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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"

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Abstract

This paper describes the analysis and study of the neutron generation experiment performed under pressurized and/or evacuated conditions between room temperature and liquid nitrogen temperature, using titanium shavings and deuterium gas packed in a cylinder. To clarify the mechanism of this phenomenon, the author has studied the experiment taking into account the characteristics of the phase equilibrium, the metal crystal construction, the theory of chemical bond and the first principle molecular orbital calculation. From the result of this study, it seems that the same phenomenon will happen in a similar experiment performed using another electron deficient metal with a suitable crystal construction.

Keywords: Crystal lattice, Deuterium, Neutron generation, Octahedron cage, Tetrahedoron cage, Titanium

1. Introduction

There are many reports on deuterium nuclear fusion at room temperature. However, some of them have not had sufficient plausible evidence to prove them and the others are doubtful.

Out of these reports, the experiments performed by ENEA, etc. appear to have been performed by suitable devices and measurement methods [1–3]. Although it is preferable that more reproducible experiments will be executed, we cannot deny the experimental results. It seems that they achieved neutron generation using titanium shavings and deuterium, which is performed in a process similar to that of deuterium adsorption and desorption.

The author has intended to study the behavior of deuterium in each process of the experiment, and has studied the conditions for deuterium atoms or deuterons to collide and the possibility of nuclear fusion occurring at room temperature, applying both the theory of chemical bond and the first principle molecular orbital calculation.

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2. The Main Process, the Conditions of the Experiment and Explanation of Each Step

According to the experiment performed by ENEA [1] and LANL [2], neutrons are generated during the course of warming the cylinder containing pressurized deuterium and titanium shavings with adsorbed and/or combined deuterium, and at the condition of nonequiliblium such as a change of particular temperature and pressure in the process of adsorption/desorption of deuterium in titanium.

The main process of the experiment and the conditions of the experiment are as follows:

Step 1: It is the generation process of the combined material of titanium and deuterium (from here on we will call it "combined material") by adsorption, etc., under the pressurized condition in the cylinder made of stainless steel. Pressure: 2–5 MPa, Temperature: room temperature

Step 2: It is the process of the cooling of the cylinder (Ca. 80 K) in the liquid nitrogen bath.

Step 3: It is the process of removing the cylinder from the liquid nitrogen bath and leaving the cylinder to warm until it reaches room temperature (we assume it is Ca. 300 K).

3. Generally Predictable Behavior of Deuterium Inside and/or on the Titanium Shavings in Each Step

In Step 1, deuterium will enter and subsequently diffuse throughout the crystal lattice of titanium metal, forming the combined material.

According to other experiments dealing with the characteristics of adsorption and desorption, the deuterium behavior in this process is similar to the graphical curve of pressure-composition isotherm adsorption with the parameter, temperature. In particular, it is similar to the characteristics of substances that also show hysteresis as shown in Fig. 1 [4].

The type of titanium crystal has a hexagonal close-packed (hcp) structure. It is said that there are three locations, where deuterium atoms or deuterons are able to be located in titanium crystal. The locations where deuterium atoms are able to locate under the suitable condition are in the tetrahedral interstice (T-site), in the octahedral interstice (O-site) formed by titanium atoms, and in the location between two titanium atoms in the c-axes of the crystal in Fig. 2 [5].

Figure 2 simply shows the structure of titanium crystal lattice and the inferred location of deuterium.

In Step 2 (the cooling of the cylinder) the saturated region of deuterium in titanium metal that expresses the length of the plateau region in the phase diagram indicated in Fig. 1, will become greater than that of room temperature, by the formation of combined material. In this step, it seems that deuterium atoms will go further into the titanium and diffuse into the lattice of titanium metal.

In Step 3, because of the temperature rise, in accordance with the characteristics of phase equilibrium, some portion of the deuterium must exit from the constrained state in titanium and the length of the plateau region in the phase diagram becomes less than that at liquid nitrogen temperature. It indicates that some portion of deuterium in the combined material is released to the gaseous phase over the course of the temperature rise, relating to adsorption phase change as written standard book.

When we compare the strength of constrained deuterium in T-site and O-site and deuterium in another site, it appears that trapping potential depth in the different sites differs with each other because the combined condition with titanium atoms differs.

According to the experimental results [1,2], it is said that substantial bursts of neutron counts (Ca. 70 and Ca. 100, respectively) were observed after the cylinder was removed from the liquid nitrogen bath. In the one experiment, it says that the average count in the active period run (at desorption phase from liquid nitrogen temperature warming to room temperature) was much higher than the previous run (at pressurized condition with thawing terms and cooling cycles). In the other experiment, the pressurized cylinder had to experience several thermal cycles before neutrons were

