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Local coherence, condensation and nuclear reaction of neutrons at crystal boundary of metal hydrides and deuterides

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Abstract

Using a concept of the neutron Bloch wave in the one-body approximation presented previously, possibilities of the following effects in boundary regions of crystals including hydrogen isotopes are pointed out: occurrence of local coherence, formation of a neutron Cooper pair, condensation of neutrons, formation of neutron drop and an effective nuclear reaction of a nucleus with thermal neutrons. It is shown that these new states and reactions will have strong effects on solid state-nuclear physics in metal hydrides (deuterides). The stochastic occurrence of localized nuclear reactions observed in CF experiments is explained by these properties of the trapped neutron. The possible application of the nuclear reactions in metal hydrides is discussed. © 2000 International Association for Hydrogen Energy. Published by Elsevier Science Ltd. All rights reserved.

Keywords: Nuclear reaction; Neutron band; Neutron Bloch wave; Local coherence; Neutron-nucleus reaction; Condensation of neutrons; Neutron drop

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1. Introduction

In the preceding paper [1], it was pointed out that a thermal neutron in appropriate crystals can have an energy spectrum with a band structure in the one-body approximation. This is a natural conclusion from the wave nature of quantum mechanical objects common to the electron, photon, neutron and others but has been overlooked for a long period with regard to the neutron due to its short decay time in free space of 887.4 ± 1.7 s.

Over the past 30 years, various aspects concerning diffraction patterns of the neutron have been developed after the work of C.G. Shull [2] on the Pendellösung fringe structure in neutron diffraction. The dynamical theory of diffraction was applied to such cases of neutron scattering as neutron interferometry [3], the change of sign of the neutron wave function in a 2π precession [4], the effect of the Earth's rotation on the quantum-mechanical phase of the neutron [5] and the effect of gravity (or of a magnetic field) on the propagation of neutrons within the perfect, single-crystal silicon slabs [6].

In the same line of investigation, properties of the cold neutron in solids with artificial potential wells have been used [7] to investigate external effects on the

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phase of neutrons using such quantum mechanical characteristics of neutrons as trapping and tunneling in and through potential walls similar to those of the electron and photon.

In the case of thermal neutrons, their periodic potential is provided by a natural crystal lattice instead of an artificial one for the cold neutron and band structure in the energy spectrum of neutrons is realized as illustrated by a simple calculation in the one-dimensional Kronig-Penny model [1].

One the other hand, neutrons in the nucleus have shown exotic features revealed by scattering experiments [8–11]. Existence of exotic nuclei far from the stability line, like ^{10}He, ^{11}Li, ^{32}Na, and so on, were observed and an explanation [12] has been tried using the relativistic Hartree theory.

In contrast to the dynamical characteristics [2–7] of the neutron-lattice system investigated hitherto, its quantum-mechanical state has remained little noticed until now. The mutual interaction of neutrons with a lower density than that in the nucleus is also left untouched due to its vague reality.

The cold fusion (CF) phenomenon [13] in solids with hydrogen isotopes, on the other hand, has been investigated from both scientific and technological points of view. Remarkable excess heat and nuclear products have been observed in several tens of systems but only with qualitative reproducibility and without reasonable explanation based on the science's present knowledge. Some necessary conditions for the phenomenon are clarified but the sufficient condition is not. It is certain that hydrogen isotopes, proton and/or deuteron, are one of necessary components in the system where this phenomenon occurs.

The purpose of this paper is to present a microscopic treatment of neutrons in an allowed band of a crystal by the physical investigation of simplified situations of a neutron-crystal lattice system using ordinary quantum mechanics. Realization of the optimum condition for CF phenomenon in metal hydrides (deuterides) is discussed. Experimental facts concerning the localization of reaction products in CF phenomenon have been explained using these concepts. Possible applications of CF phenomenon are discussed.

2. Local coherence of neutron Bloch waves in boundary layer

A simplified calculation of neutron energy in solids [1] showed a band structure in the one-body approximation similar to that of electron energy in solids. In a case where bands above zero energy level (in terms of a scale where a neutron rests far away from the solid has an energy of zero) are empty and below it are fully occupied, extra neutrons from outside and those generated by nuclear reactions in the solids enter into one of the empty bands. Properties of the band neutrons are governed by the band of the lowest energy with vacancy. Thus, the band structure of the neutron energy (neutron band) in solids has an important influence on the properties of the neutron interacting with one another and with the nucleus in the crystal.

