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Research Article

Study on the Phenomenon Reported "Neutron Generation at Room Temperature in a Cylinder Packed with Titanium Shavings and Pressurized Deuterium Gas" (3)

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Abstract

In this paper, the authors have intended to ascertain the driving force for an adsorbed deuterium atom or a deuteron to collide in titanium crystal. Recent simulation analysis results, related to the predicted cluster or cell models of deuterium atoms adsorbed in titanium crystal, together with the related calculations by Coulomb formula and Yukawa formula were investigated. Coulomb force working between deuteron–deuteron (d–d) particles is compared with the nuclear force working between them. The change of the force to each of them is evaluated in accordance with the distance between them, near the surface of the atomic nucleus. Taking into account the results of previous studies, it seems that nuclear fusion will occur occasionally without adding any specified energy. We think that there is a possibility of a collision of free deuterons through the medium of a negative charge in a deuterium atom in ligancy 2. On the other hand, we think that if a suitable amount of energy, which is far smaller than that of high temperature nuclear fusion, such as the irradiation of the alternative electromagnetic wave, for example, is supplied to adsorbed deuterium atoms and desorbed deuterons in the titanium (Ti) shavings packed in the experimental cylinder under a pressurized or evacuation condition with a suitable temperature rise, then there also will be a higher probability of nuclear fusion being achieved.
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Keywords: Adsorption, Coulomb force, Desorption, Deuterium, Nuclear force, Titanium

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1. Introduction

In the previous paper [1], we analyzed the state of deuterium atoms in the tetrahedral cage of titanium crystal using the first principle molecular orbital calculation and proposed a method to promote the neutron generation.

Recently, Giorgi et al. [5,6] have given a theoretical explanation for the formation of a combination in an electron deficient metallic system with a hydrogen (or deuterium) atom in ligancy 2, that is to say, a 3-center-2-electrons, (3c-2e) bond in the collisional mechanism which has lead to the reported neutron generation.

Furthermore, Giorgi et al. have found a metastable model including (3c-2e) bonds with respect to the structure of one octahedral subcell belonging to the hexagonal close-packed (hcp) titanium lattice. As a result of this research, we can recognize that the adsorbed deuterium atoms form a compound of deuterium atoms in ligancy 2, in many locations of titanium crystal.

In this paper, we intend to ascertain what the driving force for a deuterium atom and a deuteron to collide with one another is and what the driving force for nuclear fusion to occur is, comparing it with Coulomb force and the nuclear force working between d–d particles.

2. The Behavior of Deuterium Atoms Adsorbed in Ti Shavings

The only energy change in the process of neutron generation in the previous experiments [2–4] has been the temperature rise under a pressurized or evacuation condition. The kinetic energy change of the adsorbed deuterium atom from liquid nitrogen temperature to room temperature is ca. 26 meV.

We doubt that such a small amount of energy can make deuterium atoms overcome their repulsive force, collide with one another and then create nuclear fusion. We expect the energy of the temperature rise will only open a door to a collisional space by means of a chemical bonding environment in which a deuterium atom and/or a deuteron can collide.

To explain this concept, we think that quantitative evaluations of charge value per each deuterium atom and the working energy between deuterium atoms are necessary.

In the recent theoretical analysis, Giorgi et al. [5] have reported the impact of the deuterium adsorption on the final stress of the cell. They calculated the stress impact given by the formation of the titanium atoms combined with a deuterium atom in ligancy 2 ((3c-2e) bond) to the titanium supercells (16 and 54 atoms, respectively) and analyzed the bond formation of an electron deficient titanium matrix. Difference between the full (ions + lattice) and partial (ions) optimization [5]. T_d: tetrahedral cage, O_h: octahedral cage.

The calculated result referred to in Table 1 [5] indicates that the energy variation in the tetrahedral cage (in the matrix composed of 54 titanium atoms) is 0.028 eV. A matrix; the size of 54 titanium atoms is large enough not to give a sizable effect to the ΔE value evaluation. So, even if we calculate the ΔE value in a larger matrix, it seems that its ΔE value will not be much different as compared to 0.028 eV.

