

Solid State-Nuclear Physics of Cold Fusion Phenomenon

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ABSTRACT

First of all, it should be mentioned that the term "the Cold Fusion Phenomenon" (CFP) includes nuclear reactions and accompanying events occurring in solids with high densities of hydrogen isotopes (H and/or D) in ambient radiation.

Investigation of the cold fusion phenomenon (CFP) during the past 14 years revealed that CFP occurs in localized regions at boundaries (and surfaces) in solids containing a high concentration of either deuterium or protium or both. The occurrence is characterized by sporadicity and only qualitative reproducibility. The former means unpredictability and the latter different effects for the same macroscopic initial conditions.

Success of a phenomenological model (the TNCF model) assuming the existence of thermal neutrons in solids to explain CFP as a whole both in deuterium and protium systems suggests the existence of an unexplored field between nuclear physics and solid state physics related to neutrons in solids. Examining excited states of neutrons near the separation level of a nucleus and also excited states of protons (deuterons) in solids, we show the existence of new states of neutrons (the cf-matter) in transition-metal deuterides and hydrides, typical materials for CFP, which are responsible for exotic nuclear reactions in solids including CFP.

An excited state of a neutron in a lattice nucleus (nucleus at each lattice point) interacts with another in adjacent lattice nuclei mediated by protons (deuterons) at interstices. The result is a corresponding neutron band. Neutrons in this band form a high-density neutron matter (cf-matter) at boundary/surface regions with neutron drops (clusters of neutrons and protons) that makes nuclear reactions in solids so different from those in free space.

1. INTRODUCTION

In 1989, Fleischmann and Pons published the first paper on CFP (Fleischmann 1989). In an electrolytic system, Pd/D₂O + LiOD/Pt, they

measured excess heat, tritium and neutrons and concluded that the observed data resulted from $d-d$ fusion reactions, which are improbable to occur in solids. Succeeding investigations revealed, however, that the experimentally observed variables are also observed in systems containing only protium without deuterium. Furthermore, it became clear that there are no positive results without background thermal neutrons thus showing the essential role of thermal neutrons in CFP. More puzzling factors in CFP are poor reproducibility and the sporadic occurrence of events. In addition to these qualitative discoveries, there is an enormous amount of data of various kinds of events showing facts peculiar to CFP, which are inexplicable without invoking various nuclear reactions in materials used in the CF experiments.

A phenomenological approach was tried as an orthodox procedure to attack theoretically difficult problems with unknown variables (Kozima 1994a). We were able to obtain a consistent explanation of various experimental data sets obtained in both protium and deuterium systems. Puzzles of CFP pointed out above were explained consistently (Kozima 1998a). The key postulate of the phenomenological model (the TNCF model) is the existence of thermal neutrons in CF materials, where positive data have been obtained. The TNCF model using an adjustable parameter has been successful in explaining many quantitative relations between CF products. Also, progress has been on the neutron drop model to explain nuclear transmutations where a multi-neutron absorption by a nuclide is needed (Kozima 2000a, 2003).

In an attempt to explain quantum mechanically the several postulates assumed in the successful models, it has been shown that there are previously unknown, important new fields in nuclear physics and solid-state physics. These fields are closely related to CFP and are not explained by conventional knowledge of physics (Kozima 2004. This paper is cited as QP, hereafter.). The excited state of neutrons around the separation level (zero energy) in a nucleus is a concept not recognized to have any importance in nuclear physics. The quantum mechanical state of hydrogen isotopes in *fcc* (*hcp*) transition-metal hydrides and deuterides is another concept not recognized to have an important connection with nuclear physics in solids. Surface layers on the cathodes in electrolytic systems play important role in realization of CFP. These problems are investigated quantum mechanically in the previous paper and show peculiarity of nuclear reactions in *fcc* (*hcp*)

transition-metal hydrides and deuterides (proton conductors) completely different from those in free space (QP).

The presumption of $d-d$ fusion reactions in solids is assumed by Fleischmann et al. (Fleischmann 1989) and many of the following researchers and also by critics opposing CFP. These reactions in free space are written as follows:

$$d + d = t(1.01 \text{ MeV}) + p(3.02 \text{ MeV}), \quad (1)$$

$$= {}^3_2\text{He} (0.82 \text{ MeV}) + n(2.45 \text{ MeV}), \quad (2)$$

$$= {}^4_2\text{He} (76.0 \text{ keV}) + \gamma (23.8 \text{ MeV}). \quad (3)$$

Branching ratios of these reactions in free space are, as is well known, $1:1 \approx 10^{-7}$ and it is known that they occur effectively only if the mutual energy is above about 100 keV.

Some researchers assumed the $d-d$ fusion reactions as causes of products measured in CF experiments with materials where deuterium was occluded (Fleischmann 1989, Jones 1989). It was pointed out, however, that the $d-d$ fusion reactions in solids are not realistic from physical point of view (Leggett 1989, Ichimaru 1993) even if there are limitations of the calculation by Leggett et al. (Kim 1996b).

Simple reasoning for difficulty of the $d-d$ fusion reactions in crystals without additional accelerations can be given as follows:

Phonons have minimum wavelength about a lattice constant a ; $\lambda_{\min} \doteq a$. Therefore, they cannot distinguish two deuterons approached to less than a and can not do anything to make them approach to a distance about 1 fm where nuclear force works by overcoming the Coulomb barrier between them.

The electrons has a light mass $m_e = 9.11 \times 10^{-31}$ kg and the uncertainty principle makes the energy of an electron large when its position is confined in a small range; $\delta x \times \delta p \doteq \hbar$: In a hydrogen atom, an electron with a classical Bohr orbit with a radius $a_H \doteq a (= \delta x)$ has a kinetic energy E_e as given by

$$E_e \doteq \delta p^2/2m \approx \hbar^2/m a_H^2 \approx 10 \text{ eV} (\approx e^2/2 a_H = E_H).$$

If an electron works to lower the Coulomb barrier between two deuterons to make them fuse together, the electron has to remain between them at a distance about $r_{n.f.} \approx 1 \text{ fm} \approx 10^{-5} a_H (= \delta x)$ where works the nuclear force.

Then, the energy of the electron becomes very large showing inability of electron effect for the fusion reaction:

$$E_e \approx (\delta p)^2/2m \approx 10^{10} \hbar^2/m a_H^2 \approx 10^{10} E_H.$$

Dielectric constants ϵ 's cannot work for this object, too. Dielectric constants are concepts averaged over ions on lattice with lattice constants a 's and cannot be used for problems between two deuterons approached closer than a lattice constant a .

This simple calculation and also more elaborate reasoning (Leggett 1989, Ichimaru 1993), of course, do not exclude the possibility that there may be some mechanism to realize d - d fusion reactions in solids by overcoming the Coulomb barrier between charged nuclei.

Table 1. Matrix Substances, Agent nuclei, Direct and Indirect Evidence of nuclear reactions in cold fusion phenomenon (CFP). Q is for the excess heat and NT for the nuclear transmutation. Dependences of products on energy ϵ and position r , decay time shortening of radioactive nuclides, and fission-barrier lowering of compound nuclides give direct information of nuclear reactions in CFP.

Matrix Substances	Transition Metals (Ti, Ni, Mo, Pd, Pt, etc.) Proton Conductors (SrCeO ₃ , AlLaO ₃ , etc.) Ferroelectrics (KDPO ₄ , TGS, etc.) Others (C, Na _x WO ₃ , Stainless steel, etc.)
Agents	¹ ₀ n, ¹ ₁ H, ² ₁ H, (¹⁶ ₈ O), ⁶ ₃ Li, ¹⁰ ₅ B, ²³ ₁₁ Na, ³⁹ ₁₉ K, ⁸⁵ ₃₇ Rb, ⁸⁷ ₃₇ Rb, SO ²⁻ ₄ , etc.
Direct Evidences	Neutron Energy Spectra $n(\epsilon)$, Gamma $\gamma(\epsilon)$ Spatial distribution of NT products ($A_Z X(r)$) Decay time shortening, Fission-barrier decrease
Indirect Evidences	Excess heat Q , Number of neutrons N_n , Number of Tritium N_t , Number of ⁴ He N_{He} , X-ray spectra $X(\epsilon)$,

Experimental data sets obtained thenceforth themselves have shown that d - d fusion reactions are not fundamentally responsible for observed products in both deuterium and protium systems, first of all. Variety of these products also has told that fundamental causes of nuclear reactions in solids

producing them should be others not noticed by researchers and critics. For convenience sake, let us use a working concept *the cf-matter* to specify a state of particles (lattice nuclei and occluded hydrogen isotopes) in a part of CF samples where occurs CFP, nature of which we investigate in the course of this paper.

