

Theoretical Verification of the Trapped Neutron Catalyzed Model of Deuteron Fusion in Pd/D and Ti/D Systems

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Abstract

Theoretical estimation of factors assumed in the model proposed before are presented. The result shows that the assumptions made in the model are almost verified by the calculation to support the interpretation of the Cold Fusion phenomena as the trapped neutron catalyzed fusion of deuterons in solids.

§ 1. Introduction

Since the declarations of the discovery of the Cold Fusion phenomena (an extraordinarily big amount of heat¹⁾ and a neutron emission²⁾ in electrolytic cells with Pd and Ti cathodes, respectively, with D₂O electrolyte solution) in March 1989, there have been controversies on the reliability of experimental results on those and related phenomena.

One of the authors (H. K) proposed a model³⁾ to explain experimental data obtained in the Cold Fusion phenomena consistently but qualitatively making assumptions 1) effective trapping of thermal and cold neutrons in inhomogeneous materials, 2) effective fusion of the trapped neutrons with occluded deuterons with high probability ;

$$n + d = t(6.98 \text{ keV}) + \gamma(6.25 \text{ MeV}), \quad (1)$$

3) fusion of this triton with occluded deuterons ;

$$t + d = {}^4\text{He}(3.5 \text{ MeV}) + n(14.1 \text{ MeV}), \quad (2)$$

and 4) attenuation of the γ in the matrix to heat the lattice.

In this paper, those assumptions made in the model were investigated theoretically as rigorously as possible. The main subjects of calculation are divided into four themes corresponding to the assumptions: 1) Trapping of neutrons in a region (trapping region) surrounded by boundaries between media with different components, 2) Fusion of trapped neutrons as a standing wave with occluded deuterons, 3) Fusion of 6.98 keV triton with occluded deuterons and also deuteron acceleration by elastic collision with 14.1 MeV neutron, 4) Heating of matrix solid by the energy of 6.25 MeV photons produced in the reaction (1). The scenario contains many body problem with several constituent particles and becomes inevitably qualitative in several points. Even though, main parts are analyzed as quantitatively as possible.

§ 2. Trapping of Neutrons in Inhomogeneous Solids

A neutron of an typical energy of cosmic shower (*let's say* 1 MeV) generated up at 8 km above the earth's surface will experience elastic collisions with nitrogen and oxygen nuclei, N and O, in the air. Using average values of elastic collision cross-section⁴⁾ $\sigma_{n-N} \simeq 3$ and $\sigma_{n-O} \simeq 4$ barns, we may conclude that the neutron in a typical shower suffers fifty collisions with N and O nuclei until reaching to the earth and the energy becomes finally about 1 keV.

Furthermore, if the 1 keV neutron enter into the earth, it will make elastic collisions with a hydrogen existing there to become a thermal neutron losing energy effectively and with heavy nuclei in the earth to be reflected effectively. Quantitative estimation of this effect should take into account the structure of the matter the neutron is interacting with, and will be given in the later work.

Thus, we may assume the existence of a plenty of low energy neutrons in nature around us as is always measured in experiment. One typical example of the measurement is given by Jones et al. in their paper²⁾ (Figure 2). Number of background neutrons is estimated from the figure to be about 10^4 at above 10 keV compared 23.2 ± 4.5 neutrons with the energy 2.45 MeV. This value suggests that many low energy background neutrons less than 10 keV exist in nature. So, we may proceed our treatment with a premise there are fairly large number of background neutrons around us.

A neutron with an energy $\epsilon = p^2/2m$ carries a de Broglie wave with a wave length

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m\epsilon}}. \quad (3)$$

If the energy of the neutron is measured in eV, the wave length in Å, is given by the following relation:

$$\lambda = 2.86 \times 10^{-1} \epsilon^{-1/2}. \quad (\text{Å}) \quad (\epsilon \text{ in eV}) \quad (4)$$

Therefore, a thermal neutron with an energy of 1/40 eV (~ 300 K) has a wave length

1.80 Å comparable with lattice parameters of ordinary crystals. A neutron as a wave is reflected by a boundary of an ordered array of deuterons (and protons) in matrix lattices. The reflection occurs as results of the Bragg reflection and/or the total reflection. The Bragg reflection occurs when the Bragg condition

$$m\lambda = 2d\sin\theta \quad (5)$$

is satisfied. Here, θ is the complementary angle of an incident one, d is the lattice spacing and m is an integer.