On the other hand, Ti shavings used in the previous experiments [2–4] seem to compose of a far larger size than that of 54 titanium atoms. This calculated ΔE value, 0.028 eV, is very close to the value of the input energy, ca. 0.026 eV, caused by the temperature rise under the pressurized or evacuation condition. It appears that this energy generated by the temperature rise under the pressurized or evacuation condition is used by a deuterium atom to enter into or leave the titanium crystal lattice. Therefore, when it intends to vacate the cage or a deuterium atom in another location intends to move from its location to go to the gaseous region, its electron is taken by the titanium atom and/or surrounding titanium atoms and it will become a deuteron. After that, a collision is likely to occur between a deuteron and a deuterium atom in ligancy 2, by means of a small amount of kinetic energy, for example, alternative electromagnetic energy, and by the medium of its negative charge.

If the specified condition regarding temperature, pressure and titanium metal adsorbed deuterium gas are prepared suitably, neutron generation automatically proceeds without any additional energy required except for a temperature

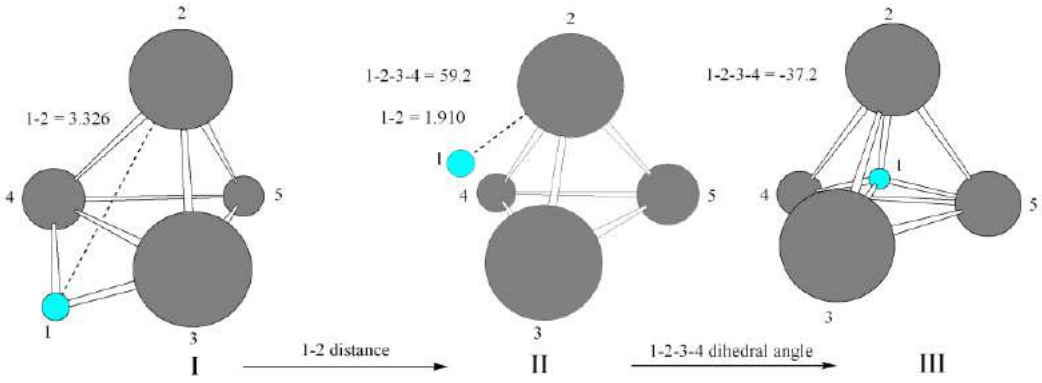

Figure 1. Set up of the trajectory of D atom entering the tetrahedral cage: the two steps approach showing the two different reaction coordinates [6].

rise under a pressurized or evacuation condition, as witnessed in past experimental reports.

Giorgi et al. performed the Density Functional Theory (DFT) study of deuterium entering a titanium tetrahedral cage [6]. In this study, the geometry of the initial Ti_4D^+ system, with the D^+ atom outside the cage, in this case a quintet spin state, and they calculated the deuteron charge from outside of the cage to the inside of the cage. Concerning the tetrahedral cage they indicated the outside–inside trajectory of the D^+ atom, provided a two step set up as indicated in Fig. 1.

In Fig. 1, Giorgi et al. have calculated the energy vs. the D^+–Ti(1–2) distance for the first step of the D^+ approach to the Ti_4 cage (from structure I to II) and calculated the energy vs. the D^+–Ti–Ti–Ti (1–2–3–4) dihedral angle for the second step of the approach to the Ti_4 cage (from structure II to III in Fig. 1).

The second step results are reported in Table 2 and show that if there is a deuterium atom in the cage, a deuterium atom in ligancy 2 outside the cage cannot enter into the cage without providing necessary energy, because they both have the same charge sign and therefore will not collide. Accordingly, we conclude that nuclear fusion will not occur inside the cage.

Table 1. Energy variation as function of adsorbed deuterium atoms. ΔE represents the difference between the full (ions + lattice) and partial (ions) optimization [5].

	ΔE (eV)
2×2×2(16 atoms)	
Ti	0.05
Ti+2D 2(3c-2e)T_d	0.12
Ti+2D 2(3c-2e)O_h	0.07
3×3×3(54 atoms)	
Ti	–
Ti+2D 2(3c-2e)T_d	0.028
Ti+2D 2(3c-2e)O_h	0.013

T_d: Tetrahedral cage, O_h: Octahedral cage.

Table 2. Calculated the Voronoi deformation density (VDD) atomic charges on D during the second step of the trajectory from outside to inside the cage (from structure II to III in Fig. 1) [6].

1–2–3–4 dihedral angle (degree)	VDD atomic charge on D (e)
50	−0.149
40	−0.29
30	−0.439
20	−0.554
10	−0.630
0	−0.693
−10	−0.744
−20	−0.760
−30	−0.781

To clarify the mechanism of the neutron generation here, we assume that there are three regions in the system of deuterium gas and Ti shavings packed in the cylinder (here after referred to as "titanium-deuterium system", or "Ti–d system"), as indicated in Fig. 2.