When a solid (say A) with empty bands above zero and fully occupied bands below zero is surrounded by another solid (say B), neutrons in A may be trapped in A if the lowest allowed band of A corresponds in energy to a forbidden band of B and if its thickness is enough to prevent tunneling of the neutron [14].

The trapped neutrons in A have a large probability density at the boundary region between A and B as shown numerically below.

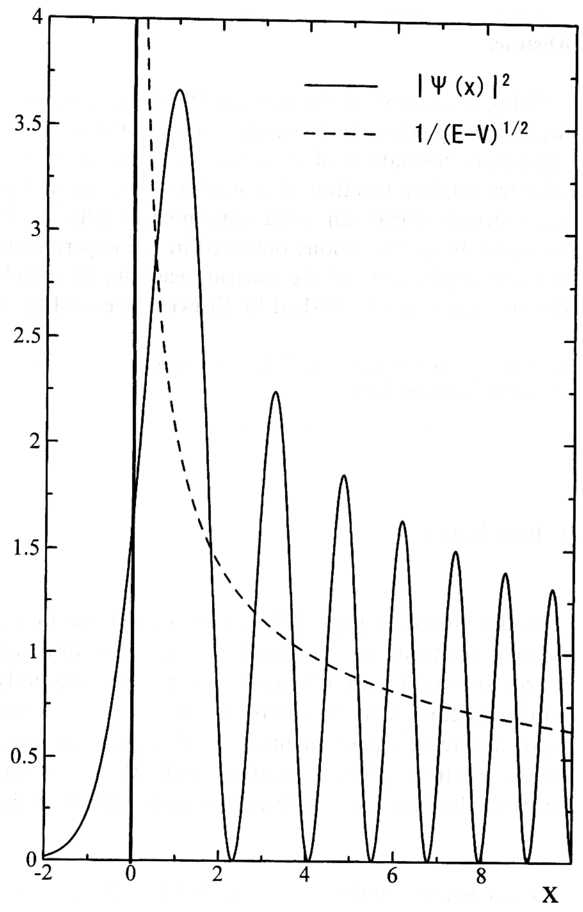

Fig. 1. Classical probability of existence (dotted line) and quantum mechanical probability density (solid line) of a particle with a mass m_n and an energy E (in arbitrary units) in the boundary region $x \sim 0$ determined by a condition $E = V(0)$ with a potential $V(x) = 0 (x_0 \leq x)$, $= \alpha(x_0 - x)(x \leq x_0)$ for $\alpha = 1$.

To investigate characteristics of the trapped neutron at a boundary between the two crystals, A and B, mentioned above, we approximate the Bloch wave in A by a plane wave and the boundary by a potential wall linearly increasing with decrease of the coordinate (say x) perpendicular to the boundary (at $x = x_0$) as the zeroth approximation:

$$V(x) = \alpha(x_0 - x), \quad (x_0 \geq x) \tag{1}$$

$$V(x) = 0. \quad (x > x_0) \tag{2}$$

Classically, a particle with a mass m_n and an energy E moving leftward to the boundary wall loses kinetic energy gradually from $x = x_0$ and reaches 0 determined by a relation $E = V(0)$ to be reflected there. The classical probability of existence at $x(\propto 1/v(x))$ is proportional to a quantity $\sqrt{m_n/E - V(x)}$ which is shown with a dotted line in Fig. 1.