On the other hand, the total reflection occurs when the θ is smaller than or equal to an critical angle

$$\theta_c = \pi/2 - \sin^{-1}n_r \quad (n_r < 1), \quad (6)$$

where $n_r = n_2/n_1$ is the relative refractive index of a medium 2 to a medium 1 when the neutron enters from 1 to 2 in the case of refraction. The refractive index n_i of the medium i is given according to the following relation :

$$n_i^2 = 1 - \lambda^2 N_i \bar{a}_{coh}^{(i)} / \pi, \quad (7)$$

where N_i is a number of nuclei per unit volume in the medium and $\bar{a}_{coh}^{(i)}$ is a weighted mean of the thermal scattering lengths of the nuclei in it. Because of a positive value of the thermal scattering length a_{coh} for deuteron, we can expect a total reflection by the occluded deuteron lattice in a matrix. However, because of a negative value of a_{coh} for proton, a neutron will be trapped in an occluded proton lattice surrounded by pure (low impurity) matrix.

Neutrons with energies of the order of or less than the thermal one behave as waves in a solid and are then possible to be reflected by a boundary of an array of occluded deuterons (protons) with a characteristic spacing a_0 when a_0 is comparable with or smaller than the wave length λ . If a region with linear dimension L larger than a_0 ($a_0 \leq L$) is bounded by walls of such a structure reflecting neutrons, a neutron might be trapped in the region for a time, say T . The time T will be determined by the state of the walls i.e. atomic species in and widths of the walls, the geometry of the region, etc.

1) Total reflection

Let us consider a plane boundary between media 1 and 2 through which a neutron passes from 1 to 2. The critical angle θ_c of the total reflection is given as follows when a neutron has a wave length λ ;

$$\theta_c = \pi^{-1/2} \lambda \langle Na_{coh} \rangle^{1/2}, \quad (8)$$

$$\langle Na_{coh} \rangle = N_2 a_{coh}^{(2)} - N_1 a_{coh}^{(1)}.$$

The thermal scattering lengths a_{coh} are listed in Table 2-1 for several nuclei along with the number density of nuclei in typical solids.

Table 2-1. Thermal scattering length a_{coh} and number density of atoms.

	¹ H	² D	⁷ Li	²⁶ Ti	²⁶ Mn	²⁸ Ni	⁴⁶ Pd
$a_{coh}(10^{-12} \text{ cm})$	0.378	0.65	-0.25	-0.38	-0.36	-0.87	0.63
$N (10^{23} \text{ cm}^{-3})$			0.463	0.566	0.800	0.903	0.688

Using these data, we can calculate the critical angle θ_c of lattices of occluded deuterons in PdD and TiD₂ for a neutron with wave length 10 Å and the results are shown in Table 2-2.

Table 2-2. The critical angle θ_c (in degree and radian) of total reflection for neutrons with $\lambda = 10 \text{ Å}$ and specific number of totally reflected neutrons $\Omega_c/2\pi$ (in percent).

	PdH	PdD	TiH ₂	TiD ₂
θ_c (degree)	0.52	0.68	0.67	0.88
θ_c (rad)	0.018	0.024	0.023	0.031
$\Omega_c/2\pi$ (%)	1.8	2.4	2.3	3.1

The critical angles for the total reflection in PdH and TiH₂ lattices by a boundary between Pd and Ti lattices, respectively, are also listed in this table.

This result shows that a neutron with wave length 20 Å ($E = 2 \times 10^{-4} \text{ eV} = 2.5 \text{ K}$) has a critical angle 1.32° in the case of Pd/D system. For an optimum situation where the neutron is in a region surrounded by 270-sided pillar and collides with each side with an angle θ_c , the neutron in the plane perpendicular to the axis of the pillar is completely trapped in this region.