- Region I: The part of Ti shavings excluding their surface part. Presumedly there are deuterium atoms in the stable location here.
- Region II: Surface part of Ti shavings, the region presumed to be where almost all the adsorbed deuterium atoms in ligancy 2 are.
- Region III: Gaseous phase region of deuterium between Region II and the inside of the cylinder wall.

We studied two cases of neutron generation based on the experimental results.

Case 1

This case inspects the neutron generation in the pressurizing condition [2–4], it pays attention to the pressure and temperature condition in the cylinder in the experiment.

Referring to a pressure-composition isotherm adsorption diagram for Ti–H_2 (assuming that this diagram is almost equivalent to the Ti–D_2 diagram) with the parameter temperature in Fig. 3 [7], we assume that the location when the

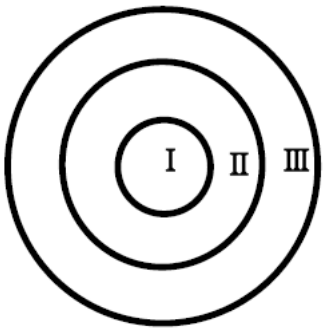

Figure 2. Spatial partition for the analysis of the neutron generation mechanism in the Ti–d system (Region I, Region II, Region III).

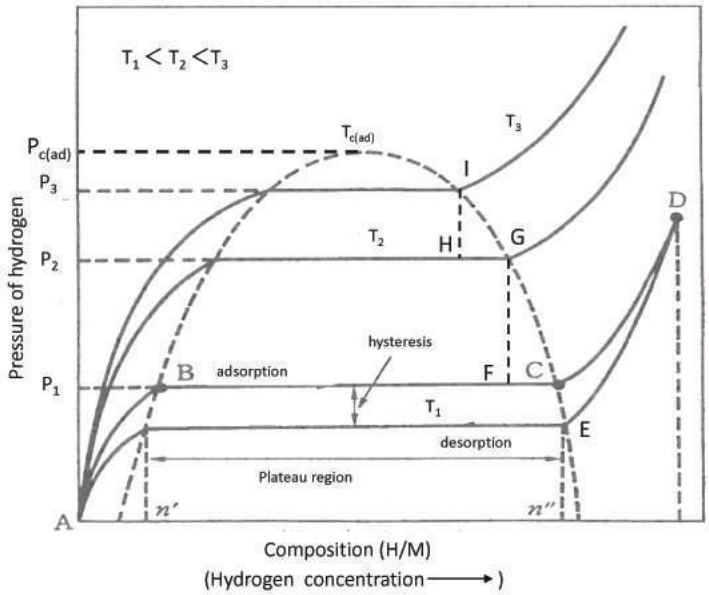

Figure 3. Pressure-composition isotherm adsorption diagram for Ti–H_2 with the parameter temperature in the adsorption diagram [7]. Where $P_i(i = 1, 2, 3), T_i(i = 1, 2, 3), P_{\text{c(ad)}}$ and $T_{\text{c(ad)}}$ denote pressure, temperature, critical pressure and critical temperature, respectively.

experiment starts is at point "C", as indicated on the curve, and the temperature is T_1 and after that, the temperature rise is from T_1 to T_2. At that time, the location of the saturation point moves from point "C" to "G".

As a result, the length of the plateau region shortens. This means that the saturation region of adsorption will shorten and the deuterium gas in the shortened portion, $\overline{CF}$, is equivalent to the deuterium gas desorbed from Ti shavings. When deuterium atoms in ligancy 2 desorb from the Ti shavings, it appears that some portion of their electrons must be taken by the titanium atoms which have adsorbed D atoms and/or the surrounding titanium atoms and become deuterons. They leave from Region I and/or Region II and enter Region III. When deuterons leave Region I and/or Region II, there is the possibility of collision with a deuterium atoms in ligancy 2 and a desorbed deuteron through the medium of their negative charges.

Case 2

Referring to the curve indicated in Fig. 3 and assuming that the experiment starts from point "G", and we change the pressure condition from P_2 to P_1 providing that the temperature T_2 is kept or only risen by a suitable temperature, theoretically; all the portions of adsorbed and saturated deuterium gas must be desorbed in accordance with the characteristics of the curve. It seems that at that time at least, the electrons of some of the desorbed portion of deuterium atoms must be taken by the titanium atoms, as in Case 1.

The working condition in the cylinder in this experiment is the evacuation condition as in neutron generation [4].

