogen (deuterium) atoms proceeds via the first and second (third) excited bands in H-Nb (D-Nb)[8]. We, therefore, confine our consideration for excited states up to the third to use in the following calculation of the super-nuclear interaction specifically for protons (deuterons) in the PdH (PdD) crystal for reasons given later. Further, we assume that protons (deuterons) are in the octahedral interstices separated from each other by  $2.49 \text{ \AA}$ , using the lattice constant  $3.89 \text{ \AA}$  of the Pd crystal[16, 17].

Although the potential felt by a proton (deuteron) in PdH (PdD) is very different from that in NbH<sub>x</sub>, (NbD<sub>x</sub>), with  $x \ll 1$  [8], we apply here the same method used for the H-Nb (D-Nb) system to PdH (PdD) to supplement the treatment in our previous paper[15]. In [15] the harmonic oscillator wave functions extrapolated to excited states from the ground state were used to estimate the interaction of protons with adjacent lattice nuclei.

To find out the height of the barrier between two interstices using experimental data for diffusion of protons (deuterons), we follow the process applied to H-Nb and D-Nb successfully by Sussmann and Weissman[8]. The experimental data on activation energies  $U$  and pre-exponential factors  $D_0$  of diffusion are used to calculate the effective mass  $m^*$  of the migrating proton (deuteron) and finally to calculate the height of the barrier for diffusion when the density of protons (deuterons) is low.

According to the assumption made in [8], we use a one-dimensional sinusoidal potential with a periodicity corresponding to the spacing between interstices. The one-dimensional Schrödinger equation with the sinusoidal potential is then written as:

$$\frac{\hbar^2}{2m^*} \frac{d^2}{dx^2} \psi(x) + \left[ U - V_0 \cos \frac{2\pi x}{\ell} \right] \psi(x) = 0 \quad (7)$$

where  $\ell$  is the distance between two adjacent interstices along the line of the crystal axis.

It should be noticed that the diffusion characteristics in PdH (D) are different from those in NbH (D) as mentioned in [8] and the use of the sinusoidal potential for diffusion problem in PdH (D) may not be appropriate for the problem of diffusion. The use of this potential is, however, legitimate as a zeroth-order approximation to investigate wave functions of interstitial protons (deuterons) in the present stage where we have no information about them.

There is an experimental datum [18] of the excitation energy of the optical mode  $\Delta E_{op} = 56 \text{ meV}$  for PdH<sub>0.68</sub>. As the value of the force constant  $K$  in PdD is less than that in PdH[15],  $\Delta E$  for PdD may be smaller than  $56 \text{ meV}$  for PdH<sub>0.65</sub>.

Simply dividing the excitation energy of diffusion  $U = 230 \text{ meV}$  by  $\Delta E_{op} = 56 \text{ meV}$ , we obtain a value 4.1 supposedly related to the excited state responsible for diffusion. Considering thermal energy of  $25 \text{ meV}$  and effective tunneling at the top of a potential barrier, we may take lower excited

states lower than the fourth in this calculation. The consistency of the following calculation gives us the number  $n = 2$  (3) for the excited band in PdH (D), which we use hereafter.

The Schrödinger equation (7) is reduced to the Mathieu equation with a variable  $\eta$ ,

$$\frac{d^2 f(\eta)}{d\eta^2} + [a - 2q \cos(2\eta)]f(\eta) = 0 \quad (8)$$

with the parameters given by

$$a = \frac{8m^* \ell^2 U(V_0)}{h^2} \quad (9)$$

$$q = \frac{4m^* \ell^2 V_0}{h^2} \quad (10)$$

Using experimentally determined values[17] of  $U$  and  $D_0$  tabulated in Table 1, we can determine the height of the barrier  $2V_0$  as follows [8].