The longer the wave length of the neutron, the less the number of side of the pillar is needed to satisfy this condition. This is, of course, an extreme example but shows a possibility making the time T very long compared with the transit time τ of the neutron for the region ;

$$\tau = L/v = \sqrt{L^2 m / 2E}$$

2) Bragg reflection.

If a neutron is in a region surrounded by a lattice with spacing d satisfying the condition (5), the neutron with wave length λ can not pass through the lattice and reflected totally by the lattice.

Let us consider a simple example of a one dimensional lattice with spacing d where a neutron travels. From knowledge of the band calculation in solids, it is known that at the wave vector $k = m\pi/d$, there is a energy band gap $\Delta E = 2|V_n|$, where

$$V_n = \frac{1}{d} \int_0^d V(x) \exp(2\pi i n x / d) dx \tag{9}$$

and $V(x)$ is the periodic potential for the neutron with a period d .

In three dimensional lattice with a value $d = 2(3) \text{ \AA}$ for $\theta = \pi/2$, the energy at the center of the gap is given by

$$E\left(\frac{\pi}{d}\right) = \frac{\hbar^2}{2m_n} \left(\frac{\pi}{d}\right)^2 = 5.12(2.28) \times 10^{-3} \text{ eV.}$$

This value corresponds to the energy of the cold neutron. So, some cold neutrons coming from outside with an energy in the range of $E(\pi/d) \pm |V_n|$ are reflected totally by the lattice :

$$E(\pi/d) - |V_n| < E < E(\pi/d) + |V_n| \quad (10)$$

The value of $|V_n|$ was estimated for the deuteron using the Fermi pseudopotential

$$\hat{V}_N = \frac{2\pi\hbar^2}{m_n} b\delta(\mathbf{r} - \mathbf{R}). \quad (11)$$

to be $0.211(0.063) \times 10^{-6} \text{ eV}$. The bound scattering length b is taken as $0.67 \times 10^{-12} \text{ cm}$ (for D) in the above calculation (S.W. Lovesey, Theory of Neutron Scattering from Condensed Matter, Vol. 1, Oxford U.P.).

The value given above for \hat{V}_n means that 0.01 % of the cold neutrons are trapped by a single gap at $k = \pi/d$. This number of neutrons seems sufficient to explain the ordinarily observed amount of excess heat and the number of emitted neutrons⁵⁾ from inhomogeneous Pd/D and Ti/D systems if we consider the large number of background neutrons as explained in the beginning of this section.

In the case of the proton, $b = 0.37 \times 10^{-12} \text{ cm}$ (average value for singlet and triplet states), and $|V_n|$ is 55 % of that for deuteron. If, however, it is possible to use polarized state of proton and neutron, the scattering lengths for triplet and singlet states can be used for effective trapping ;

$$b^{(+)} = 1.04 \times 10^{-12} \text{ cm, triplet} \quad (12)$$

$$b^{(-)} = 4.70 \times 10^{-12} \text{ cm. singlet} \quad (13)$$

In the case of singlet scattering, the band gap ΔE becomes wider by a factor of $4.74/0.67 = 7.1$ than in deuteron lattice. On the contrary, in the case of the deuteron, the difference of the scattering length is not so large (0.95 and $0.10 \times 10^{-12} \text{ cm}$), and the use of polarized state makes not so large effect as in the proton lattice.

Then, the neutron is fully trapped in the region if it satisfies some conditions. In reality, however, the lattice has a finite width and there is a penetration probability for a neutron in the region even if the condition (5) be satisfied. But, for an optimum situation where the surrounding lattices have such an enough thickness as the neutron trapped in the region fuse with one of deuterons in it, we can take the trapping time T as infinity.

From our knowledge of the band structure of electron spectrum in solids, it is possible to infer that in a fixed direction the shorter the wave length satisfying the condition (5) for a fixed d is, the wider the energy range of neutrons reflected by the lattice is. So, the longest wave length reflected effectively by this mechanism is d when the neutron

collides with $\theta = \pi/2$. Thus, the Bragg reflection is preferable for thermal neutrons with large θ if the Bragg condition (5) is satisfied while the total reflection is preferable for cold neutrons with small θ .