As was experimentally shown, CFP includes various events (phenomena) in various kinds of crystals as shown in Table 1 (Table 1 of QP).

We can see in this table that the CF materials where the cf-matter is formed include various substances. We, however, concentrate our discussion on *fcc* transition metals in this paper to investigate characteristics of CFP because of rich data in them.

Observations of neutrons in CFP (Jones 1989, De Ninno 1989, and others) can be taken as an opening of a new era of solid state-nuclear physics. In the process of development of CF research, there are several signals showing importance of the role of neutrons in CFP. The first signal was the experiment by Shani et al. (Shani 1989) showing several orders of magnitude larger effect of thermal neutrons on neutron emission from PdD_x compared with those from deuterium gas. Several succeeded works have shown enhancement of CFP by thermal neutron irradiation to CF materials (Yuhimchuk 1992, Celani 1992, Stella 1993, Lipson 1995, 1996, Oya 1996, Notoya 1998). The second was absence of CFP in experiments without background neutrons (Ishida 1992, Jones 1994, Taylor 1994, Forsley 1998). There are also peculiar experimental data showing trapping and later release of neutrons perhaps related to the effects just mentioned (Cerofolini 1993, Samgin 1996, Lipson 2002, and others).

The background neutron is abundant around us (Carpenter 1989) and should be considered its role in CFP seriously as we done in the TNCF model (Kozima 1998a). Furthermore, observations of a lot of neutrons with energies up to about 10 MeV (upper limits of measurements) (Sato 1991, Botta 1999, and others) indicate experimentally occurrence of other nuclear reactions than Eq.(2) in solids (Kozima 1999b).

Interesting works related to neutrons in solids were performed about 30 years ago in relation to the problem of theoretical verification of the neutron star by simulation (Baym 1971, Negele 1973). When there is a neutron liquid with densities more than 10^{35}cm^{-3} , there appears a so-called Coulomb lattice of clusters of neutrons and protons (and electrons) with a definite lattice

constant. The lattice constant and proton to neutron ratio in a cluster decrease with increase of the average neutron density and finally stable homogeneous distribution of pure neutrons are realized as a neutron star at densities more than about 10^{38}cm^{-3} . If we extrapolate the result of their simulation to lower density region of about 10^{30}cm^{-3} attainable in surface layers (Kozima 2000a), we obtain a Coulomb lattice with a lattice constant about 10^{-3}Å and almost the same proton to neutron ratio to that of Pd nuclei (Kozima 2002) (cf. Section 3.3).

There are recent developments in neutron physics in solids. We will give some examples in relation to our TNCF model (Kozima 1998a): Multi-layer structures of crystals, for instance Ti (100 Å)/ Ni (100 Å)/ --- and Permalloy (100 Å)/ Ge (800 Å)/ Permalloy (100 Å), have been used to reflect cold neutrons (Ebisawa 1998) and to investigate trapping and tunneling characteristics of cold neutrons (Achiwa 1998, Hino 1998). Here is a new direction of low energy neutron physics where the property of a neutron in a potential is an object of research instead of the external effect of a crystal or a potential structure on the neutron investigated hitherto (Shull 1956, Williams 1988).

The cold fusion matter (*the cf-matter*) is, as defined above, a working concept used in the following chapters to specify a state of composite particles in a part of CF materials where occurs CFP. The part of CF materials where the cf-matter is formed, is usually localized at boundary/surface regions of samples used in CF researches (CF samples) but sometimes it should be considered to be a whole volume of the CF materials. The size of the localized region is known to be measured by micrometers (μm).

Standard of energy for nucleons in a nucleus is taken at the threshold energy of neutron emission or the separation level except otherwise stated. This means that *the zero of energy* is about 8 MeV higher than the ground level of nuclides with a medium nucleon number while it corresponds to the energy scale of thermal neutrons in free space.

2. QUANTUM MECHANICAL INVESTIGATION OF INTERDISCIPLINARY FIELD BETWEEN NUCLEAR PHYSICS AND SOLID-STATE PHYSICS USING DATA OF CFP

2.1 *Neutrons in crystal*

2.2 *Hydrogen isotopes in fcc transition metals*

2.3 *Energetics of nuclides related to CFP*

2.4 *Excited states of a nucleus around the separation level (zero energy)*

The cold fusion phenomenon (CFP) could not be independent of physical properties of CF materials and also of properties of nuclides included in them. In this Chapter, therefore, we survey these properties of nuclides and occluded hydrogen isotopes seemingly relevant to CFP investigated in solid-state physics and nuclear physics. It is interesting to find out following facts that there are riddles in properties of solids and nuclides not fully understood in each fields but they seems have close relations to CFP. The solution of the riddles in solid-state physics might be related to interactions of hydrogen isotopes and nuclei, which we discuss partly in Chapter 3. The CFP is a probe of the physics in the cf-matter, the solid state-nuclear physics, from our point of view and we can investigate the nature of the assumed cf-matter through events of CFP.

2.1 *Neutrons in Crystal*

The neutron is unstable in free state and decays by beta disintegration with a constant of 886.7 ± 1.9 s (half-life 616 s) into a proton, electron and neutrino liberating energy of 0.782 MeV (Caso 1998).

As the experimental data sets in CFP and their explanation by the TNCF model have shown, the ambient background neutron (Carpenter 1989) plays an important role in CFP. Little is known, however, about their nature in materials even if the neutron diffraction and the chain reaction in atomic piles are used largely in worldwide research and in industry where neutron behaves as a wave and as a particle, respectively.

In this section, we summarize the fundamental nature of neutron first and then explain its relation with the TNCF model.

2.1-1 *Wave Nature of Neutron and Interaction with Lattice Nuclei*

It is well established now that any particle has wave nature and it is true for the neutron, too. This nature of neutron is widely used in many applications as neutron diffraction and neutron optics.

The neutron as an elementary particle exhibits wave property with a

characteristic wavelength λ (called de Broglie wave length) expressed by Eq. (4) of QP which takes a value 1×10^{-8} cm for a kinetic energy of 88 meV and 1.80×10^{-8} cm for 25 meV (the thermal energy at 300 K).

A neutron with mass m_n and de Broglie wave length λ comparable with lattice constants of the crystal behaves as a wave and interacts with nuclei on the lattice points (lattice nuclei) through nuclear force. The interaction could be treated approximately by Fermi pseudo-potential (zero-radius potential) as expressed by Eq. (5) of QP with a parameter b , the effective scattering length, with a dimension of length. This potential of lattice nuclei gives band structure in energy spectrum of neutrons in crystal in the rigid-lattice approximation (Kozima 1998c). The effect of thermal motion on the band structure should be considered in real crystals that will make the band structure blurred.

In natural conditions on the earth, there are a lot of background thermal and epithermal neutrons generated by the cosmic ray in the upper atmosphere (Carpenter 1989). These neutrons with a flow density of about 10^{-2} neutrons/cm²s enter into crystals of transition-metal hydrides and deuterides we are considering now. They behave as Bloch waves in a neutron band in crystals (Kozima 1998c) and may be trapped in the crystals by several mechanisms (Kozima 1998a). Rather effective mechanism of neutron trapping may be one by the nature of neutron band in a crystal (Kozima 1996a, 1998b).

The trapped neutrons in neutron bands above zero (neutron conduction bands) can be de-excited to neutron bands below zero (neutron valence bands, cf. Section 3.5). Furthermore, neutrons in lattice nuclei are able to be excited into the bands from the ground state getting enough energy (\approx a few MeV) liberated in nuclear reactions between trapped neutrons and lattice nuclei.