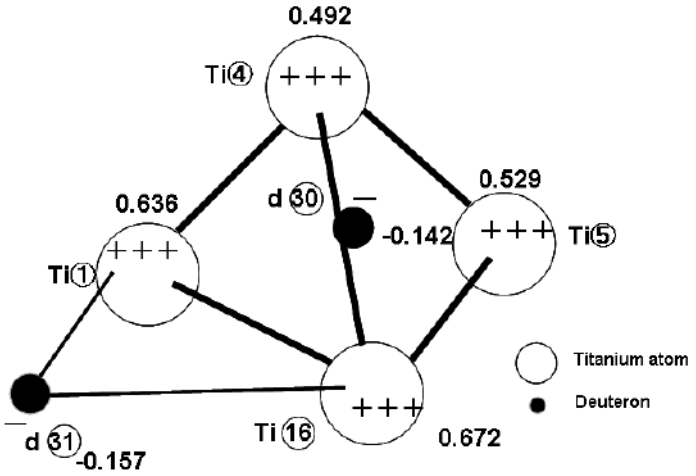

Figure 4. Atomic charge value (bold) in the cluster model 3, in the previous paper [1], a deuterium atom and a deuteron are located inside and outside the cage, respectively.

3. Working Force and Potential Barrier between Two Particles (d–d)

3.1. Working force

Providing that the condition indicated in Fig. 4 is assumed, we think that it is important to consider how strong or large the estimated force (or potential barrier) is between a deuterium atom outside the cage and a negatively charged deuteron inside the cage. We should therefore try to evaluate the numerical value.

Providing that a deuterium atom in ligancy 2 and a deuteron with a negative charge are located at the inlet and inside the cage as in Fig. 4, we can evaluate the working force between them applying Coulomb formula.

$$F = (1/4\pi\varepsilon_0)(qq'/r^2), \tag{1}$$

where F, ε_0, q, q' and *r* denote Coulomb force, vacuum dielectric constant, charge (q, q') and the distance between the two charges, respectively.

Providing that d31 is detected only in the inlet of the cage in Fig. 4; the distance *r*, between q30 and q31 would be ca. 0.604 Å in a tetrahedral cage without distortion and the charge of d30, q30 would be -0.142 eV (q30 $= -0.142 \times 1.602 \times 10^{-19}$ C). If we assume that the charge value does not change at the inlet of the cage, then the charge of a deuterium atom in the front of the inlet of the cage, with a charge of d31, q31 would be -0.157eV (q31 $= -0.157 \times 1.602 \times 10^{-19}$ C) [1], Coulomb repulsive force between them at the inlet should be about 1.41×10^{-9} N (1.44×10^{-10} kg force).

The minimum necessary energy for two deuterons to collide should be greater than that of the potential barrier. When we make d31 collide with d30 by accessing the distance between them from l to D_{d}, where l and D_{d} denote the optional distance and a pion-range or shorter distance than l between them, respectively; and if we substitute the value of each charge q30 and q31 to Eq. (2), respectively, then the energy necessary to make d31 collide with d30 is calculated from

$$W = \int_{D_\mathrm{d}}^{l} (1/4\pi\varepsilon_0)(\mathrm{q30q31}/r^2)\,\mathrm{d}r = (1/4\pi\varepsilon_0)(\mathrm{q30q31})[-1/r]_{D_\mathrm{d}}^{l}. \tag{2}$$

3.2. The potential barrier for two particles to overcome based on Coulomb formula in order to collide

The potential barrier in each condition is calculated in the following.

(1) The potential barrier between two deuterons with the same charge sign and 1 eV each, stems from the following conditions.

The evaluated energy is the worked energy $W_{\text{d-d}}\,(1)$, that two deuterons each accessed from infinite to the distance, $D_\mathrm{d}(D_\mathrm{d} \sim 5.4$ fm).

If two deuterons approach 1.4 fm, the gap between them, is a pion-range, and these two particles will collide with subsequent nuclear fusion. Providing that the radius of a deuteron is 2 fm and the pion-range is 1.4 fm, and we substitute $D_\mathrm{d} = 5.4$ fm and $l = \infty$ to Eq. (2), the calculation result is as follows:

$$W_{\text{d-d}}(1) = (1/4\pi\varepsilon_0)\,(1.0)(1.602 \times 10^{-19})(1.0)(1.602 \times 10^{-19}) \times [-1/r]_{D_\mathrm{d}}^{l} = 267\ \mathrm{keV}. \tag{3}$$

This value is equivalent to the potential barrier in this condition and coincides fairly with the value in Tanimoto's paper [8].