We would like to emphasize here the stochastic nature of the formation of boundaries around a region favorable to trap the neutrons. This nature reflects in the lack of reproducibility of experimental data of the Cold Fusion phenomena, which is one of main reasons why the phenomena could not get full confidence from some researchers.

Another trapping mechanism in terms of the neutron Moessbauer effect (the Lamb effect) will be treated in the other work published elsewhere.

§ 3. Fusion of Trapped Neutron with Deuterons

Using an optical model with square well potential, we calculated the fusion cross section of low energy neutrons with a deuteron. The result is shown in Fig. 3-1. In this figure, the fusion cross section in barns are plotted as a function of neutron energy in eV. This data is consistent with existing data at higher energy⁴⁾ and shows $E^{-1/2}$ increase of the capture cross section with decrease of neutron energy. So, the multiplication factor for the fusion probability due to the neutron trapping is more larger than assumed before³⁾ where only trapping time was taken into account. In the process of deceleration

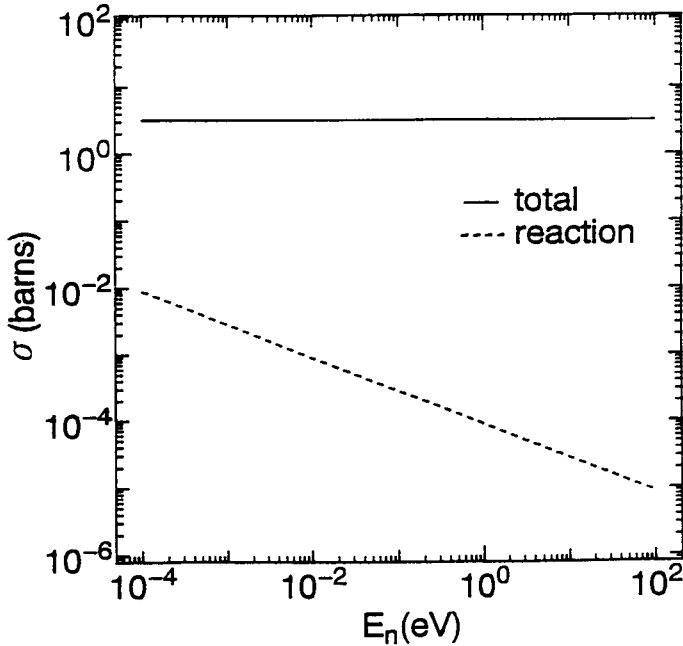


Fig. 3-1. Fusion cross section (barns) of neutron (energy E_n with deuteron extrapolated to low energy with use of the optical model.

in matrix, the neutron loses its kinetic energy and becomes thermal or cold neutron having a large probability of trapping and also a large fusion cross section with a deuteron when it is trapped.

This result verifies the assumption of the effective occurrence of fusion reaction (2) made in the model³⁾. The effect of the neutron trapping (the existence of a standing wave) will work further positive for our model at least by a factor T/γ .

We did not consider a possibility of neutron fusion with matrix nuclei in this paper. In reality, the fusion reaction may occur and the difference of the matrix will influence some features of the Cold Fusion phenomena.

§ 4. Fusion of 6.98 keV Triton with Deuterons occluded in Solids

The triton generated by the reaction (1) in a matrix occluding deuterons has an energy of 6.98 keV. The triton passes through the matrix and collides with deuterons occluded there. The $t + d$ fusion cross section of the reaction (2) as a function of triton energy E is given by the following formula (D.I. Book, Plasma Formulary, Naval Research Laboratory):

$$\sigma(E) = \frac{A_5 + [(A_4 - A_3 E)^2 + 1]^{-1} A_2}{E [\exp(A_1/\sqrt{E}) - 1]} \quad (14)$$

Here, σ is in barns, E in keV, and the coefficients have following values :

$$\begin{aligned} A_1 &= 56.27, & A_2 &= 7.53 \times 10^4, & A^3 &= 0.912 \times 10^{-2} \\ A_4 &= 1.076, & A_5 &= 614. \end{aligned} \quad (15)$$

For the triton energy 6.98 keV, this formula gives the fusion cross section of 3.05×10^{-6} barns.