It is interesting to notice here that the notion of the neutron band has not been used hitherto in neutron physics even though the nature is used to confine neutrons in a crystal (Hino 1998). The neutron band in solids proposed for the first time by the author (Kozima 1996a, 1998c) is a novel one corresponding to the popular electron band in solids and the photonic band (Yeh 1988, Joannopoulos 1995) in artificial periodic structures. It is also interesting to remind that these three particles have been used in structural analysis as electron, X-ray and neutron diffractions widely and complementally in science and technology.

2.1-2 *Nuclear Interaction in Solids and Neutron Mössbauer Effect*

In the discussion of CFP, it should be kept in mind at least following facts about nuclear interactions in solids. To accomplish a nuclear reaction where works the nuclear force with an action range $\approx 10^{-13}$ cm, the reactant nuclei must approach each other to this distance. On the other hand, separation of nuclei in atoms in ordinary materials is several Å, i.e. $\approx 10^{-8}$ cm that is 10^5 times the distance necessary to get work of the nuclear force. To make two deuterons approach together close in a distance about 10^{-13} cm overcoming the Coulomb barrier between them, it needs too large energy of more than 10 keV for nuclides with the thermal energy of about 25 meV.

It is also advisable to confirm an essential point in the explanation of the Mössbauer effect, one of typical phenomena revealing an effect of phonons in the solid state-nuclear physics. The energy of the relevant nuclei in the Mössbauer effect is the same order of magnitude of the average phonon energy. For instance, $^{67}_{30}\text{Zn}$ emits a photon with energy 93.26 keV that is used in the Mössbauer spectroscopy. In this case, the recoil energy of the Zn atom is about 7.0×10^{-2} eV which corresponds to a thermal energy at a temperature 840 K, about three times room temperature. This is the reason that the Mössbauer effect can occur in crystals at room temperature. The same consideration guarantee the neutron Mössbauer effect in solids to occur for thermal neutrons (Kozima 1994b), which may have relation with CFP.

2.2 *Hydrogen Isotopes in fcc Transition Metals*

The behavior of hydrogen isotopes in transition metals has been investigated for more than 100 years and there are abundant data on diffusion and vibration characteristics of protons and deuterons in them. Several interesting features are introduced here from our point of view in relation to CFP.

There are two groups of metals in which H diffusion has been measured (Sussmann 1972). The first consists of Nb, V, and Ta and the second consists of Ni, Pd, and Ti. Sussmann et al. excluded the second group from their treatment "because the potential felt in them by the hydrogen is very different from sinusoidal," which is in the first group. This is an expression showing difference of physics of diffusion in the former *bcc* transition metals and the latter *fcc* (*hcp*) ones.

Springer (Springer 1978) explains some peculiar properties of Pd deuterides compared with hydrides. "In the *fcc* palladium lattice, hydrogen or deuterium atoms occupy octahedral sites.... The zone center frequency (in PdH_{0.63}) is more than two times lower than it is in the case of NbD_x which implies a relatively weak Pd-D interaction." "The pronounced maximum appearing in the longitudinal optic branch indicates strong second neighbor D-D interactions whose strength is comparable to the first neighbor D-D interaction."

There are contradicting facts about physical properties of Pd-H systems: In low-density samples (i.e. H/Pd ratio ≈ 0 , where diffusion experiments were usually performed), H is in rather low energy states showing large values of activation energy for self-diffusion. In high-density samples (i.e. H/Pd ratio ≈ 1 , where elastic measurements were usually performed) H-Pd interaction is comparable to H-H interaction even if H-Pd distance (2.03 Å) is less than that of H-H ($\sqrt{2} \times 2.03$ Å) and the large value of the nuclear charge $Z = 46$ of Pd.

The latter fact probably reflects the nuclear interaction between a proton and Pd nucleus, which is attractive as we can guess from nuclear property of Pd isotopes discussed in Section 2.3-1.

Puska (Puska 1984) further explains difference of *fcc* and *bcc* transition metals about hydrogen diffusion. "Our results suggest a diffusion model for hydrogen in *fcc* metals that is totally different from the one described for *bcc* metals. First we note that in the high-temperature region the diffusion activation energy in *fcc* metals is typically 0.2 - 0.4 eV, which is much more than the calculated self-trapping energies in the octahedral sites. On the other hand, according to the calculations, *self-trapping in the tetrahedral site is unprobable, and thus hydrogen would not be localized at the tetrahedral site during the activation process, but its wave function should be spread over several interstices.*"

The behavior of proton in the tetrahedral site remind us proton conductors that also show CFP as tabulated in Table 1 (Chapter 1).

Furthermore, there is a peculiarity of elastic properties in PdH and PdD. Wicke (Wicke 1978) explains strange character of interactions in them: "Consequently, Burch introduced the idea of a repulsion of H atoms on next-nearest neighbor sites, which would overcompensate the attraction of nearest neighbor H atoms at high concentrations."

It seems that characteristics of CFP tabulated in Table 1 show another difference in properties of *fcc* transition metals and *bcc* ones. From our point of view, these characteristics of *fcc* transition metals should have interrelation among them.

2.3 Energetics of Nuclides Related to CFP

It is interesting to notice that there exist stable nuclides with proton- and nucleon-number differences of $\Delta Z = 1$ and $\Delta A = 1$ and 2, respectively; A_ZX , ${}^{A+1}_{Z+1}X'$, and ${}^{A+2}_{Z+1}X''$. These nuclides correspond to absorption of proton ($\Delta Z = 1$, $\Delta A = 1$) and deuteron ($\Delta Z = 1$, $\Delta A = 2$) by the smaller nuclide, respectively. We investigate their energetics concretely in relation to CFP in this Section leaving their dynamics aside.

2.3-1}. ${}_{22}^{A_{22}}\text{Ti}$, ${}_{28}^{A_{28}}\text{Ni}$, ${}_{46}^{A_{46}}\text{Pd}$, and ${}_{78}^{A_{78}}\text{Pt}$ Group (*fcc* crystals)

First, we investigate nuclides in *fcc* transition metals where CFP occurs effectively.

The nuclide ${}^{48}_{22}\text{Ti}$ (natural abundance 73.94%) can absorb a deuteron, and ${}^{49}_{22}\text{Ti}$ (5.51%) and ${}^{50}_{22}\text{Ti}$ (5.34%) can absorb a proton to form a stable nuclide ${}^{50}_{23}\text{V}$, and ${}^{50}_{23}\text{V}$ and ${}^{51}_{23}\text{V}$, respectively. This fact may be related to experimental facts that deuterium works to produce CFP in experimental systems with Ti, especially in gas contact experiments (De Ninno 1998, Menlove 1991, Chicea 2001). We can expect also some effect of CFP in Ti-H systems.

The nuclide ${}^{62}_{28}\text{Ni}$ (3.61%) can absorb a proton to form a stable nuclide ${}^{63}_{29}\text{Cu}$. This fact may be related to experimental facts that only protium works to produce CFP in experimental systems with Ni, especially in gas-contact systems (Focardi 1994, Campari 2000). In electrolytic systems, the combination Ni/H/K is very effective to give CFP (Notoya 1993, Sankaranarayanan 1996, Swartz 1996). This shows also special chemical relation of NiH_x and K to form surface layers on the sample. CFP in the Ni-H system may be also related to the fairly large cross section of neutron absorption by ${}^{39}_{19}\text{K}$.

The nuclide ${}^{105}_{46}\text{Pd}$ (22.33%) can absorb a deuteron to form a stable nuclide ${}^{107}_{47}\text{Ag}$, ${}^{106}_{46}\text{Pd}$ (27.33%) and ${}^{108}_{46}\text{Pd}$ (26.71%) can absorb a proton to form a stable nuclide ${}^{107}_{47}\text{Ag}$ and ${}^{109}_{47}\text{Ag}$, respectively. This fact may be related to experimental facts that protium and/or deuterium work well to produce CFP

in experimental systems with Pd. The combination Pd/D(H)/Li is very popular as a system for CFP and shows special chemical relation of PdD(H)_x and Li to form surface layers on the sample. This may be also related to the large cross section for neutron absorption by ⁶₃Li.

There are a few positive data in electrolytic systems with Pt cathodes and both H₂O and D₂O (Mizuno 1998, Notoya 1998, Storms 2000).