**Table 1:** Experimental data on the activation energy  $U$  and pre-exponential factor  $D_0$  for the diffusion of H and D in the metal Pd at low concentrations. (Data for Nb-H are given for comparison)

	H-Nb	H-Pd	D-Pd
$U$ (meV)	$106 \pm 4$	230	206
$U$ ( $\times 10^{-13}$ erg)	1.7	3.7	3.3
$10^4 D_0$ ( $\text{cm}^2\text{s}^{-1}$ )	$5.0 \pm 1$	29.0	17.0

The width  $\delta_n$  of the  $n$ -th excited state responsible for diffusion is related with the parameter  $D_0$  determined experimentally by the relations:

$$v_0 = 1.57 \frac{\delta_n}{h} \quad (11)$$

$$D_0 = \frac{d^2}{24} v_0 \quad (12)$$

where  $d$  is the lattice constant of the crystal and  $v_0$  is the diffusion jumping frequency. Then, the experimental values  $U$  and the  $\delta_n$  determine  $\delta_n/U$  which is used to calculate the value of  $q_n$  for a  $n$ -th excited band responsible for diffusion using the Mathieu equation (8).

The value of  $q_n$  thus determined further determines the parameter  $a$  and then the effective mass  $m^*$  in Eq.(9). Using the  $q$ - and  $m^*$ - values thus determined we can finally obtain the height of the barrier  $2V_0$  by Eq.(10). The resulting values are given in Table 2.

The result shown in Table 2 shows that it is appropriate to use the second (third) band for PdH (PdD) system in this approximation as the band responsible for the diffusion of protons (deuterons) considering the consistency of the start (values of  $U$ ) and the final result (values of  $2V_0$ ).

**Table 2:** Values  $\delta_n$ ,  $\delta_n/U$ ,  $q$ ,  $a_n$ ,  $m_n$  and  $2V_0$  for the relevant excited bands calculated using experimental data of the proton (deuteron) diffusion in the metal Pd at low concentrations. It is assumed that diffusion is related with 2nd (2nd and 3rd) excited state in PdH (PdD). The values for the second excited state ( $n = 2$ ) in PdD are given only for reference.

System	H-Pd	D-Pd	
Excited band $n$	2	2	3
$\delta_n$ (meV)	148	86	86
$\delta_n/U$	0.64	0.42	0.42
$q$	1.38	2.24	2.78
$a_n(q)$	4.6	5.4	9.7
$m_n^*$ ( $m_p$ )	0.06	0.04	0.12
$2V_0$ (meV)	272	343	231

The height of the barrier  $2V_0$ , in turn, is a reflection of the interaction between a proton (deuteron) in an interstice and lattice nuclei in adjacent lattice points in the tight-binding approximation which has been not taken explicitly into consideration in the previous work[15].

### 3. Super-nuclear Interaction and Neutron Energy Bands Mediated by Protons (Deuterons) in Transition-metal Hydrides (Deuterides)

Using the knowledge of the state of protons (deuterons) occluded in transitionmetal hydrides (deuterides), we can investigate interaction of nuclei on the lattice points (the lattice nuclei) mediated by the occluded hydrogen isotopes. The interaction of the lattice nuclei results in formation of a band structure in energy spectra of neutrons occupying nuclear excited states of the lattice nuclei.

#### 3.1. Protons (Deuterons) in Transition-metal Hydrides (Deuterides)

The treatment given in the previous section is based on the diffusion data where the density of hydrogen isotopes is low. In the case of transition-metal hydrides (deuterides) such as PdH (D) where density of hydrogen isotopes is high and almost all interstices are occupied by protons (deuterons), the situation is very different. It is true that the interaction between protons (deuterons) on the adjacent interstices becomes rather important in considering the state of hydrogen isotopes. In the following calculation, however, we have to remain in the zeroth approximation neglecting the effect of neighboring interstitials on the state of a hydrogen isotope at an interstice.