This result means that in a Pd metal sample (density 12.16 g/cm³) of 1 mol occluding the same number of deuterium as palladium atoms, the triton suffers about 10^{-6} fusion reactions before it comes out from the sample.

The 14.1 MeV neutron generated in the reaction (2) may make elastic collision with deuterons in the sample and give them kinetic energy. When the collision is head-on, the neutron loses its 8/9 of the initial energy and on the average its 16/27. So, in an optimum situation, the collision of the neutron and deuterons occluded in the sample occurs frequently, and a neutron accelerates about 9 deuterons to higher energies than 100 keV necessary to accomplish $d + d$ fusion effectively :

$$d + d = {}^3\text{He}(0.82 \text{ MeV}) + \text{n}(2.45 \text{ MeV}) \quad (16)$$

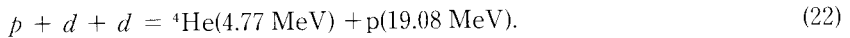
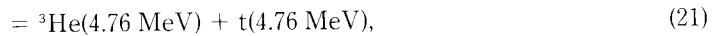
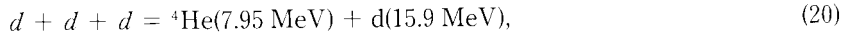
$$= t(1.01 \text{ MeV}) + p(3.02 \text{ MeV}) \quad (17)$$

$$= {}^4\text{He}(76.0 \text{ keV}) + \gamma(23.8 \text{ MeV}) \quad (18)$$

Branching ratios of these reactions are known as 1 : 1 : 10^{-7} in the nuclear physics and the last reaction may be ineffective. Thus, the neutrons with an energy 2.45 MeV observed

sometimes²⁾ should be explained by the successive reactions (1), (2) and (16). As in the case §3, we did not consider interactions of the triton with matrix nuclei which certainly occur with finite probability. We will postpone this problem to future.

If we don't accept the neutron catalyzed fusion mechanism, it is necessary to solve riddles of much ⁴He, tritium and large excess heat (see next section) without remarkable neutron counts. There were some trials to take up following rather difficult reactions to occur in solids as done in some literatures ;



These reactions may have some connections with the Cold Fusion phenomena but would not take main roles in them.

§ 5. Photon Attenuation in a Medium occluding Deuterium and Hydrogen

For photons passing through a homogeneous medium of density ρ (g/cm³) and thickness t (cm), the intensity I remaining is given by the expression

$$I = I_0 e^{-\mu t} \equiv I_0 e^{-\rho t / \lambda_m}. \quad (23)$$

Here μ is the mass attenuation coefficient (cm⁻¹), $\lambda_m = \rho / \mu$ is the mass attenuation length (g/cm²), and I_0 is the initial intensity (number of photons). The data for elements Pb, Fe, Ar, C and H in the energy range from 10⁻² to 10² MeV are given in TRIUMF Kinematics Handbook (Table VII-16). Interpolation to other atomic number Z are done by scaling the cross section (cm²)

$$\sigma = \frac{A}{\lambda_m N_A}, \quad (24)$$

where A is the atomic weight of the absorber material (g/mol) and N_A is the Avogadro number (mol⁻¹). For a mixture, the formula

$$\lambda_{eff}^{-1} = \sum_i f_i \lambda_m^{-1} \quad (25)$$

is used, where f_i is the proportion by weight of the i -th component.

The plot of the cross section σ as a function of Z is shown in Fig. 5-1 for a photon energy $E = 6.25$ MeV. From this figure by interpolation, we can estimate σ for Ti and Pd metals as 0.22×10^{-23} and 0.66×10^{-23} cm², respectively.

Using these values of σ , we calculated the e-folding length $\ell = 1/\mu$ for the 6.25 MeV photon in Ti and Pd using a relation

$$\ell = \mu^{-1} = \frac{\lambda_m}{\rho}. \quad (26)$$

The result is shown in Table 5-1.