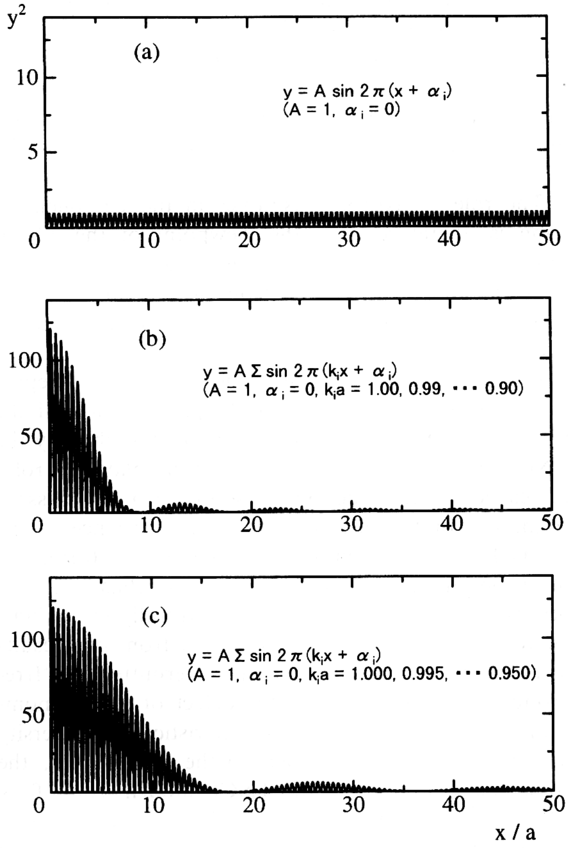

Fig. 2. Illustration of local coherence of neutron Bloch waves near the boundary region by sinusoidal waves in phase at $x = 0$. Probability amplitudes of (a) a single sinusoidal wave with $k = k_0 \equiv \pi/a$, (b) eleven sinusoidal waves with different wave numbers between $k = 0.90\pi/a$ and $k_0 \equiv 1.00\pi/a$ and (c) eleven sinusoidal waves with different wave numbers between $k = 0.95\pi/a$ and $k_0 \equiv 1.00\pi/a$ where a is the period of the Kronig-Penny potential.

Quantum mechanically, the corresponding quantity, the probability density $\rho(x) \equiv |\psi(x)|^2$, is calculated numerically [14] with the Airy function for the wave function $\psi(x)$, and shown with a solid line in Fig. 1. As is well known in quantum mechanics, e.g. for a case of harmonic oscillator, quantum behavior of a microscopic object approaches to classical one with an increase of the quantum number and the similarity of two curves in Fig. 1 is an example of this nature. Qualitative investigation of a quantum object at boundary is therefore partly given by behavior of a classical particle.

The neutron Bloch waves in a band above zero with an energy minimum at Brillouin zone boundary, have almost the same energy and their behavior in the classical forbidden region ($x \leq 0$) is expressed by similar exponential functions with almost the same decreasing factor. Therefore, the behavior of the Bloch functions in the classical allowed region ($0 \leq x$) determined by the shape of the function in the forbidden region is coherent for a finite length determined by the difference of the wave number vectors. Range of this local coherence in the phase factor of wave functions is longer for two waves with a smaller difference of the wave number vectors.

In the case of the model calculation of the Kronig-Penny potential [1], the energy of the lowest band above zero does not change much from $k_0 = \pi/a$ to $k' = 3\pi/4a$ (in one quarter of k_0 from the zone edge) and the local coherence of the Bloch waves exists at least for a region with a length l_{coh} from the turning point determined by $(\pi/a - 3\pi/4a)l_{\mathrm{coh}} = \pi$, or $l_{\mathrm{coh}} = 4a$ for $N/4$ neutrons in the band where a = lattice constant as shown numerically in Fig. 2 and N is the number of states in the band.

3. Formation of neutron cooper pair, neutron-proton (deuteron) cluster and neutron drop in a boundary region

There are two remarkable possibilities for the new quantum states of neutrons in solids due to the existence of the empty bands above zero.

First, in the situation where there is an empty band with energy minimum at the zone edge $k = \pi/a$, it is conceivable to have a neutron Cooper pair of two neutrons with opposite spins and quasi-momenta $\boldsymbol{k}$ and $-\boldsymbol{k}$ just as in the case of electrons shown in the BCS theory of superconductivity. If this is the case, the whole system will be in a more stable state with a lower energy than if in the state without them, even though the mutual interaction of neutrons are ignored.

Second, in the situation where the trapped neutrons are in a band above zero of a crystal surrounded by another satisfying the condition described in Section 2, it was shown already there that neutron density in the boundary region becomes very large in the one-body approximation. Neutrons interact with each other through an attractive nuclear force and therefore the one-body approximation loses its applicability as shown drastically by the existence of superconductivity in metals. It might be possible to form a cluster of neutrons with several protons in it (neutron drop) which has not been treated appropriately in neutron physics in solids and also not observed by now. Reality of this speculation is shown as follows.