2.3-2. ^A₂₃V, ^A₄₁Nb, ^A₇₃Ta, ^A₂₄Cr, ^A₂₆Fe, and ^A₄₂Mo Group (*bcc* crystals)

In this group where CFP occurs rarely at room temperature, there are, however, nuclei of transition metals to form stable nuclides by absorption of a proton or a deuteron.

The wave function of an occluded proton or deuteron in *bcc* transition-metal hydrides is localized around an interstitial site (cf. Section 2.2) in their ground and lower excited states and therefore has nothing to do with the proton (deuteron)-neutron interactions responsible to the neutron valence bands (cf. Section 3.2) and to CFP, from our point of view, in consistence with experimental results.

Data of nuclides shows that these *bcc* transition metals except Fe may be used for CFP *with protium and deuterium* at high temperatures where the occluded hydrogen isotopes are in higher excited states with widespread wave functions to mediate the super-nuclear interaction between neutrons in lattice nuclei (cf. Section 3.2).

One positive data with vanadium deuterides was obtained by Yuhimchuk et al. (Yuhimchuk 1992) in VD_{1.2}. They observed neutron emission proportional to background neutrons showing an effect of the latter to the former (Kozima 1996b, 1998a)

Chromium exhibits extremely low solubility for hydrogen even though a hexagonal monohydride CrH and a cubic dihydride CrH₂ are reported (Shavely 1949). There are no CFP data in chromium hydrides and deuterides. However, ⁵³₂₄Cr (9.55%) and ⁵⁷₂₆Fe (2.19%), and ⁵⁴₂₄Cr (2.38%) and ⁵⁸₂₆Fe (0.33%) can absorb a deuteron, and a proton, respectively to produce stable Mn, and Co isotopes. Therefore, the stainless steels Fe_{1-x-y}Cr_xNi_y, widely used in technology, may be responsible for CFP at high temperatures where hydrogen isotopes can permeate through them. Experimental data of CFP in the stainless steel with D₂ and H₂ in discharge experiments are reported by Dufour (Dufour 1993).

Molybdenum is responsible to CFP if it includes either protium or deuterium. There are no data of the hydride formation of molybdenum at room temperature but hydrogen isotopes permeate it at high temperature ($T \gtrsim 900^\circ\text{C}$). Molybdenum has been used in discharge systems with D_2 gas to produce tritium constantly (Romodanov 1995). In this case, temperature of the metal is very high ($\approx 3000^\circ\text{C}$).

There are another characteristic of nuclides related to neutrons in addition to those related to hydrogen isotopes discussed above. A concept *the neutron affinity* introduced by us (Kozima 1998a, cf. Section 3.4) may have a connection with the characteristic properties of transition-metal nuclei Ti, Ni, Pd, Pt and Mo. The neutron affinities of these transition metals (Ti, Ni, Pd, Pt) and *bcc* one (Cr, Fe, Mo) has positive values while those of other *bcc* ones have negative. Definition of the neutron affinity is given in Section 3.4.

2.4 *Excited States of a Nucleus Around the Separation Level (Zero Energy)*

The excited neutron states near zero energy, i.e. the threshold energy of neutron emission (or the separation energy), are not well known in nuclear physics, yet. There are several theoretical estimations and recent experimental observations about these states.

Theoretically, Weisskopf (Weisskopf 1950) has shown that a wave packet built by linear combinations of wave functions of a number of neighboring stationary excited states (neglecting any radiative transitions to lower levels) is such that they correspond to a relatively well defined grouping of particles in space with given velocities, within the limits of accuracy set by the uncertainty principle. The movement of these quasi-particles (or better, of the maxima in the square of the wave function) corresponds to a good approximation to the movement calculated by classical mechanics. If we define the period T as a time after which the initial grouping of particles re-occurs, then the time T is intimately connected with the level distance D of the states used in the linear combination: A relation between T and D (Eq. (6) of QP) is obtained for the case where the levels are equally spaced. It remains, however, qualitatively valid for more complicated systems using the average level spacing D as an indication of the period of the internuclear motion. The resulting values for the period are large, much larger for example than the ones of a one-body problem in a potential well of nuclear size. This is due to the interaction between nucleons, which makes the

motion much more involved so that the time interval between the re-occurrences of the same configuration becomes large. Therefore, these states have rather sharp energy.

Thus, we can consider the excitation levels of the nuclear system which have energies only a little below zero and the motion is periodic which gives rise to an energy quantization and to the existence of discrete, stationary states. The series of discrete energy values exist below zero, which extend above zero in an approximation.

Then, these stationary states with energies $-\varepsilon$ ($\varepsilon \ll$ binding energy B) have exponentially decreasing parts of wave functions expressed by Eq. (7) of QP with a damping factor $\eta \approx \eta(|\varepsilon|)$.

There is another approach to this problem. The wave function Eq. (7) of QP corresponds to a structure in elastic scattering cross-sections of slow neutrons as shown by quantum mechanics: For a slow neutron with an energy $E (\geq 0)$, the elastic scattering cross-section is given by a formula (Landau 1965) Eq. (8) of QP with a parameter $-\varepsilon$, the energy of a level below zero. The wave function of the neutron with an energy $E = -\varepsilon$ is expressed as Eq. (9) of QP. This shows the damping factor $\eta \equiv \eta(|\varepsilon|)$ in the Eq. (7) of QP is $\sqrt{(2m|\varepsilon|)/\hbar}$.

Experimentally, investigation of the energy levels close to zero has recently started in relation to experiments to check parity violation in neutron resonances of palladium (Crawford 1998, Smith 2002). It should be also noticed that the neutron halo of extremely neutron-rich nuclei is recently observed in small mass number nuclei (Hansen 1987, 1993). Its wave functions spread out to distances far away from the binding potential as Kim et al. (Kim 1996a) have investigated for loosely bound systems. For medium mass number nuclei, the neutron halo probably exists even though it has not been observed yet.

These theoretical and experimental results about shallow levels below zero suggest that wave functions of neutrons with energies near zero in Ti, Ni, Pd (and Pt) may spread out from nuclei and contribute to CFP as investigated in the next Chapter.

3. NEUTRON BANDS AND CF-MATTER IN *fcc* TRANSITION-METAL HYDRIDES AND DEUTERIDES

- 3.1 *Perturbation treatment of many-body system*
- 3.2 *Neutron valence band in fcc transition-metal hydrides and deuterides*
- 3.3 *Energetics of neutron drops*
- 3.4 *The Neutron Affinity*
- 3.5 *The cf-matter –neutron drops in thin neutron gas formed in solids*
- 3.6 *CFP or nuclear reactions induced by neutron drops in the cf-matter*

In this Chapter, we give a semi-quantitative treatment of neutron valence bands, one of new characteristics in *fcc* transition-metal hydrides (deuterides), formed below zero composed of excited states of neutrons in lattice nuclei by mediation of occluded hydrogen (deuterium) in a PdH (PdD) crystal. Then, we show appearance of neutron drops at boundary/surface regions due to the local coherence of neutron Bloch waves realized by a characteristic of the bands.

The proton (deuteron) band in *fcc* transition metals as explained in Section 3.2 is a common characteristic of *fcc* transition-metal hydrides (deuterides) and proton conductors where CFP has been observed. On the other hand, the neutron-nuclide A_ZX reactions without the Coulomb barrier are a well-known fact in nuclear physics. Combining these two factors in solid-state physics and nuclear physics, we can show a possible occurrence of CFP in *fcc* transition-metal hydrides and deuterides and in proton conductors. We confine our investigation to *fcc* transition-metal hydrides (deuterides) in this Chapter.

3.1. *Formulation of Perturbation Treatment of Many-Body System in fcc Transition-Metal Hydrides and Deuterides*

A system composed of lattice nuclei and occluded hydrogen isotopes is semi-quantitatively investigated in this Section by the second-order perturbation approximation using a data obtained in nuclear physics and solid state physics explained in Chapter 2.

3.1-1. *Neutron Wave Functions in Lattice Nuclei*

Let us consider a neutron in one of excited states $\{n\} \equiv (n, l, m, s)$ (with an energy $E_{(n)}$) of one of lattice nuclei at a_i given by Eq. (10) of QP.

Neutron wave functions $\phi_{\{k,s\}}(\mathbf{x})$ in a crystal are expressed in the single-particle approximation as a linear combination of wave functions (Eq.