(2) The potential barrier for two deuterium atoms to overcome in order to collide is associated with the following conditions.

We must assume that each charge value of q and q′ is 1.0 and -0.157 eV, respectively, and each charge value does not change while two particles have access to the distance, 25 fm.

(As the distance between two deuterons is ca. 25 fm, the nuclear force between them is nearly equal to zero, we therefore selected this value.)

(a) When one particle is a deuterium atom in ligancy 2 and another particle is a deuteron

We assume that each charge value of q and q′ is 1.0 and -0.157 eV, respectively. The worked $W_{\text{d-d}}(2)$, accessed from $l = \infty$ to $D_\mathrm{d} = 25$ fm is calculated below. It is likely that this energy can be accessed as long as a deuterium atom in ligancy 2 does not change its negative charge before a collision.

$$W_{\text{d-d}}(2) = (1/4\pi\varepsilon_0)(-0.157)(1.602 \times 10^{-19})(1.0)(1.602 \times 10^{-19}) \times [-1/r]_{D_\mathrm{d}}^{l} = -41.92\ \mathrm{keV}. \tag{4}$$

(b) When two particles are deuterons

The potential barrier between two deuterons at a distance ca. 25 fm is calculated in the following.

$(I = \infty, D_\mathrm{d} = 25$ fm)

$$W_{\text{d-d}}(3) = (1/4\pi\varepsilon_0)(1.0)(1.602 \times 10^{-19})(1.0)(1.602 \times 10^{-19}) \times [-1/r]_{D_\mathrm{d}}^{l} = 57.7\ \mathrm{keV}. \tag{5}$$

These calculation results indicate that the difference in the combination condition between a titanium atom and a deuterium atom makes the superficial charge value of a deuterium atom change. As a result, the potential barrier also greatly changes.

However, the evaluation of the force between two particles in the region where the nuclear force influences them, is not included in the previous calculations and neither is the possibility of the access to the distance, (25 fm) between two particles.

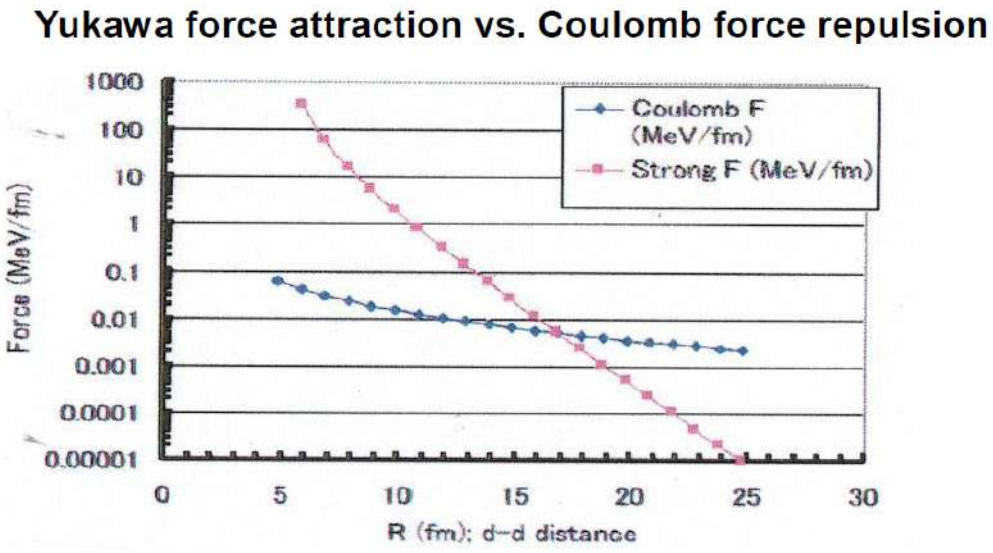

Figure 5. Comparison of repulsive force by Coulomb force and attractive force ("Yukawa force attraction" or "Strong F" in Fig. 5) by nuclear force between two deuterons. Attractive force is calculated by an improved Yukawa formula [9].

4. Coulomb Force and Nuclear Force between d–d Particles

According to the reports of Takahashi [9,10], the comparison of the nuclear force (Yukawa force) and Coulomb force in the near nucleus surface is indicated in the graph, in Fig. 5.