The density of the nuclear matter in the nucleus, or number density n_A (cm^{-3}) of nucleons in the nucleus with a mass number A and a radius R, is well defined quantity in nuclear physics [15] and is given as follows:

$$R = 1.5 \times 10^{-13} A^{1/3}\ \mathrm{cm}, \tag{3}$$

$$n_A \equiv \frac{A}{(4\pi/3)R^3} = 7.07 \times 10^{37}\ \mathrm{cm}^{-3}. \tag{4}$$

The nucleons in the nucleus with this density are interacting with one another and with the nuclear force, the so-called strong interaction. Existence of the exotic nuclei, ^{10}He, ^{11}Li, ^{12}Be, ^{32}Na, and so on, is a clear evidence of the nuclear force between neutrons in this state, with a density of this order.

Local coherence of the trapped neutrons in the boundary layer illustrated in the preceding section, 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 neutrons as a whole as high as 10^{12} times that of a single neutron in the coherent region of a thickness $10a$, or ~ 30 Å $= 3 \times 10^{-7}$ cm as shown in Fig. 2. If we assume all neutrons in a unit volume accumulate in this region, the effective density becomes very high $(10^{12})^2/3 \times 10^{-7}\ \mathrm{cm}^{-3} = 10^{31}\ \mathrm{cm}^{-3}$. This is a fairly large value, expected to be in the outer region of the neutron halo of exotic nuclei, and we can expect the effect of neutron–neutron interaction to form neutron drop from a neutron-proton cluster $n_x p_y (y \ll x)$ as a seed like condensation of vapor from gas into liquid or solid phase.

This possibility will be enhanced by the formation of the neutron Cooper pair, a boson, which is favorable for the formation of a cluster of neutrons because of probable Bose-Einstein condensation.

It is necessary, here, to detail one of the necessary conditions for the CF phenomenon — the existence of hydrogen isotopes. In the trapped neutron catalyzed fusion (TNCF) model [13,16] of the CF phenomenon, we have only used hydrogen isotopes as components relevant to the trapping condition for thermal neutrons, which participates in nuclear reactions with a neutron and one another. Considering the existence of the exotic nuclei, where proton and neutron are interacting together to realize a stable state of the ensemble, it is definitely necessary to take hydrogen isotopes into the consideration of the state of neutrons in the boundary region where the neutron drop could be formed.

Thus, hydrogen isotopes in metal hydrides used in CF experiments may be an inevitable component in the formation of a stable state of neutrons with high density at crystal boundary through the formation of a neutron–proton or neutron–deuteron cluster; $n_x p_y$ or $n_x d_y$.

In the process of the neutron drop formation, or neutron condensation, it is probable that the neutron–proton and/or neutron–deuteron cluster plays a key role as, for instance, a seed of condensation. The scenario could be to form the neutron–proton (deuteron) cluster first and then the cluster emerges into a neutron drop by condensation of neutrons. This is only an idea and has not been investigated quantum-mechanically yet.

The role of hydrogen isotopes in the CF phenomenon is, therefore from the viewpoint of the TNCF model, to establish the trapping condition of thermal neutrons and to form a neutron–proton (or deuteron) cluster in the boundary region where neutron Bloch waves have local coherence.

It is appropriate to mention here about the irreproducibility of the cold fusion (CF) phenomenon. If the physics of the CF phenomenon are as described by the TNCF model, where trapped neutrons play key roles to realize nuclear reactions in solids, then a necessary condition for the phenomenon is the existence of the trapped neutron which is conditioned by the formation of an optimum structure realized by stochastic atomic processes. This mechanism results naturally in qualitative reproducibility with wide diversity from null results to events in high times occurring intermittently. "Irreproducibility" is, then, not the defect of CF phenomenon but its fundamental characteristic. The diversity of the results reflects a variety of the values of n_n, the adjustable parameter in the TNCF model, from $10^6 \sim 10^{12}$ cm^{-3} for observed events of the CF phenomenon.

These problems of neutron states and reactions in solids should be treated quantum-mechanically taking the strong interactions between neutrons, between a neutron and a proton (a deuteron) and the neutron–nucleus interaction into consideration, all of which have previously been ignored in neutron physics in crystals. This is a new phase of neutron physics in solids, similar to the exotic nucleus in nuclear physics as treated by the relativistic Hartree theory [12] to explain the existence of the neutron skin and the neutron halo. This phase of the properties of neutrons in solids in relation to the TNCF model, remains to be studied in the future.