(10) of QP) where the regularity of the crystal lattice determines the coefficients of the linear combination as required by the Bloch's theorem (Mott 1958). Thus, $\psi_{\{k,s\}}(\mathbf{x})$ is expressed by a neutron Bloch function with a band structure in its dispersion relation as Eq. (11) of QP.

The concept of the neutron band, and therefore the neutron Bloch waves is applicable as far as experimental results (Ebisawa 1998) show and theoretical expectation of weak interaction between neutrons suggests it.

3.1-2. Proton (Deuteron) Wave Functions in fcc Transition-Metal Hydrides and Deuterides

The dynamical behavior of a proton (deuteron) occluded in fcc transition-metal hydrides (deuterides) is described as a harmonic oscillator in its ground and lower excited states (Sicking 1972) or rather as a proton (deuteron) Bloch state with a wave function spread over several interstices during activation processes (Puska 1984). The proton-neutron interaction differs from the deuteron-neutron interaction and therefore we have to treat two cases separately, in principle. In this paper, however, we consider only the proton-neutron interaction semi-quantitatively and the deuteron case is considered implicitly to be treated in another chance.

Let us write these localized wave functions of a proton as $\phi_{\{p\}}(R-b_j, \sigma)$ in a state $\{p\} \equiv (n_p, l, m, s)$ (with an energy $\varepsilon_{\{p\}}$) at an interstice b_j of a rigid lattice. The wave functions may have finite probability density at a nearby lattice point a_i , a nearest neighbor of b_j as expressed by Eq. (12) of QP.

If we ignore the mutual interaction of Z protons on different interstices, the total proton wave function may be expressed as a product of wave functions on the interstices (neglecting anti-symmetrization) as Eq. (13) of QP.

When the proton (deuteron) is in its extended Bloch states, we have to use Bloch functions $\phi_{\{B\}}^{(b)}(R)$ expressed as Eq. (14) of QP corresponding to Eq. (11) of QP for neutron wave functions instead of Eq. (12) itself of QP.

It should be noticed a following fact of the single-particle approximation. The ion-band state should not be understood as a state where two or more ions are overlapping to interact at a point. Instead, this state means there is a situation where the single-particle approximation applicable (Pines 1952). This means that two protons (deuterons) can be treated as independent particles in solids as a result of many-body interactions including electrons

and lattice nuclei together with protons (deuterons).

3.1-3. *Total Wave Function*

Therefore, the total wave function of a system composed of a neutron Bloch wave $\phi_{\beta}(r)$ and Z occluded protons in the state $\{p_{\alpha}\} \equiv \{p_1, p_2, \dots, p_z\}$. at interstices is expressed as (omitting spin parts) Eq. (15) of QP.

3.1-4. *Neutron-Proton (Deuteron) Interaction in fcc Transition-Metal*

The overlapping of the proton wave function $\phi_{\{j\}}(R_j - b_j)$ (Eq. (12) of QP) on an interstice at b_j with a nucleon (neutron) wave function $\phi_{\{i\}}(r - a_i)$ (Eq. (10) of QP) on an adjacent lattice nucleus at a_i results in a proton-neutron interaction through the nuclear force. The nuclear interaction is expressed by a potential whose form is taken, for example, as the square-well type (neglecting spin-dependence and the imaginary part):

$$\begin{aligned} V_s(r-R) &= -V_s^{(s)}_0, \dots (|r-R| < b) \\ &= 0, \dots (|r-R| > b) \end{aligned}$$

where $V_s^{(s)}_0 \approx 3.5$ MeV and $b \approx 2.2 \times 10^{-13}$ cm (Blatt 1952). The choice of this potential out of several possible types does not make a large difference to the result for the low energy phenomena we are considering in this paper.

This interaction pulls two neutron states in different lattice nuclei into coupling as shown below. We will call this coupling the "super-nuclear interaction." In the following investigation, we concentrate on excited neutrons rather than on protons in lattice nuclei, which need more energy to be raised to the excited levels due to the fact $Z \ll N$. (In Pd, $Z = 46$ and $N = 56 - 64$.)

3.1-5. *Total Energy of fcc Transition-Metal Hydrides and Deuterides*

In the second-order perturbation approximation taking the square well potential (Eq. (16) of QP) for the nuclear interaction, the total energy $E_{k,\{p_{\alpha}\}}$ of this system composed of occluded protons (deuterons) and a neutron in an excited level of lattice nuclei expressed as a Bloch state is expressed as Eqs. (17) and (18) of QP.

In the calculation of the matrix elements (Eq. (21) of QP), we used simplification that the neutron wave functions (Eq. (10) of QP) was

expressed as the Dirac delta-function (Heitler 1954).

An order of magnitude estimation of the effective potential energy $v_{np}(ii'j)$ for PdH is, then, semi-quantitatively calculated using following simplifications; the proton wave function $\phi_{\{p\}}(R)$ is slowly varying in the range of the nuclear force, and the nuclear wave function $\phi_{\{n\}}(r)$ is approximated by a delta-function as given in the Eq.(22) of QP. Then, an order of magnitude of the matrix elements $\langle n p; ij | V | n' p'; ij \rangle$ is given as Eqs. (24) and (25) of QP giving

$$|\langle n p; ij | V | n' p'; ij \rangle| \approx = 3.2 \times 10^{-14} \quad \text{eV.}$$

3.1-6. *Level Density of Excited Nucleon States in a Nucleus*

The result of the calculation of the total level density for the Fermi gas in a nucleus ${}^A_Z X$ is given as follows (Bohr 1969) and used for an order of magnitude estimation of $\rho_n(E)$ given by Eq. (26) of QP.

A high density of nuclear levels at high excitation energies, amounts of the order 10^6 times higher than that corresponding to single-particle motion, has been revealed by densely spaced, sharp resonances in slow neutron capture reactions (Tsukada 1966) giving experimental verification of the formula (26) of QP. This fact results in formation of a compound nucleus in a nucleus with $A \approx 100$ (Bohr 1969). To take this fact into our consideration of level densities to be used in this paper, let us assume a factor α (an enhancement factor) to give a level density at around zero level including collective modes as $\alpha g(\epsilon)$ multiplying to the single particle level density $g(\epsilon)$. Then, the experimental data (Tsukada 1966, Bohr 1969) shows that we may take the maximum value of α as $\alpha_{\max} \approx 10^6$.

The single-particle level spacing of excited levels near zero in several nuclides has been investigated recently (Smith 2002) in relation to parity violation in neutron resonances. It was shown that the level spacing in the 10 to 100 eV energy regions for the heavy even-even nuclides are about 20 eV. So, we might be able to take it as 20 eV for our general discussion of excited bound levels around zero, considering a relationship of scattering cross-sections and bound levels (Landau 1965). Then, the level density as a whole at around the separation level may be taken as $10^2 \alpha / \text{keV}$ taking into account of collective modes giving a factor α for the level density ($\alpha_{\max} = 10^6$) even if applicability of Eq.(26) of QP and discussions following it to this case are not clear at present.

The figure $10^2 \alpha / \text{keV}$ might be several times larger at most by the separation of a level by the weak interaction where values of matrix elements are $1 \approx 2 \text{ meV}$ (Smith 2002). In the following discussion, we will use the level density of $\alpha g(\varepsilon) = 10^3 \alpha / \text{keV}$ in Subsection 3.2-3 taking this fact into our consideration.

3.1-7. *Width of Neutron Valence Band in fcc Transition-Metal*

To show briefly the crystal-structure dependence of the bandwidth Δ of the neutron valence band, we will make a simplification of the super-nuclear interaction (Eq. (18) of QP) between adjacent nuclei at a_i and a_i' assuming that it depends only on the magnitude of the vector $a_i \equiv a_i - a_i'$.

Then, we can rewrite the total energy (Eq. (17) of QP) and have energy spectrum of the neutron Bloch waves in the fcc lattice (a is the side of the lattice cube) (Mott 1958) as given by Eq. (29) of QP.

The energy level shifts from $E_{\{n,p\}}$ by $-\gamma_{n,p}$, which may be negative in appropriate situations. A characteristic of this energy band formation is the contributions from nearest neighbors ($(0, \pm a/2, \pm a/2)$, etc.) and also from next nearest neighbors ($(\pm a, 0, 0)$, etc.) to the k -dependent terms.