In previous reports [9,10], the nuclear force between d–d results attractive. Figure 5 indicates that Coulomb force (repulsive force) is stronger than the nuclear force between d–d until the distance is nearly equal to ca. 17 fm. The attractive nuclear force works for two deuterons so as to be inversely proportional to the distance between them. On the other hand, nuclear force only works a bit until two deuterons access to ca. 25 fm. When the two deuterons access to ca. 17 fm, the absolute values of repulsive and the attractive forces are nearly the same and after closer access, the attractive force exceeds the repulsive force.

Two curves indicate that if we can add a suitable amount of energy at a specified distance between two deuterons when the nuclear force exceeds the repulsive Coulomb force to an accessing deuteron, then they will be able to collide each other, even if each of the two particles have the same charge, 1 eV.

Using the original Yukawa formula regarding nuclear potential, the formula of nuclear force between each nucleus is introduced in the following:

$$F_n = -ge^{\kappa r}(1/r^2 + \kappa/r), \tag{6}$$

where g and κ are constants. (Constants g and κ are produced by fitting them to the improved Yukawa formula, $g = -8.501 \times 10^4, \kappa = 0.804$.) r is the distance between two nuclei (fm) and F_{n} is the nuclear force (MeV/fm). The results of the calculations regarding $F_{\mathrm{n}}, F_{\mathrm{lig2}}$ and F_{c} are indicated in Fig. 6. Where $F_{\mathrm{n}}, F_{\mathrm{lig2}}$ and F_{c} denote nuclear force and Coulomb forces between d-d including a deuterium atom in ligancy 2 and pair charge values of each force are F_{n}: (1 eV, 1 eV), F_{lig2}: (1 eV, -0.157 eV) and F_{c}: (1 eV, 1 eV), respectively.

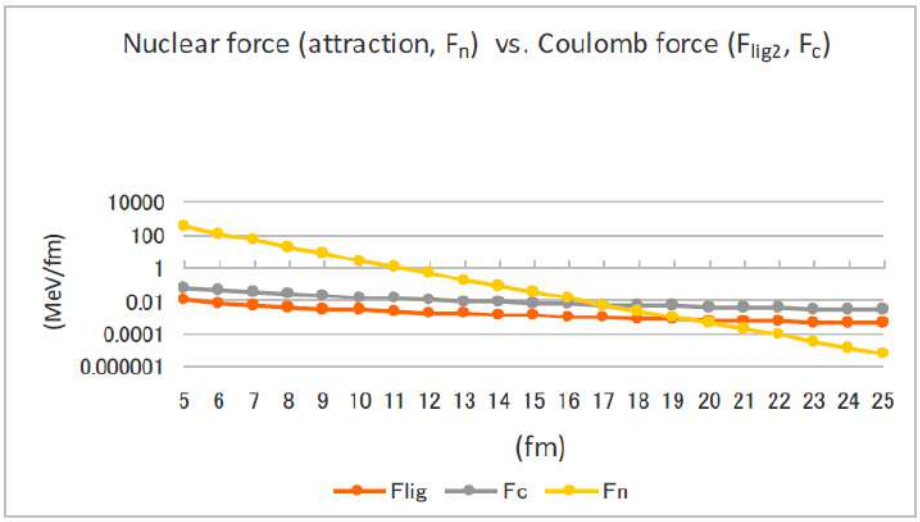

Figure 6. Comparison of Coulomb forces and attractive nuclear force. All the forces are indicated in their absolute values. F_{n}: nuclear force (attraction), F_{c}: Coulomb force (repulsion), F_{lig2}: Coulomb force (attraction).

In the Ti shavings adsorbed deuterium atoms, there are deuterium atoms in ligancy 2 in a Ti–d system which locally forms polar compounds. So if the suitable alternative electromagnetic wave is irradiated to a Ti–d system, desorbed deuterons and deuterium atoms in ligancy 2 must periodically move changing in opposite directions of each other with a positive and negative charge respectively in accordance with the frequency change.

It appears that the electron deficient titanium atoms constrain the electrons of deuterium atoms or take them. As a result, it means that the potential barrier will change. It seems that the absolute value of energy to add may only be a little bit or it may not be necessary at all by the tunnel effect, if the nuclear force is equal to or greater than the repulsive Coulomb force at ca. 17 fm. Even if two particles each have the same charge, 1 eV, the nuclear force will dramatically increase in inverse proportion to the distance between two nuclei.

For two particles to collide, we think that it is preferable to add additional energy to an accessing deuteron. However, it is most important to note how a deuteron will be able to access distance $<$ 17 fm from a deuterium atom in ligancy 2, without changing either charge.