4. Interraction of neutron Bloch waves with a nucleus in a boundary region of metal hydrides (deuterides)

In many metal hydrides and deuterides used in cold fusion experiments, structure of the samples is generally complex. Metals are usually composed of several components, e.g. Pd–Li, Ni–K, Cu–Ti–Pd–Ti, Cu–Pd, and so on. In the process of hydrogenation, a density gradient of the relevant hydrogen isotope is usually formed in the sample crystal. The resultant material should be accepted as a multi-layer multi-component, even if the original sample is of a single component with homogeneity. The inhomogeneity due to regions of different components or compositions, works as a crystal boundary to reflect the neutrons treated in previous sections.

As shown in Section 3, the trapped neutrons in the lowest band above zero in a crystal A surrounded by another B, have a large probability density at the boundary region of the two crystals if the boundary is expressed by a potential wall $V(x)$ in Eq. (1). In the boundary region between A and B, the atomic arrangement and composition in reality, vary gradually from those of A to those of B. If thickness of the crystal B is enough to prevent tunneling of the neutron in an allowed band in A, which corresponds energetically to a forbidden band in B, the potential wall against the neutron may be approximated by an increasing function of x and the potential of Eq. (1) is considered as its zeroth order approximation.

The fusion probability of a neutron and a nucleus is known to be proportional to an interaction time, i.e. a time that the neutron stays in a range where the nuclear force is working. This property results in the well-known general energy dependence of the fusion cross section of $1/\sqrt{E}$ for the reaction of a neutron with a target nucleus. In the case of interaction of the trapped neutrons with a lattice nuclei in a surface layer, the reaction time is reduced to the probability density of the neutrons in the surface layer.

Therefore, the trapped neutrons in the band above zero, which is quasi-stable unless it suffers large perturbation, fuse with a heterogeneous nucleus at an aperiodic position seen from the periodic lattice, where the neutron is trapped, with a large cross section in the boundary region.

In three-dimensional crystal with a volume of 1 cm^3, there are about 10^{22} atoms and therefore there are $\sim 10^{22}$ states in a band. In a one-dimensional scheme, this corresponds to 10^7 states in such a band, as calculated using one-dimensional Kronig-Penny potential.

If the number of the trapped neutrons in the band is as large as 10^6, the local coherence discussed in Section 3 makes the fusion probability 10^6 times that of a single neutron in the boundary region, fairly deep (l_{coh}) into the crystal A determined by a relation $(\pi/a - 9\pi/10a)l_{\text{coh}} = \pi$, or $l_{\text{coh}} = 10a$. This coherence lasts partially further into the crystal decreasing its multiplicity to 1/10 of this value (to 10^5) at $100a$. The amplification of the fusion probability increases in the surface region if formation of the neutron drop occurs, or the condensation of neutrons, considered in Section 3.

5. Stabilization of neutrons trapped in solids

In a situation such as one where the highest band below zero is partially filled in the solid A discussed in Section 2, the extra neutrons entered into the band from outside are in lower energy states to prevent their spontaneous transmutation into proton by β-decay. In such cases, the neutrons trapped in the solid accumulate gradually to a high density where the mutual interaction of neutrons through such a strong interaction as that exhibited by the exotic nucleus, enforces stability of the system. It is, of course, necessary to take into consideration the neutron-lattice nucleus interaction in this case, which introduces greater complexity to the state of a system, composed of neutrons and crystal lattice, than in the case of the exotic nucleus.

Anyway, there is a great possibility that the trapped neutrons stabilize, in an optimum situation, conditioned by a combination of structure and components of the system. A more concrete treatment for this problem will be given elsewhere.

6. Discussion

The duality of a microscopic object, a characteristic of the quantum mechanical point of view, has been an interesting property which sometimes attracts and sometimes confuses people. An example which clearly expresses the beauty of quantum mechanical logic, is the production of a cloud-chamber track by a fast electron [17]. The same can be said about the nuclear reaction of the trapped neutrons and a nucleus in a boundary region as investigated above. The local coherence due to behavior of the neutron Bloch waves in the boundary region, and also perhaps to the Cooper pair formation, should be responsible for tremendous nuclear reactions previously unnoticed in the region.