The neutron energy bands originating in the excited states of lattice nuclei are energetically located below zero in contrast to those originating in free neutron states above zero worked out in a previous paper (Kozima 1998b). The former could be called the *neutron valence band* and the latter the *neutron conduction band* to distinguish them in the following discussion of nuclear reactions in solids.

We obtain a semi-quantitative estimation of the bandwidth Δ of the neutron valence band as Eq. (31) of QP:

$$\Delta_{n,p} = 24 v_{np}(\text{ii}'\text{j}).$$

3.2. *Calculation of Neutron Valence Band in fcc Transition-Metal Hydrides and Deuterides*

There are two factors to magnify the band width Δ in *fcc* transition-metal hydrides and deuterides, i.e. in *CF materials*, in their excited states: i) excited neutron states near zero largely extending outward that makes matrix elements (Eq. (21) of QP) larger, ii) wide-extended excited proton (deuteron) states at tetrahedral interstitials $0.2 - 0.3 \text{ eV}$ higher than

octahedral interstitials (Puska 1984). Here, we show the effects of these two factors on the neutron valence band.

3.2-1. *Excited Neutron States near Zero Energy.*

As discussed in Section 2.4, we can determine possible wave functions of neutrons in excited states at and below zero energy (the separation level) using two methods: wave functions suggested by neutron scattering cross sections (Landau 1965) and wave packets of neutrons in excited bound levels in a semi-classical model (Weisskopf 1950). Thus, wave functions of the neutron with an energy $E = -|\epsilon|$ near zero are expressed as Eq. (9) of QP:

$$\xi(\mathbf{r}) = \text{constant} \times \exp(-r\sqrt{(2m|\epsilon|)/\hbar}).$$

Therefore, when the energy E of the state is less than but close to zero, the wave function of a neutron in a nucleus ${}^A_Z\text{X}$ outside the nucleus is approximated by Eq. (32) of QP.

In general, excited nucleon states have finite lifetime in an isolated nucleus. It should be pointed out, however, that there is a possible stabilization of the excited states when they are coupled with each other mediated by occluded hydrogen isotopes to have long-range coherence as discussed in Section 3.3.

3.2-2. *Excited States of Proton (Deuteron) in CF Materials (fcc Transition-Metal Hydrides and Deuterides)*

When the occluded proton (deuteron) is excited to a $0.2 \approx 0.3$ eV higher tetrahedral site from a octahedral site by some causes (e.g. excitation by energies liberated by nuclear reactions between neutron drops (Kozima 2000a) and other nuclei), the wave function $\phi_{\{p\}}(\mathbf{R}-\mathbf{b}_j)$ of the proton (deuteron) becomes not localized and its wave function should be spread out over several interstices (Puska 1984) and overlapping with the neutron wave function $\phi_{\{n\}}(\mathbf{x};\mathbf{a}_i)$ increases; Eq.(14) of QP becomes rather appropriate than Eq.(12) of QP to express a proton wave function in these cases. When the $\phi_{\{p\}}(\mathbf{R}, \sigma)$ is an appropriate wave function to express a proton (deuteron) in a crystal, neglect of spins in Subsection 3.1-3 becomes not inadequate. The summation on (i,i') in Eq. (17) of QP on the super-nuclear interaction (Eq. (18) of QP) should, then, be extended over whole lattice points making neutrons in all lattice nuclei to couple together with the interaction with a proton (deuteron).

Thus, when the proton (deuteron) wave function is not localized around an interstice, the matrix elements Eq. (21) of QP becomes very large by an enhancement factor β^2 approximately given by a square of a ratio $|\phi_{\mathbf{k}}(\mathbf{x}_N)/|u_n(\mathbf{x}_N)| \equiv \beta_n$ ($n = 2, 3, \dots$), the maximum value of which is roughly calculated as 10^{10} for $n = 3$ by plane wave approximation for the wave function $\phi_{\mathbf{k}}(\mathbf{R})$, i.e. $\beta_{\max} = 10^{10}$, $\beta_{\max}^2 = 10^{20}$. $u_n(\mathbf{R})$ is a harmonic oscillator wave function for the proton (deuteron) wave function (Eq. (12) of QP) and \mathbf{x}_N is the lattice point nearest to the interstitial where is $u_n(\mathbf{R})$; $|\mathbf{x}_N| = 1.95\text{\AA}$ (PdH).

The plane wave approximation to calculate $\phi_{\mathbf{k}}(\mathbf{x}_N)$ surely overestimate the value β_n and the use of delta-function approximation for nuclear wave function underestimate the matrix elements (Eq. (21) of QP) in the band width calculation and are in the direction to cancel each other. Estimation with those approximations may be allowable for our semi-quantitative discussion of such an extremely complicated system as transition-metal hydrides (deuterides) composed of lattice nuclei and occluded protons (deuterons) we are treating.

3.2-3 Matrix Elements of Super-Nuclear Interaction and Band Width

Thus, the matrix elements (Eq. (21) of QP) calculated for neutron states around the separation level and proton (deuteron) states of Bloch functions are at most 10^{20} times larger than the value calculated for a lower excited state of a neutron in nucleus and a localized state of a proton (deuteron).

Finally, the effective potential $v_{np}(ii')$ (Eq. (18) of QP) except enhancement factors α and β is calculated as a function of the principal value of the integration appeared in that equation using Eq.(25) of QP and assuming the insensitiveness of the matrix elements to the energy as Eq. (33) of QP:

$$v_{np}(ii') \approx 1 \times 10^{-27} I \quad (\text{eV}^2),$$

$$I \equiv P \int (\rho_n(E)/E) dE,$$

where the integral is from $-\infty$ to $+\infty$ and P represents the principal value is taken in the integral.

We can, then, estimate the approximate value of the integral (principal value) I , taking following values $\rho_n(E) \approx 10^3 \text{ keV}^{-1}$, $\delta \varepsilon \approx 10^{-3} \text{ keV}$, and $\Delta \varepsilon \approx 1 \text{ keV}$ on the assumption that single-particle energy-level difference is

≈ 1 keV and the level density increases to 10^3 times larger than that of single particle motion (Eq. (34) of QP):

$$I \approx (\rho_n(\epsilon) / \delta \epsilon) \Delta \epsilon = 10^6 \text{ eV}^{-1}.$$

Thus, an order of magnitude of $v_{np}(ii'j)$ in PdH becomes

$$v_{np}(ii'j) \approx 1 \times 10^{-24} \text{ (eV)}.$$

Including the enhancement factors, we obtain final result:

$$v_{np}(ii'j) = 10^{-24} \alpha^2 \beta^2 \text{ eV},$$

where $\alpha_{\max}^2 = 10^{12}$ and $\beta_{\max}^2 = 10^{20}$.

Putting the value $v_{np}(ii'j) \approx 10^{-24} \alpha^2 \beta^2 \text{ eV}$ in $\Delta_{n,p}$ above, we obtain the bandwidth Δ as follows (Eq. 37) of QP):

$$\Delta_{n,p} \approx 2.5 \times 10^{-23} \alpha^2 \beta^2 \text{ eV}$$

with an enhancement factor α for the level density of neutrons in a nucleus (defined in Section 3.1-6) and an enhancement factor β for the probability amplitude of a proton (deuteron) wave function at a lattice nucleus (defined in Section 3.2-2).

The value of the bandwidth $\Delta_{n,p} \approx 2.5 \text{ GeV}$ for $\alpha_{\max} = 10^6$ and $\beta_{\max} = 10^{10}$ is obtained by the assumption that the level density at excited levels around the separation energy is similarly strongly magnified by collective modes as observed by neutron resonance absorption experiments (Tsukada 1966) and plane waves for excited proton states. The first assumption has no experimental bases at present and seems too exaggerating the situation to be real. We may assume rather small factor as $\alpha = 10^2$ or 10^3 instead of 10^6 (Tsukada 1966, Bohr 1969). Then, the bandwidth may have a value about $1 \approx 10^2 \text{ eV}$ for $\beta_n = \beta_{\max}$.