5. The Presumed Nuclear Fusion Process in the Titanium Crystal Adsorbed Deuterium Atoms

When deuterium gas and titanium crystal adsorbed deuterium atoms are in an equilibrium state under a suitable pressure and temperature, even a slight temperature rise will break this equilibrium state and they will proceed to a new equilibrium state. As a result, it seems that the electrons of some portion of the desorbed deuterium atoms in Regions I and II (Fig. 2) are then taken by the titanium atoms or by the surrounding titanium atoms at desorption and proceed to Region III via Region II, where there should be a large quantity of deuterium atoms in ligancy 2 at saturation.

The authors envision that if the charge sign of the deuterium atom becomes positive and Coulomb force, based on the above mentioned concept, works between the deuterium atom in ligancy 2 outside the cage and the deuterons which move from Regions I and II, and the suitable amount of energy by alternative electromagnetic wave is irradiated,

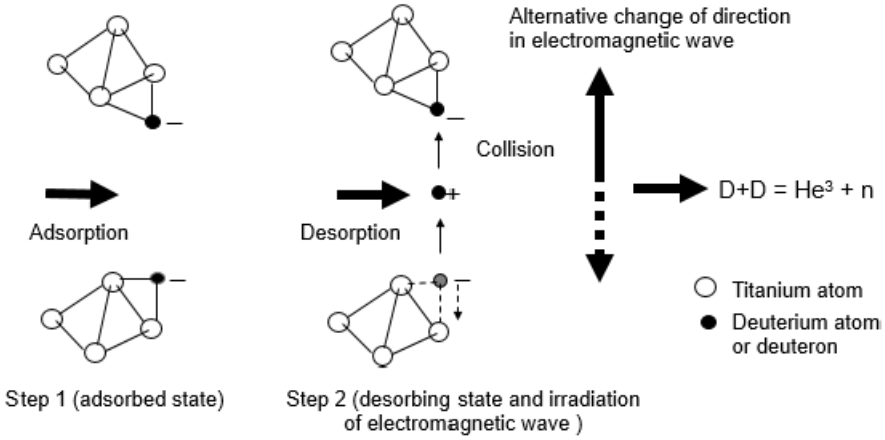

Figure 7. NFP model 1 in the titanium crystal adsorbed deuterium atoms.

there is a high possibility of a collision.

If the additional energy to overcome the repulsive force by Coulomb force before entering into the superior field of the attractive nuclear force in the near surface of the nucleus is added at the distance l for example, $17 < l < 25$ fm, to such a non-equilibrium condition in the Ti–d system, especially to free deuterons, it appears that there will be a higher probability of nuclear fusion being achieved because the nuclear force in d–d is attractive.

Nevertheless, it seems that if the deuterium atom in ligancy 2 with the charge -0.157 eV, does not lose its negative charge until the distance between it and the accessing free deuteron is less than ca. 17 fm, then the two particles will be able to collide with each other. After these particles access a distance closer than ca. 17 fm, the attractive nuclear force will begin to work, even if the charge of the deuterium atom in ligancy 2 changes from -0.157 to 1 eV.

Evidently, it is unconceivable for a free deuteron to directly enter into the plane within the orbit, including the nucleus and its related electron, without being given suitable kinetic energy, because each particle may change its charge and the power balance between them at that time would be unstable.

Presumed nuclear fusion process (here after referred to as "NFP") models in the titanium crystal adsorbed deuterium atoms are indicated in Fig. 7 (NFP model 1) and Fig. 8 (NFP model 2).

To accurately evaluate the energy required to increase the probability of nuclear fusion, we think that the information of the electron orbit and each charge of atoms relating to the deuterium atom in ligancy 2 are necessary, especially, the orbit form and each radius length in periapsis and apoapsis. Based on these information, the energy needed for nuclear fusion to occur will be calculated.

In NPF model 2, we think there may be a possibility of double or triple collision of deuterons.

The most important matter is how accessible the minimum distance between two particles is, after the collision with a negative charged deuterium atom in ligancy 2. Then, if the distance of two particles is within the attractive region that is stronger than that of the repulsive region, there will be chance of nuclear fusion.

6. Conclusion

Based on computational results and published reports, we have investigated the possibility of the nuclear fusion in titanium crystal.