To investigate the interaction of a proton (deuteron) with lattice nuclei in a compound PdH (PdD), therefore, we use the value  $2V_0$  of the barrier height, determined above from diffusion data in low concentrations, to calculate wave functions of a proton (deuteron) at an interstice assuming that it is insensitive to the density of protons (deuterons). Further, the potential for a proton (deuteron) in an interstice is assumed to be a harmonic oscillator with spherical symmetry (cf. Eq. (2)) which has a value  $2V_0$  at the middle point  $x_{1/2}$  of a line connecting adjacent interstices, i.e. at  $x_{1/2} = 2.75/2 \text{ \AA} = 1.375 \text{ \AA}$ ;

$$2V_0 = Kx_{1/2}^2$$

Using  $2V_0$  given in Table 2, we obtain the force constant  $K_H$  and  $K_D$  for PdH (2nd band) and PdD (3rd band), respectively, as follows;

$$K_H = 1.44 \times 10^{19} \text{ (eV/m}^2\text{)}, \quad K_D = 1.22 \times 10^{19} \text{ (eV/m}^2\text{)}.$$

In the tight-binding approximation, the probability density of a proton-band wave function  $\phi_k^p(\mathbf{R})$  (Eq.(1)) at a lattice nucleus at  $\mathbf{a}_l$  is determined essentially by the wave function  $\varphi_p(\mathbf{r}-\mathbf{b}_m)$  at one of the nearest interstices  $\mathbf{b}_m$ .

Using these force constants and the harmonic oscillator wave functions  $u_n(x)$  (Eq. (4)) determined by them with  $n = 2$  (3) for PdH (PdD), we can calculate the probability density  $|u_n(x_N)|^2$  at an adjacent lattice point  $x_N \equiv |\mathbf{a}_l - \mathbf{b}_m|$ , i.e. at  $r = 3.89/2 \text{ \AA} = 1.95 \text{ \AA}$ .

$$|u_2(x_N)|^2 = 2.5 \times 10^3 \text{ m}^{-1} \text{ (PdH)}, \quad |u_3(x_N)|^2 = 1.0 \times 10^2 \text{ m}^{-1} \text{ (PdD)}. \quad (13)$$

The values of the barrier height  $2V_0$  of the sinusoidal potential, which are given in Table 2 and used in the above calculation, were calculated according to the recipe given by Sussmann et al. [8]. If we use the values of the activation energy  $U$  of 230 (206) meV for PdH (PdD), given in Table 1 for  $2V_0$ , we obtain following values for the probability densities;

$$|u_2(x_N)|^2 = 1.3 \times 10^4 \text{ m}^{-1} \text{ (PdH)}, \quad |u_2(x_N)|^2 = 4.2 \times 10 \text{ m}^{-1} \text{ (PdD)}. \quad (14)$$

It is difficult to discuss the meaning of the differences of values in Eq.(13) and in Eq.(14) at the present stage of investigation. We use the values in Eq.(13) in this paper, hereafter.

### 3.2. Neutron Bands based on Excited States of Lattice Nuclei

A neutron as a quantum mechanical particle behaves similarly to an electron even if their masses differ by three orders of magnitude. Both are used for structural analysis of matter by neutron and electron diffraction, which rely on their wave nature. Electrons in a periodic potential have band structure in their energy spectrum. This has been widely utilized in microelectronics. On the other hand, the corresponding state of neutrons has not attracted scientific attention.

We have investigated the energy state of thermal neutrons in solids, using the approximation of quasi-free neutrons in a previous paper[13]. It has been shown with a simplified potential in one dimension that there is a neutron band above zero with its energy minimum at Brillouin zone edges at an energy close to the thermal energy, using appropriate parameters for the potential. The

calculated energy band of neutrons corresponds to the conduction band in semiconductors and can be called *the neutron conduction band*.

To investigate energy states below zero corresponding to the valence bands of electrons in semiconductor crystals, we consider here neutron states in metal hydrides originating from excited states of neutrons in lattice nuclei, using the tight binding approximation used in the case of electron bands.

Here, we can consider these neutrons in the excited states as basic states to construct neutron bands corresponding to the valence bands in semiconductors and we can call them *the neutron valence bands*.

The Schroedinger equation for a neutron in the field of an isolated nucleus at a lattice point  $\mathbf{a}_\ell$  is

$$\nabla^2 \phi_n(\vec{r} - \vec{a}_\ell) + \frac{2m}{\hbar^2} (E - U(\vec{r} - \vec{a}_\ell)) \phi_n(\vec{r} - \vec{a}_\ell) = 0, \quad (15)$$

where  $U(r)$  is the potential of a nucleus for the neutron. We consider, for simplicity, a solution  $\phi_n(\mathbf{r})$  with a quantum number  $n$ , which corresponds to an excited s-state and is therefore spherically symmetrical. Let  $E_n$  be the corresponding energy and let the state be non-degenerate.