The neutron has been an object difficult to control due to its weak interaction with other particles except in the nucleus, where neutron density is very high, although there are recent advanced treatments of the cold neutron [7]. As a natural conclusion of its wave nature, the concept of a neutron band in the one-body approximation has been deduced, and an energy spectrum with a band structure above zero is shown for the one-dimensional Kronig-Penny model with appropriate parameters. This is applicable to a real situation with two-dimensional homogeneity by a simplified numerical calculation [1].

The neutron band structure, a result of its wave nature, brings in the trapping of the neutron in a crystal with an appropriate boundary condition. In the case of the lowest allowed band with a vacant level below zero, it is expected that the stabilization of neutrons trapped in the solid will occur. In cases where the level is above zero, accumulation of neutron density at crystal boundaries is expected in the one-body approximation, resulting in the formation of the neutron drop.

The particle nature of the neutron, however, appears in the absorption of the neutron by a nucleus which gives a strong perturbation on the neutron Bloch wave. The interaction in the boundary region considered above, is just such a perturbation due to the large probability density of neutrons in it, and reveals the particle nature of the neutron in the reaction with a nucleus in it.

When the number of the trapped thermal neutrons in an allowed band above zero is very large, the interaction of a nucleus with trapped neutrons with almost the same energy in the boundary region can induce a drastic change of properties of the nucleus, e.g. a change of its decay characteristics, by summation of the individual interaction due to almost the same phases of the wave functions at the classical turning point.

Thus, the thermal neutrons in solids expressed by neutron Bloch waves in one-body approximation can induce qualitatively new phases of mutual interaction of neutrons, and also reactions between neutrons and a nucleus in solids not noticed before, and could be the basis of a new science in solid state-nuclear physics. The idea of the polyneutron used to explain the mass spectrum of nuclear products [18] might be a reflection of the neutron drop discussed in Section 3.

A part of this new feature of the trapped neutron-lattice nucleus system in the boundary region is exhibited by the occurrence of localized nuclear products observed in CF experiments [19–29,33]. There are various events showing the production of new elements in materials, mainly in electrodes electrolyzing water or heavy water, observed in CF experiments.

The first confirmation of the localized existence of reaction products is, as far as the authors know, the detection of ^{4}He in the surface layer of a thickness of 40 μm by Morrey et al. [19] and of less than 1 mm by Bockris and Minevski [23]. The occurrence and the amount of ^{4}He observed in these experiments have been explained by the so-called TNCF model [13,16,30] using a single parameter n_n and premises related with effective nuclear reactions in the boundary layer justified in this paper.

The origin of ^{4}He is supposed to be due to the first of the following neutron reactions expected in the Pd/D(H)/Li system:

$$n + {}^6_3\mathrm{Li} = {}^4_2\mathrm{He}(2.1\,\mathrm{MeV}) + t(2.7\,\mathrm{MeV}), \tag{5}$$

$$n + p = d(1.33\,\mathrm{keV}) + \gamma(2.2\,\mathrm{MeV}), \tag{6}$$

$$n + d = t(6.98\,\mathrm{keV}) + \gamma(6.25\,\mathrm{MeV}). \tag{7}$$

Assuming the ^{4}He detected in the surface layer of the Pd cathodes to be a reduced percentage of that produced in it, the data were shown to be consistent with ^{4}He detected later in the gas phase of the system by others [31,32].

Further evidence of local nuclear reactions in the surface layer, is the detection of nuclear transmutation products. There are several data showing the localized existence of new elements and we can refer to the first data of nuclear transmutation explained by fission by Bockris and Minevski [23] and others [24–28,33].

These data show the localization of reaction agents, trapped neutrons in the TNCF model, in the surface layer. If the explanation of the CF phenomenon based on the model is plausible, hydrogen isotopes in metals are one of the key elements in the realization of optimum conditions for the nuclear reaction in solids. As was already shown at the end of Section 3, this mechanism realizes its possibility by stochastic atomic processes in compound solids and explains the controversial irreproducibility, i.e. qualitative reproducibility in our terminology, of events in the CF phenomenon. A variety of conditions for its realization is reflected in values of the parameter n_n in the TNCF model from 10^6–10^{12} cm^{-3}. It is worth tracing this route of reaction mechanism as far as possible.

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