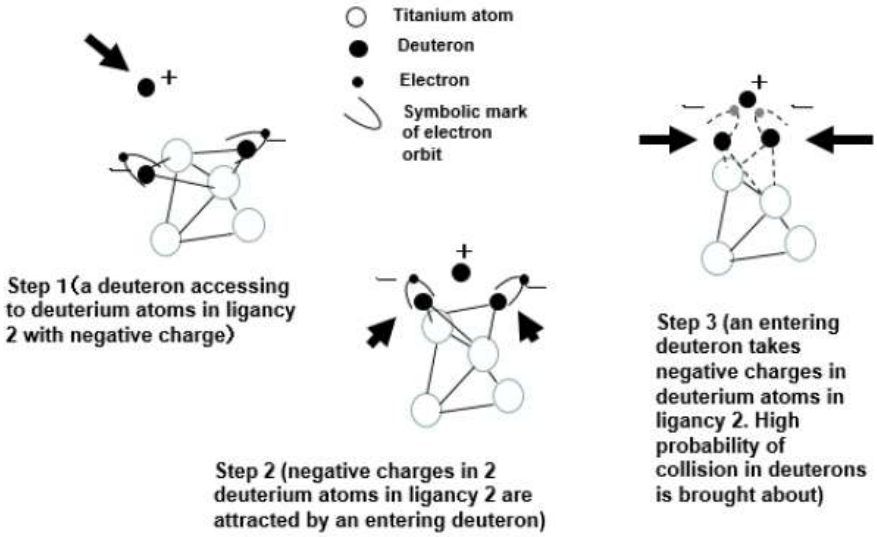

Figure 8. NFP model 2 in the titanium crystal adsorbed deuterium atoms.

We thought that the temperature at which a non-equilibrium state occurs was not at one single specific value, but that there were several temperatures which are lower than the temperature $T_{c(ad)}$ indicated in Fig. 3. This presumption confirms the past experimental results [3,4]. That is, that there are several conditions in which a non-equilibrium state occurs in both pressurization and evacuation conditions.

Regarding a non-equilibrium state, firstly, deuterium atoms locally form a polar compound in ligancy 2 with titanium atoms in titanium crystal and each deuterium atom in ligancy 2 has a negative charge. Under the pressurized or evacuation condition and with an additional suitable temperature rise, it appears that some portions of adsorbed deuterium atoms desorb from the titanium atoms and they become deuterons with a positive charge.

Secondly, as there are some particles (deuterons) which have a positive charge within them and others (deuterium atoms in ligancy 2) that have a negative charge inside, and providing that these charges do not change, they are then able to access one another within the working region of Coulomb force.

According to Takahashi's report, the nuclear force between d–d is attractive and it is nearly equal to the repulsive Coulomb force at the distance of ca. 17 fm at the dividing distance of ca. 17 fm when they have the same charge, +1 eV. For larger distances ($>$ 17 fm), the repulsive Coulomb force is stronger than the attractive nuclear one [9,10].

We think that even if the charge sign of a deuterium atom in ligancy 2 is changed during the accessing process of a deuteron, the added suitable amount of energy and the nuclear force will be able to overcome the repulsive Coulomb force and the two particles will be able to access each other, therefore colliding and nuclear fusion will be achieved.

To promote the nuclear fusion effectively, a necessary amount of energy needs to be added to the desorbed deuterons to overcome the Coulomb force and it needs to be determined by means of a more detailed theoretical and experimental setup.

To increase the probability of nuclear fusion in a Ti–d system, we now believe that it is necessary to add a suitable amount of energy. As a possible means to provide energy, the irradiation of an alternative electromagnetic wave energy is a possibility we would like to confirm in a future experiment.

Addendum

The authors had the information of a case study which was to reserve the hydrogen in a cylinder for the use of a fuel tank of an automobile.

At that time, we intended to similarly apply the example of a reservation cylinder of acetylene. In the cylinder, we packed Ti–Fe alloy grain with 5–10 mm equivalent diameter size to adsorb hydrogen gas instead of diatom earth and acetone.

When we reserved the hydrogen gas, we found that at first the adsorption quantity of the hydrogen was smaller than after conducting the adsorption and desorption operation several times. Therefore, it is recommendable that preliminary adsorption-desorption operations are executed before starting the adsorption operation. For example, the pressurizing and depressurizing of hydrogen in the cylinder can be repeated between ambient pressure and 2.5 MPa. After this operation, the adsorption quantity of hydrogen will increase greatly.

The authors think that this tendency is also the same in Ti shavings as that of the Ti–Fe alloy grain. In the experimental operation, caution is necessary as repeatedly pressurizing and depressurizing will cause the pulverizing of the Ti–Fe grain. This pulverized Ti–Fe powder sticks inside the piping. So, it is recommendable to equip a filter at both the inlet and the outlet of the cylinder packed with Ti shavings.

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