Table 5-1. The e-folding length ℓ of 6.25 MeV photons in Ti and Pd.

	Z	A(g/mol)	σ (barns)	λ_m (g/cm ²)	ρ (g/cm ³)	ℓ (cm)
H	1	1.00	0.07	23.7		
D	1	2.01	0.14	23.7		
Ti	22	47.9	2.2	36.2	4.5	8.0
Pd	46	106.4	6.6	26.8	12.16	2.2

The effective e-folding length ℓ_{eff} of photon attenuation for hydrides and deuterides of Ti and Pd are given in Table 5-2, where the volume of the sample is assumed to be the same as the metal without hydrogen isotopes.

Table 5-2. Effective e-folding length ℓ_{eff} of 6.25 MeV photons in hydrides

	λ_{eff} (g/cm ²)	ρ (g/cm ³)	ℓ_{eff} (cm)
TiH	35.8	4.6	7.8
TiH ₂	355.5	4.7	7.6
PdH	26.8	12.3	2.2
TiD	35.5	4.7	7.6
TiD ₂	34.8	4.9	7.1
PdD	29.7	12.4	2.2

This table shows the effect of the hydrogen isotope occlusion on the photon attenuation is not large if the volume change is neglected. The volume change of the order of 5 % observed in the experiments gives density change of the same order to the opposite direction. This change of the density will give the fractional decrease of ℓ_{eff} by the same order of percentage.

The large value of the attenuation length of photons in Pd may be relevant with the large excess heat generation observed in Pd/D system. If the Pd sample used in the Cold Fusion experiments has a linear dimension larger than 2 cm in the longest direction of the sample, the photon emitted in this direction in an optimum case will almost decay out in the sample. The photon energy given mainly to electrons in this process will dissipate into kinetic energy of electrons and ions in the sample and the temperature of the sample will be raised by this amount.

Thus a photon generated simultaneously with the triton will be captured with probability ~ 1 in Pd, while the t + d fusion probability is determined by the cross section 3×10^{-6} barns and only 10^{-6} neutrons will be generated by the reaction (2) in the Pd sample of 1 mol. This difference may have close relation with the $10^7 \sim 10^8$ difference of numbers of events which contribute to neutron emission and to excess heat generation

observed in the experiments¹⁾, one of riddles in the Cold Fusion phenomena.

The maximum excess heat measured by Fleischmann et al.¹⁾ corresponds to $10^{11} \sim 10^{12}$ atoms/cm³s reactions by their estimation (assuming the sample volume as 1 cm³ from their Table 1). If this heat be supplied by the gammas generated in the reaction (1), its quantity corresponds to 10^{18} reactions/cm³s. Using the fusion cross section of 10^{-2} barns for 10^{-3} eV neutron given in §3 and number of deuterons occluded in the sample 6.9×10^{22} cm⁻³ (assuming the ratio of atoms Pd/D ~ 1), we can estimate the number of neutrons responsible to the reaction as 4.1×10 cm⁻³. This number is too large to be considered as that of the trapped neutrons according to the experimental data, e.g. given in §2. However, if a mechanism to breed neutrons in an deuteron occluded material work effectively, 10^3 breeding rate in a sample with linear dimension ~ 1 cm could be expected⁶⁾ and the above number $\sim 10^{15}$ is an conceivable one. If the effect of neutron trapping to the fusion cross section be taken into account, this number will become smaller by several orders.