Consider now the wave function  $\psi_k(\mathbf{r})$  of a neutron in the field of the lattice nuclei as a whole plus protons in the interstitial sites  $\mathbf{b}_m$ . Let  $\mathbf{a}_\ell$  denote the position of any lattice nucleus and  $\mathbf{R}$  the position of any proton with a wave function  $\varphi_p(\mathbf{R} - \mathbf{b}_m)$  with a quantum number  $p$  in any interstitial site at  $\mathbf{b}_m$ . Then, since the direct influence of one lattice nucleus on the neutron in another lattice nucleus is negligible, the wave function of a neutron in the field of the nucleus at  $\mathbf{a}_\ell$  will be approximately  $\phi_n(\mathbf{r} - \mathbf{a}_\ell)$ , which is just the unperturbed wave function of a neutron in the nucleus with its center at  $\mathbf{a}_\ell$ . We therefore set for  $\psi_k(\mathbf{r})$

$$\psi_k(\vec{r}) = \sum_{\ell} c_{\ell} \phi_n(\vec{r} - \vec{a}_{\ell}) \quad (16)$$

where the coefficients  $c_{\ell}$  for a neutron in the field only of the lattice nuclei may be determined from the theorem of Bloch, that  $\psi_k(\mathbf{r})$  is the product of a periodic function and a factor  $e^{i(\vec{k}\vec{r})}$ ; this gives  $c_{\ell} = e^{i(\vec{k}\vec{a}_{\ell})}$ , and hence for a state  $\mathbf{k}$ :

$$\psi_k(\vec{r}) = \sum_{\ell} e^{i(\vec{k}\vec{a}_{\ell})} \phi_n(\vec{r} - \vec{a}_{\ell}), \quad (17)$$

the summation being over all lattice points of the crystal.

Using an approximation of tight binding similar to that used in solid state physics to calculate electron bands, we obtain an energy spectrum of a neutron in the second order perturbation calculation



$$E = E_n + \sum_{\ell} e^{-i(\vec{k}\vec{a}_{\ell})} v_{nnp}(\vec{a}_{\ell}) \quad (18)$$

where  $E_n$  is the energy of a neutron with a quantum number  $n$  in a lattice nucleus, and  $v_{nnp}(\vec{a}_{\ell})$  represents the effective interaction energy of two neutrons with the same quantum number  $n$  in one ( $\vec{a}_{\ell} = 0$ ) and also in adjacent lattice nuclei ( $\vec{a}_{\ell} =$  nearest neighbors of 0) through the super-nuclear interaction via a proton with a quantum number  $p$ .

The total energy  $E_{tot}$  of the system is expressed as follows;

$$E_{tot} = E_n + \varepsilon_p + \sum_{\ell} \exp(-i\vec{k}\vec{a}_{\ell}) v_{nnp}(\vec{a}_{\ell}), \quad (19)$$

$$v_{nnp} = \sum_{m, n', p'} \frac{[n, p | V | n', p'] [n', p' | V | n, p]}{E_{n', p'} - E_{n, p}} \quad (20)$$

$$E_{n, p} = E_n + \varepsilon_p, \quad (21)$$

$$V(\vec{r}) = \kappa \frac{e^{-r/r_0}}{r}, \quad (22)$$

$$[n, p | V | n', p'] = \int \int d\vec{r} d\vec{R}, \quad (23)$$

$$\psi_n^*(\vec{r} - \vec{a}_{\ell}) \varphi_p^*(\vec{R} - \vec{b}_m) V(\vec{r} - \vec{R}) \psi_n(\vec{r} - \vec{a}_{\ell}) \varphi_p(\vec{R} - \vec{b}_m), \quad (24)$$

where  $E_n$  is energy of a neutron in a state  $\psi_n(\vec{r} - \vec{a}_{\ell})$  in a lattice nucleus at  $\vec{a}_{\ell}$ ,  $\varepsilon_p$  is energy of a proton in a state  $\varphi_p(\vec{R} - \vec{b}_m)$  at an interstice  $\vec{b}_m$ .