The assumption, on the other hand, of a plane wave for the proton (deuteron) Bloch state ($\beta_n = 10^{10}$) may overestimate the matrix elements (Eq. (21) of QP) by several orders of magnitude making the bandwidth down to $10^{-2} \approx 1 \text{ eV}$ if we take $\beta_n = 10^8 - 10^9$.

If the bandwidth Δ is less than the thermal energy ≈ 25 meV of ions at room temperature, the neutron band structure may be not realistic and the neutrons should be treated as localized at lattice nuclei. This requires $\alpha^2 \beta_n^2 \geq 10^{21}$ for a realistic neutron valence band. This means that the parameters to realize the neutron valence band should be $\alpha \geq 10^{5.5}$ for $\beta_n = 10^5$ and $\beta_n \geq 10^7$ for $\alpha = 10^3$.

3.3. *Energetics of Neutron Drop*

It was known since 1932 when the neutron was discovered as a kind of nucleons, a component particle of nucleus, that they are attracting each other and also with protons, another nucleon. Astonishingly enough, we have been shown existence of such exotic nuclei as ^{10}He , ^{11}Li , ^{32}Na , and so forth recently by scattering experiments in nuclear physics (Hirata 1991, Tanihata 1992, Korshennikov 1994, Suzuki 1995). This is an evidence of very strong attraction not only between neutron and proton but also between neutrons in nucleus where their density is very high.

The same situation will be realized even in solids to form neutron-proton (deuteron) clusters and finally neutron drops (clusters of neutrons containing several protons in it) in the solids when the density of neutrons becomes high enough at boundaries (Kozima 2000a, 2000c) where average distance between neutrons is the same order of the force range of the strong interaction. It is rather probable that formation of a neutron-proton (deuteron) cluster and further a neutron drop occurs like condensation of molecules in a gas into a liquid or a solid where the density of molecules differs by a factor $\approx 10^4$. The possibility of such a situation of high neutron density in solids is pointed out by us (Kozima 2000a).

The density of the nuclear matter in the nucleus, or number density n_A (cm^{-3}) of nucleons in the nucleus, is well defined quantity in nuclear physics (Fermi 1950, Blatt 1952) and is given by Eqs. (38) and (39) of QP:

$$\begin{aligned} n_A &= A/(4\pi R_A^3/3) = 7.07 \times 10^{37} \quad \text{cm}^{-3}, \\ R_A &= 1.5 \times 10^{-13} A^{1/3} \quad \text{cm}, \end{aligned}$$

where R_A is the radius of a nucleus with a mass number A .

Another consideration can be added to show possible formation of the neutron drop. Local coherence of the trapped neutrons in the

boundary/surface layer (Kozima 2000c) makes the neutron density in this region very high; if the density of the trapped neutron is as high as 10^{12} cm^{-3} determined in several situations observed in CF experiment, the local coherence makes the probability amplitude of whole neutron as high as 10^{12} times that of a single neutron in the coherent region of a thickness $10a$ where a is the lattice constant of the metal, or $\approx 30 \text{ \AA} = 3 \times 10^{-7} \text{ cm}$. If we assume whole neutrons in a unit volume accumulate in this region, the effective density in coherence becomes very high as $(10^{12})^{2/3} \times 10^{-7} \text{ cm}^{-3} = 10^{31} \text{ cm}^{-3}$. This is fairly large value expected in the outer region of the neutron halo of exotic nuclei and we can expect effect of neutron-neutron interaction to form a neutron drop. For this process to occur, existence of hydrogen isotopes with an appropriate density is an inevitable necessary condition and will work positively as shown by successful experiments in CFP.

Interesting works related with neutrons in solids were performed about 30 years ago in relation with the problem of theoretical verification by simulation of the neutron star (Baym 1971, Negele 1973). When there is a neutron liquid with densities more than 10^{35} cm^{-3} , there appears a so-called Coulomb lattice of clusters of neutrons and protons (and electrons) with a definite lattice constant as a stable state. The lattice constant and proton to neutron ratio \underline{x} in a cluster decrease with increase of the neutron density and finally stable homogeneous distribution of pure neutrons are realized as a neutron star at densities more than about 10^{38} cm^{-3} . If we extrapolate the result of their simulation to lower density region of about 10^{30} cm^{-3} attainable in surface layers of solids (Kozima 2000c), we obtain a Coulomb lattice with a lattice constant about 10^{-3} \AA and almost the same proton to neutron ratio \underline{x} to that of Pd nuclei as shown in Table 2 of QP (Kozima 2002).

This possibility will be enhanced by formation of the neutron Cooper pair (Kozima 1998a), a boson, which is favorable to form a cluster because of probable Bose-Einstein condensation.

3.4 *The Neutron Affinity*

Let us assume that the neutron Bloch wave transforms into a proton Bloch wave when it suffers a β -decay. Furthermore, let us estimate the stability of the neutron wave interacting with a nuclide ${}^A_Z\text{X}$ with a *neutron affinity* η defined by a following relation;

$$\eta \equiv -(A+1_Z X - A+1_{Z+1} X) c^2.$$

Here, c is the light speed in vacuum, $A_Z X$, in this formula, is the mass of the nuclide with a nucleon number A and a proton number Z composing the lattice nuclei.

This definition tells us that the neutron affinity is a quantity expressing an energy difference of two nuclear states, one with an extra neutron and the other with an extra proton. The positive value of η means the former is in lower energy than the latter and is more stable. Therefore, the neutron Bloch wave interacting with lattice nuclei with a positive neutron affinity is stable for a β -decay, in the meaning of the above assumption.

Looking into a table of the neutron affinities (Kozima 1998a), we know all lattice nuclei in CF materials have positive values of the neutron affinity if there obtained positive results in them. Typical transition metals are Ti, Ni, Pd, Pt and Mo (cf. Table 1 and Section 2.3).

3.5 *The CF-Matter – Neutron Drops in Thin Neutron Gas Formed in Solids*

Neutrons in solids are not fully investigated until now perhaps because of its short lifetime of about 887 seconds in free space (Case 1998). However, the wave nature of the low energy neutron has been used more widely in technology (the neutron guide and others) and science (the neutron trap to study nature of neutrons). From our point of view, however, the research is in infantile stage and we have much to study neutron physics in solids, especially *fcc* transition-metal hydrides and deuterides.

Thus, we can expect new states of neutrons in transition-metal hydrides and deuterides when there is an optimum situation where several conditions are fulfilled to realize the neutron valence bands below zero as discussed above and also expect new phenomena related to the neutron valence band.

It should be added several words to the states of neutrons in the boundary/surface regions in solids. At boundaries/surfaces of a crystal, there is aperiodicity of the crystal lattice and disturbance to the neutron Bloch waves. There appear new states due to the disturbance such as surface states different from the Bloch states with different energies. We ignore, however, occurrence of these states in this paper and confine our investigation to the neutron Bloch waves.

3.5-1 *Local Coherence of Neutrons and Surface Reaction of Trapped Neutron*

When there are many neutrons in a neutron band, there appear interesting features of neutron behavior at boundary/surface regions that reflect neutrons back into the original region of the crystal; the *local coherence* of neutron Bloch waves appears there due to almost the same energies and slightly different wave number vectors (Kozima 1999a). Neutrons thus accumulated in boundary/surface layers by the local coherence tend to form stable neutron drops stabilizing themselves (Kozima 2000a).

Some properties of the neutron drop can be investigated on the evaporation model of nuclear reaction (Blatt 1952). In an equilibrium state, evaporation and condensation are reverse processes in balance and the same situation is also in quasi-equilibrium state in CFP (Kozima 2000a).

As was noticed in Chapter 1, there are many evidences of nuclear reactions in CFP difficult to explain without participation of neutrons, including those called decay-time shortening and NT in surface layers of metal electrodes in electrolytic systems and in surface regions of cathodes in discharge systems. In the TNCF model, this fact is taken into the model by the instability factor ξ of the trapped neutron assuming a value 1 ($\xi = 1$) in the surface layer and another 0.01 ($\xi = 0.01$) in volume (Kozima 1998a, 1999a).