In a very rare situation where the reactions (1), (2) and (16) occur successively in a short time, the number of neutrons in the sample will increase rapidly to reach the value to explain such an extraordinary events as observed in some experiments where were

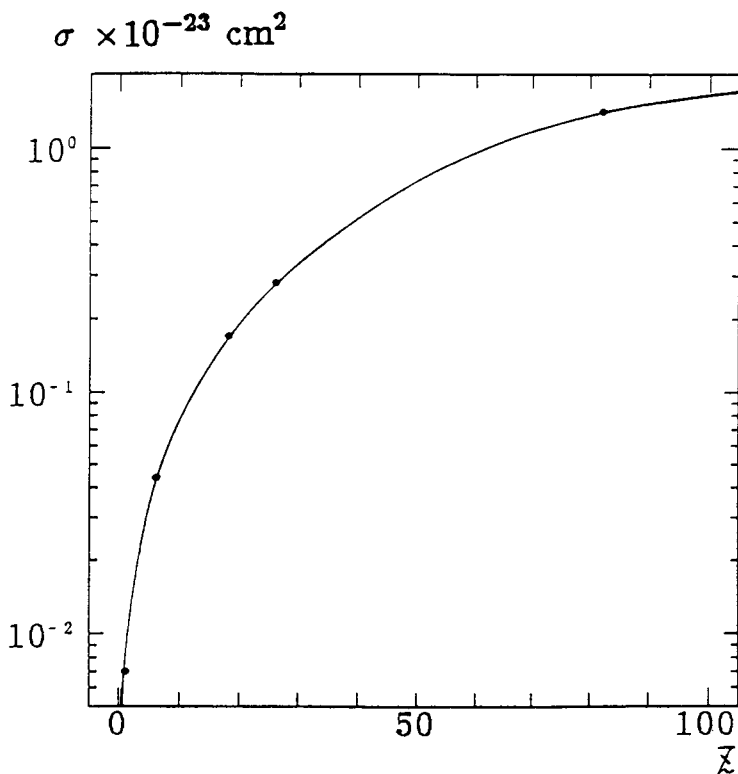


Fig. 5-1. Cross section of photon absorption by Eq. (29) to interpolate the photon mass attenuation coefficient for Ti and Pd.

explosions in Pd/D system⁷⁾ including very large excess heat by Fleischmann et al.¹⁾ A model estimation of the neutron breeding rate will be published in the following paper⁶⁾ giving a maximum value of 10^6 neutrons per second in an infinite lattice of saturated Pd-D crystal in an optimum situation. On the average, the size effect will reduce the value by three orders of magnitude for a sample with a linear dimension of 1 cm. Therefore, to get the same order of magnitude for the breeding rate, it will be necessary to have a three orders of magnitude larger initial neutron density. Details will be shown in the paper⁶⁾.

The four-fold longer e-folding length of 6.25 MeV photons in Ti than in Pd metal may be relevant to the fact that the large excess heat has not been observed in Ti but in Pd. Because of this situation in Ti metal, the neutron breeding process by 14.1 MeV neutron collision with deuterons may work effectively without hindrance from thermal bursts and neutron bursts might be observed⁵⁾.

§ 6. Conclusion

The discussion given above is not fully quantitative in points that it is not derived only from the first principle and that the absolute value of the excess heat generated in Pd/D system is not determined. Not considering the former claim, it is necessary to know the exact situation of the sample and environments in the experiments to solve the latter problem and it is not possible to realize. Even so, the Cold Fusion phenomena observed in Pd/D and Ti/D solids are explained consistently in terms of the trapped neutron catalyzed mechanism of deuteron fusion. Especially, several hitherto unsolved problems in the phenomena, such as the stochastic nature of the occurrence of phenomena, the large excess heat without appropriate neutron production¹⁾, the large amount of tritium with no neutron emission⁸⁾, the large amount of ^4He observed with some amount of heat and tritium⁹⁾, and the fact that the large excess heat is observed mainly in Pd/D but not in Ti/D system, are explained satisfactorily. In addition, the higher energy neutrons than 2.5 MeV were observed in several experiments in Pd/D¹⁰⁾ and in other metal deuterides¹¹⁾. These data will be explained by the neutron generated in the reaction (2).

Thus, it is possible to say that the Cold Fusion phenomena are the trapped neutron catalyzed fusion of deuterons occluded in Pd, Ti and other materials in its essential parts. To make the resulting energy thermal, it is desirable to use elements as large Z as possible in the hydrogen occluding material. If a ceramics is possible to use for this object as the matrix solid, we will have a large variety of choice in this point.

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the manuscript.

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