The potential between a proton (deuteron) and a neutron is approximated by a three-dimensional square-well potential

$$\begin{aligned} V_s(\vec{r} - \vec{R}) &= -V_0^{(s)}, & (|\vec{r} - \vec{R}| < b) \\ &= 0, & (|\vec{r} - \vec{R}| > b) \end{aligned} \quad (\text{Square well}) \quad (25)$$

where  $V_0^{(s)} \sim 3.5$  MeV,  $b \sim 2.2 \times 10^{-13}$  cm.

Thus, as shown by numerical calculations given below, neutrons in excited states of lattice nuclei are combined together to form an energy band by the super-nuclear interaction mediated by protons (deuterons) occluded in the Pd lattice. There appear, therefore, neutron energy bands corresponding to excited neutron states in lattice nuclei. The neutron energy band, then, is responsible for nuclear reactions at boundary region as shown in a previous paper[4].

### 3.3 Width of the Neutron Valence Band

To show structure dependence of the bandwidth, we will make a simplification of the super-nuclear interaction between adjacent nuclei assuming that it depend only on the magnitude of vector  $\mathbf{a}_\ell$ . We can rewrite the expression (19) as follows;

$$E = E_n + \varepsilon_p - \alpha - \sum_{\ell} \gamma_{\ell\ell'} e^{-i(\bar{k}\bar{a}_{\ell})}, \quad (26)$$

$$-\alpha = v_{nnp}(0) \quad (27)$$

$$-\gamma_{\ell\ell'} = v_{nnp}(\bar{a}_{\ell\ell'}), \quad \bar{a}_{\ell\ell'} = \bar{a}_{\ell} - \bar{a}_{\ell'}, \quad (28)$$

where  $a_{\ell\ell'} = |\bar{a}_{\ell\ell'}|$  is the nearest neighbor distance. If we can assume that the effective potential is independent of direction,  $\gamma_{\ell\ell'}$  is replaced by a constant  $\gamma$ .

For the three cubic structures, we have from this equation, if  $a$  is the side of the cube;

$$E = E_n - \alpha - 2\gamma(\cos k_x a + \cos k_y a + \cos k_z a) \quad (\text{s.c.}), \quad (29)$$

$$E = E_n - \alpha - 8\gamma \cos \frac{1}{2} k_x a \cos \frac{1}{2} k_y a + \cos \frac{1}{2} k_z a \quad (\text{bcc}), \quad (30)$$

$$E = E_n - \alpha - 4\gamma(\cos \frac{1}{2} k_y a \cos \frac{1}{2} k_z a + \cos \frac{1}{2} k_z a \cos \frac{1}{2} k_x a + \cos \frac{1}{2} k_x a \cos \frac{1}{2} k_y a) \quad (\text{fcc}) \quad (31)$$

The energy of a neutron consists, therefore, of a constant term  $E_n - \alpha$ , together with a term, which depends on the wave vector  $\mathbf{k}$ . Thus, for the energy state of a neutron in the free nucleus, there exists a band of energies in the crystal with a high density of protons in interstitial sites. Without further calculation of the effective potential (28), we cannot give the value of the integral  $\gamma$ , and hence the breadth of the band in metal hydrides. It is noticed here that the band structure of neutron energy depends on the lattice structure and therefore the interaction of particles in solids is influenced strongly by the symmetry and lattice constants of the crystal.

The effective interaction energy  $v_{nnp}(\mathbf{a}_\ell)$  depends generally on the quantum numbers  $n$  and  $n'$  of two neutrons and on  $p$  of a proton and should be written as  $v_{nn'p}(\mathbf{a}_\ell)$  if we consider the possible change of the neutron state in the adjacent lattice nucleus. This makes expression (19) more complicated, thus giving wide variety to the structure of the band.