3.5-2 *Condensation of Neutrons – Formation of CF-Matter*

Neutrons thus accumulated in boundary/surface layers by the local coherence interact with each other and with protons/deuterons through the nuclear force losing the single-particle nature and may tend to form the cf-matter, i.e. neutron drops (Kozima 2000a) in a thin neutron liquid stabilizing themselves as shown by a simulation calculation in the neutron star matter (Negele 1973) where appear the Coulomb lattice of the neutron-proton clusters (neutron drops in our terminology). This formation of stable neutron states in solids is a characteristic of the system of lattice nuclei in *fcc* (*hcp*) transition-metal hydrides/deuterides (and proton conductors).

Even if the excited neutron states in lattice nuclei are unstable, neutrons entered into the neutron band instantaneously become stable forming neutron drops in the boundary/surface regions and accumulate there. The

cf-matter, i.e. neutron drops in a thin neutron gas at boundary/surface regions may interact with exotic nuclei there to induce new kinds of nuclear reactions in the boundary/surface region that may be observed in phenomena such as the cold fusion phenomenon (CFP) in *fcc* and *hcp* transition-metal hydrides and deuterides (Fleischmann 1989, Kozima 1997, 1998a).

Thus, the role of hydrogen isotopes in the CFP is, from the viewpoint of our model, (1) to establish the trapping condition of thermal neutrons by inhomogeneous distribution in solids, (2) to participate in reactions with neutrons and each other if accelerated by energetic particles, (3) to mediate super-nuclear interaction between neutrons, and (4) to participate in formation of the neutron drop in the boundary/surface regions where appears the local coherence of neutron Bloch waves.

3.6 CFP or Nuclear Reactions Induced by Neutron Drops in CF-Matter

Nuclear reactions between neutron drops and other nuclei are essentially the same to those occur in free space except new dissipation channels of surplus energies. In free space, isolated nuclei in their excited states can mainly de-excite emitting a gamma photon, or alpha or beta particle in the case of radioactive nuclei. However, in the case of CF materials, the surplus energies can be effectively dissipated (or carried away) by surrounding neutron drops and a thin background neutron gas. This results in gammaless nuclear reactions and decay-time shortening in CFP. When there occurs nuclear fission of a nuclide with a large excess number of neutrons formed by interaction with a neutron drop, the reaction becomes mild by the interaction of surrounding neutron drops thus emitting no high-energy neutrons.

4. CONCLUSION

The cold fusion phenomenon (CFP), which is perplexing and puzzling from conventional points of view in nuclear physics and solid-state physics, is explained as a phenomenon of solid state-nuclear physics where new states of neutrons play essential roles to induce nuclear reactions different from those in free space. It seems that the realization of the neutron valence band is a form of self-organization in complex chaotic systems, *fcc* (*hcp*) transition-metal hydrides and deuterides (and proton conductors).

CFP was explained, for the first time, consistently by phenomenological

models, the TNCF and the neutron drop models. The neutron drop model assumes neutron drops ${}^A_Z\Delta$ made of Z protons and $(A-Z)$ neutrons in the thin neutron gas, which is formed in the cf-matter at boundary/surface regions.

The working concept, the cf-matter, is defined as "the field where the CFP occurs in CF materials." This is used to explain complex events in the CFP. It became clear through the investigation in this paper that the cf-matter is spread over CF materials in general. At boundary/surface regions, the cf-matter contains high-density neutron drops in a thin neutron gas while in the volume it contains only a few of them in accordance with experimental data.

The neutron drop ${}^A_Z\Delta$ interacts with a nucleus A_ZX to accelerate the decay process of A_ZX if it is unstable or to give ν neutrons and ν' protons to A_ZX ($\nu, \nu' = 0, 1, 2, \dots$) thus inducing nuclear transmutations (NT). Especially, an explanation of mass spectra of nuclear products observed in CFP (e.g. Miley 1996) can be explained as fission products of unstable nuclides ${}^{A+\nu+\nu'}_{Z+\nu}X'$ formed by the above process as done by Fisher using a hypothetical polyneutrons (Fisher 1998).

A brief microscopic scenario for these phenomenological models is given as follows. Formation of neutron valence bands in *fcc* transition-metal hydrides and deuterides was shown using relevant knowledge in nuclear physics and in solid-state physics. Excitation of occluded protons (deuterons) from ground octahedral sites to excited tetrahedral sites with spatially extended wave functions, on one hand, and excitation of neutrons in lattice nuclei to excited states near zero with spatially extended wave functions, on the other, make the state favorable for the neutron valence bands.

Trigger reactions between trapped thermal neutrons in neutron conduction and/or valence bands and exotic nuclei A_ZX liberate energy which is used for the excitation of occluded hydrogen isotopes to higher energy levels and also for the excitation of neutrons in lattice nuclei to levels near zero.

Then, the local coherence of neutron Bloch waves at boundary/surface regions of a sample enhances the density of neutrons at these regions, making the density of the thin neutron gas higher there. Formation of the cf-matter, neutron drops in the thin neutron gas, is realized by the local coherence in neutron valence bands at boundary/surface regions. It is

possible deuterides are favorable for the cf-matter formation than hydrides due to the existence of a neutron in a deuteron unless other conditions differ so much. In the process of the cf-matter formation, such concepts related with neutrons in solids as neutron Mössbauer effect (Kozima 1994b) and the neutron affinity (Kozima 1998a) may work positively.

The neutron drops ${}^A_Z\Delta$ make specific reactions in CF material possible: (a) Rare emission of gamma rays in CFP means that main decay channels of excited states of a nucleus in CF materials are through neutron drop-nuclear interactions rather than intranuclear conversions such as in free space. (b) Various nuclear transmutations of nuclides become possible in the cf-matter through multi-nucleon transfer to nuclides: NT_D , NT_F , NT_A are explained by absorption of ν neutrons by a nuclide A_ZX ($\nu \geq 1$); $\nu = 1$ for NT_D accompanied by decays, $\nu \gg 1$ for NT_F accompanied by fissions, and ν and $\nu' \geq 1$ for NT_A with ν' a number of protons absorbed simultaneously with neutrons. Frequent observation of Fe in CFP might be explained by transitions of neutron drops ${}^A_Z\Delta$ into stable nuclides A_ZX in the cf-matter.

Only one characteristic of the neutron wave function in excited states and one of the proton (deuteron) wave function in *fcc* transition-metal hydrides (deuterides) were taken up in Chapter 3 to show possible formation of the neutron valence band even though other characteristics pointed out in Chapter 2 should be relevant to CFP.

Several crucial factors not properly treated yet are as follows: (1) the first is spin-dependence of nuclear interactions, (2) the second is the effect of the imaginary part of the neutron-nucleus interaction resulting in absorption of neutrons by lattice nuclei not considered in our treatment, (3) neglect of hybridization of wave functions $\psi_{\{n\}}(x, a_i)$ with different $\{n\}$'s in band formation, and (4) the fourth is the difference in the proton-neutron and the deuteron-neutron interactions on the super-nuclear interaction. (5) The fifth is correct wave functions of occluded protons and deuterons at their excited band states. (6) The sixth is the thermal motion of lattice nuclei which will make the band structure blur unless the super-nuclear interaction is strong enough to overcome the effect of the thermal motion. (7) The seventh is the surface states of neutrons at boundaries different from the Bloch states taken up in this paper. (8) The eighth is roles of electrolytes in formation of surface layers with extraneous composition from matrices of cathodes in electrolytic systems. These factors should be properly considered to make the

estimation given in this paper more quantitative.

The spin-dependence of the nuclear interaction between neutron and proton (deuteron) will be detected as reinforcement of CFP when spins of occluded protons (deuterons) are polarized by the proton-spin (deuteron-spin) polarization technique.

We can add several words on application of CFP. Realization of necessary and sufficient conditions for creation of the cf-matter in solids is subtle problem depending on many factors such as neutrons in excited states of lattice nuclei and protons (deuterons) in excited states in solids, as shown in this paper theoretically. On the other hand, realization of CFP is with the qualitative reproducibility and sporadicity, experimentally. If we know how to realize the optimum condition in samples, however, it will be possible to use CFP for such applications as energy generation, nuclear transmutation, acceleration of nuclear decay process, and so forth with high efficiencies. Elucidation of physical mechanisms of CFP will help to attain this goal.

ACKNOWLEDGEMENT

The author would like to express his heart-felt thanks to John Dash of Portland State University, USA. Many collaborators have worked with him during these more than ten years.

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