For numerical estimation of the width  $\Delta E$  of the neutron energy band mediated by protons (deuterons), we assume the energy difference  $\varepsilon_{n'p',np} \equiv E_{n',p'} - E_{n,p}$  in the denominator in Eq.(16) to be a constant value of  $\sim 100 \text{ meV} = 1.6 \times 10^{-13} \text{ erg}$  suggested by experimental data of low-energy neutron scattering by medium nuclei[19]. The region where the interaction potential Eq.(21) has a large value is confined to the nucleus. We may put the following values for the matrix elements Eq.(20), neglecting details of neutron wave functions;

$$\psi_n^* \psi_n \cdot d\bar{r} \sim 1, \quad \phi_p^* \phi_p \cdot d\bar{R} \sim 1.4 \times 10^{-12}.$$

In reality, however, it is obvious that the distribution of neutron density in the nucleus depends sensitively on the value of the matrix element (20), and this estimation is necessarily qualitative.

Then, we obtain the following values using relations suggested by experimental data of nuclear reactions between neutrons;

$$\begin{aligned} \langle n, p | V | n', p' \rangle &\sim 5 \times 10^{-3} (\text{meV}) \\ v_{nnp} &\sim 3 \times 10^{-6} \sum_{m, n', p'} (\text{meV}) \sim 3 \times 10^{-5} \sum_{n', p'} (\text{meV}) \\ \Delta E &\sim \sum_{\ell} v_{nnp} (a_{\ell}) \sim 10 v_{nnp} \sim 10^{-4} \sum_{n', p'} (\text{meV}) \end{aligned}$$

For quasi-continuous levels of excited states in a lattice nucleus, we have to calculate such integrals as the following one;

$$\sum_{n', p'} \frac{|\langle n, p | V | n', p' \rangle|^2}{E_{n', p'} - E_{n, p}} = \int_{-\infty}^{\infty} d\varepsilon \rho_p(\varepsilon) \int_{-\infty}^{\infty} dE \rho_n(E) \frac{|\langle n, p | V | n', p' \rangle|^2}{E + \varepsilon}, \quad (32)$$

where  $\rho_p(\varepsilon)$  and  $\rho_n(E)$  are densities of states for proton and neutron quantum states, respectively, and  $\varepsilon = \varepsilon_{p'} - \varepsilon_p$ ,  $E = E_{n'} - E_n$ . We leave investigation and exact calculation of this integral for future work.

Thus, the width of the neutron energy band mediated by the super-nuclear interaction has a following value as an order of magnitude for a choice of  $\varepsilon_{n'p', np} = 100$  meV;

$$\Delta E \sim 10^{-4} \sum_{n', p'} (\text{meV})$$

which depends strongly on the number of quantum states of the system around the zero-energy where we can expect widely extended neutron wave functions  $\psi_n(\mathbf{r} - \mathbf{a}_{\ell})$  and high density of states  $\rho(\varepsilon)$ .

It, also, depends very strongly on the distribution of probability densities of neutron wave functions in the lattice nucleus and of proton (deuteron) wave functions at lattice nuclei which depend drastically on the value of  $2V_0$ , the height of the potential barrier between interstices. For instance,  $|u_2(x_N)|^2$  becomes  $10^4$  larger when  $2V_0 = 230$  meV rather than that for  $2V_0 = 270$  meV used in the above calculation.

For the summation over the states  $n'$  and  $p'$ ,  $\sum_{n', p'}$ , in the above relation for  $\Delta E$ , we may take rather arbitrarily a value of  $10^6$ , considering dense distribution of excited levels in heavy nuclides around zero energy [20]. Then we obtain  $\Delta E \sim 0.1$  eV. This is a narrow but finite width of the neutron energy band mediated by occluded hydrogen isotopes in Pd. It should be noticed that the summation  $\sum_{n', p'}$  has originally a summand expressed in Eq. (22) and the above choice depends on the constant value  $\varepsilon_{n'p', np} = 100$  meV which we assumed before.

Therefore, the calculations given above show clearly the possible existence of the super-nuclear interactions between neutrons in adjacent lattice nuclei mediated by protons (deuterons) in PdH (PdD). This generalizes the treatment [15] where we used wave functions calculated with an extrapolated form of the harmonic oscillator potential  $V_{h.o.}(\mathbf{r})$  suggested by low-level excited states.

#### 4. Relation between the Nuclear Energy Band and Cold Fusion Phenomenon explained by the TNCF Model

The TNCF model (Trapped Neutron Catalyzed Fusion model) was proposed [21] as a phenomenological model and has been successful in explaining various features of CFP [2-5, 9-11]. As a phenomenological model, it is naturally based on several assumptions, and it has an adjustable parameter. The basic supposition of the model is the assumed existence of neutrons in solids (trapped neutrons) with a density (denoted as  $n_n$ ) at the reaction region.

The value of  $n_n$  was determined by experimental data in CFP as  $n_n = 10^8 \sim 10^{13} \text{ cm}^{-3}$ .

On the other hand, as was shown in this and previous papers [13-15], it is conceivable that neutrons in appropriate crystals are in band states with energies near zero. Neutrons in a band state exhibit a characteristic localized coherence in boundary regions designated as a local coherence [4,12]. Therefore, the density of neutrons in a band becomes very large at boundary regions of a crystal next to another appropriate crystal.

This neutron density is a consistent result with a supposition of the TNCF model that reaction cross-sections of a trapped neutron with other nuclides are large in the boundary region. This supposition is consistent with results, which show localized production of new elements in CFP.

The large value of  $n_n$  determined from experimental data could be well understood if neutrons in lattice nuclei occupy the energy band responsible for the above-mentioned reaction and they are accumulated at surface regions of crystals by the local coherence.

Furthermore, the gammaless de-excitation of unstable nuclides, daughters of nuclear reactions in CFP, even if not treated explicitly in the model, may be explained by their interaction with neutrons in band states. In short, nuclides in CFP are not isolated as those treated in ordinary nuclear physics but interacting with each other through super-nuclear interaction mediated by occluded hydrogen isotopes. This is the new fundamental feature of nuclear interactions in solids, which was not known until CFP was discovered. It is assumed phenomenologically in the TNCF model to explain various events in CFP.

It is also possible to explain other characteristics of CFP, for instance the qualitative reproducibility, sporadic occurrence of events and surface nature of nuclear reactions. These are qualitatively explained by the necessary conditions that facilitate the appearance of the super-nuclear interaction.

In relation with the successful explanation of CFP by the TNCF model, assuming quasi-stable neutrons in solids, the existence of other models for CFP based on assumed neutral particles should be mentioned. One of plausible assumptions of neutral particles is the unstable polynutron proposed by J.C. Fisher [22]. Mass spectra of nuclear products in an experiment by G.H. Miley et al.[23] were successfully explained as results of fission reactions of nuclei formed from lattice nuclei

by the absorption of several neutrons from a polynutron, a hypothetical temporal assembly of neutrons in crystals. The role of these fictitious neutral particles can be replaced by the neutron drop[24] proposed as an assembly of neutrons and protons (and electrons to neutralize charge) in relation with the TNCF model and verified from another point of view of neutron star matter [25].

## 5. Discussion

The result of our calculation for the probability density of the proton (deuteron) wave function with a quantum number  $n = 2$  (3) is compared with the result using an extrapolated harmonic oscillator potential from the first-excited wave function. The conclusion of the latter calculation was that the state with  $n = 9$  (12) is responsible to the super-nuclear interaction if we simply extrapolate the potential for a proton (deuteron) to such higher levels. The result given in this paper shows that the formation of proton (deuteron) bands makes the lower excited states effective to mediate the super-nuclear interaction, which we could anticipate beforehand without numerical calculation. Thus, the present treatment seems rather reasonable if we consider that diffusion of protons (deuterons) occurs with an excited energy of  $U = 230$  (206) meV.

It is interesting to notice a fact shown in Eqs.(13) and (14). While the barrier height  $2V_0$  is lower and therefore diffusivity is higher for deuterium than for hydrogen, the probability density at an adjacent lattice nucleus is smaller for the former than for the latter. This means that the neutron energy band mediated by hydrogen isotopes is easier to be realized in hydrides than in deuterides in the case treated in this paper.

This conclusion might be related with experimental results where nuclear transmutation seems to occur sometimes rather frequently and massively in hydrides than in deuterides. Some of typical experimental results in hydrides[5] showing large amount of new nuclides explicable only by nuclear transmutations are by R.T. Bush et al.[26, 27], G.H. Miley et al.[23, 28], R. Notoya et al.[29], T. Ohmori et al.[30, 31] and D.W. Mo et al.[32].

Even if the treatment given in this paper is qualitative, especially the use of the Mathieu functions to express ion bands in PdH (PdD), the result showing definite effects of the proton (deuteron) wave functions on the lattice nucleus is not absurd. Thus, the interaction of protons (deuterons) with lattice nuclei will have substantial effects on the nuclear interactions in solids observed as the so-called cold fusion phenomenon (CFP). This is the decisive reason that CFP occurs predominantly in transition-metal hydrides and deuterides with high densities of hydrogen isotopes to make the crystal structure regular. The closer to stoichiometric density, the higher the regularity of the crystal structure, and the easier it is to form neutron energy bands.

The characteristics of CFP have been a controversial problem difficult to explain with simple assumptions based on the usual crystal structure and on nuclear reactions between nuclei with electric charges. As we proposed in previous papers [2-5, 9-11], it is necessary to assume the existence of neutrons (or neutral particles) to explain nuclear reactions in solids at or near ambient temperature. The super-nuclear interaction mediated by occluded hydrogen (deuterium) given in this paper describes the give a possible participation of neutrons in excited states of lattice nuclei for realization of nuclear reactions in solids, especially in transition-metal hydrides and deuterides.

The CFP has several characteristics, which are remarkable from various points of view. From the applications point of view, the huge excess heat is attractive for an almost inexhaustible energy source and nuclear transmutation without hazardous radiation for effective remediation of nuclear waste from atomic reactors used to produce electricity. To develop techniques for their application, however, it is necessary to know the physics of reactions occurring in systems showing CFP.

Tests based on the TNCF model (2-5, 9-11) have given consistent explanations of such events of CFP as excess heat generation, production of nuclear products, neutron spectra and a mechanism of gammaless de-excitation of nuclei.

Quantitative relations between amounts of products have been given using a single adjustable parameter in the TNCF model [2-5, 9,10]. This explanation alone shows the effectiveness of the phenomenological model and suggests that the physics of CFP is related to neutrons in solids. The fundamental factor making CFP different from nuclear reactions in free space is that nuclear reactions pertinent to CFP are in an environment full of neutrons but not in free space; lattice nuclei are interrelated with each other through neutrons like the situation of neutron star matter elaborated by J.W. Negele et al.[25] and others. Dissipation of nuclear energy in excited states of nuclei occurs not by gamma or beta emission but by giving energy to neutrons. This may be the reason for gammaless nuclear transmutation, a riddle that perplexed people for so long.

Now, it is possible to contemplate necessary conditions for and to depict the processes of the CFP.

(1) **Existence of background neutrons:** It is suggested by experimental facts that CFP occurs only in presence of background neutrons [5]. (2) **Heterogeneous structure of crystals:** To make trapping effective, the crystal should have heterogeneous structure (usually near its surface). Then, thermal neutrons supplied from background neutrons can be trapped and then cause trigger reactions with nuclei in the lattice. Furthermore, the neutrons in band states concentrate at boundary regions where neutron Bloch waves are reflected and have local coherence. (3) **Lattice nuclei with appropriate excited neutron levels near zero energy:** Products of the trigger reactions raise neutrons in lattice nuclei to their excited states with rather wide-spread wave functions. (4) **High-density of hydrogen isotopes in interstices:** The excited neutrons in lattice nuclei interact with each other through the super-nuclear interaction mediated by hydrogen isotopes in interstices and there are formed band states of the neutrons in the excited states. (5) **Formation of neutron drops** High-density neutrons at the boundary region form neutron drops, which react with lattice nuclei and with hydrogen isotopes resulting in anomalous nuclear reactions observed in CFP.

The attempt given in this paper is far from complete from the quantitative point of view, but it gives a glimpse of interrelations between CFP and solid-state physics of transition-metal hydrides (deuterides). We will continue our effort in this direction using modern physics as a tool to make clear physics of CFP and facilitate the development of techniques to enhance it.

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