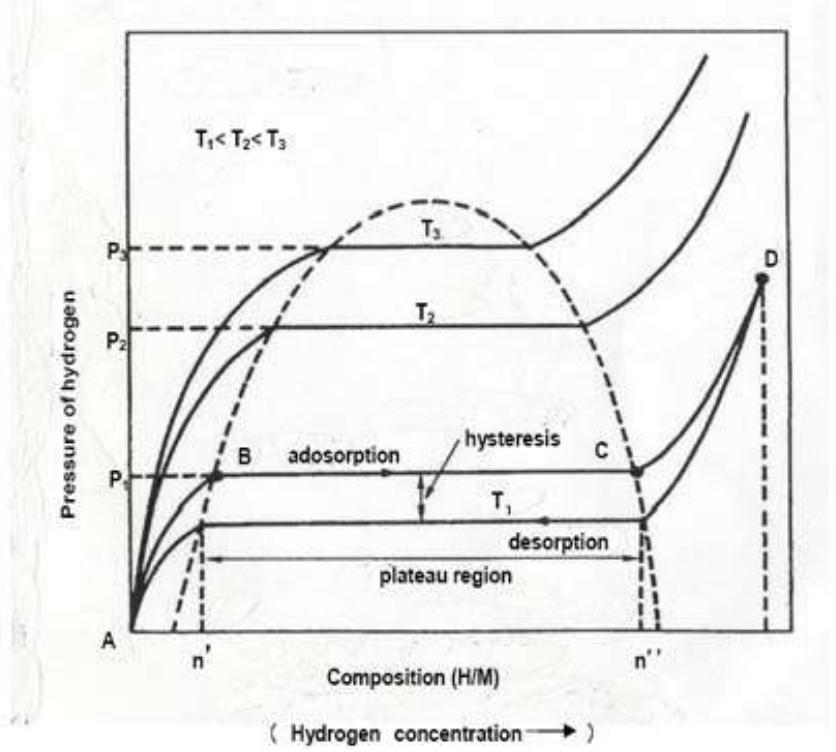

Figure 1. Pressure-composition isotherm adsorption with the parameter, temperature [4].

detected. About 1 h into the warm up cycle, when the pressurized cylinder was at –30°C, high neutron counts (∼85) were observed, followed by smaller bursts.

It is inferred that any reaction must occur in a condition of nonequilibrium, such as a change of pressure and/or temperature.

4. The State and Behavior of Deuterium Atoms in Titanium Crystal

4.1. Analysis of the state of deuterium atoms in titanium crystal based on the theory of chemical bond

4.1.1. *Bonding state of the deuterium atoms and the titanium atoms in the tetrahedron cage*

In the following, the author will study the mechanism of the bonding of deuterium atoms with titanium atoms in accordance with the theory of chemical bond, taking into account the electron orbits of titanium.

The reason why the deuterium atoms are stable in that location must be because they combine with the titanium atoms by a specified chemical bond. As an example of an electron-deficient substance, when boron forms diborane (B_2H_6), the boron atoms cause adjacent hydrogen atoms to have ligancy (number of stable positions (potential well) for H(D)) 2 as indicated in Fig. 3 [6,7].

It seems that a deuterium atom and the titanium atoms jointly own the valence electron located outside the argon shell in the electron orbits of the titanium atom; the deuterium atom and titanium atoms form a coordinate bond. In the

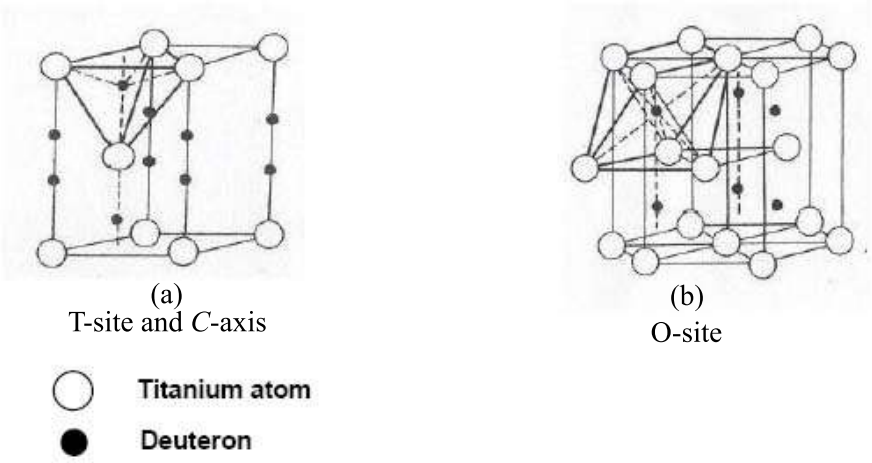

Figure 2. The location of deuterons in the titanium crystal lattice [5].

following, we will study why this combination is formed.

By the same process as the formation of diborane, it seems that the titanium atoms forming the cage can also cause the entering deuterium atom to have ligancy 2. The reason why it is deemed so is because the electron orbits and their respective number of electrons regarding a titanium and argon atom are as follows:

Titanium: $(1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6)\ 3d^2\ 4s^2$

Argon: $(1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6)$

According to the theory of chemical bond explained by Pauling [8], there are nine stable orbits, $3d^5 4s 4p^3$, outside this shell. Even if these nine orbits are occupied by nine electrons, 0.72 is allocated as metallic orbit, leaving 8.28 for occupancy by bonding electrons and unshared electron pairs.

On the other hand, the titanium atom has four electrons outside the saturated orbits (argon shell). As compared to the number of electrons, four, in the part of the titanium electron orbits outside the argon shell and nine, the total

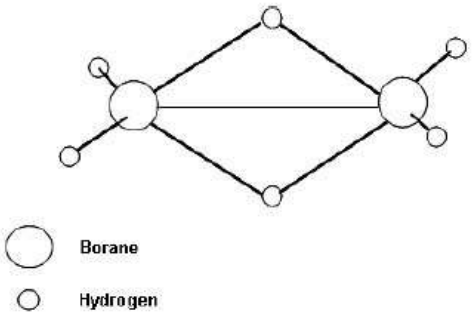

Figure 3. The configuration of atoms in diborane, $B_2\ H_6$ [6, 7].

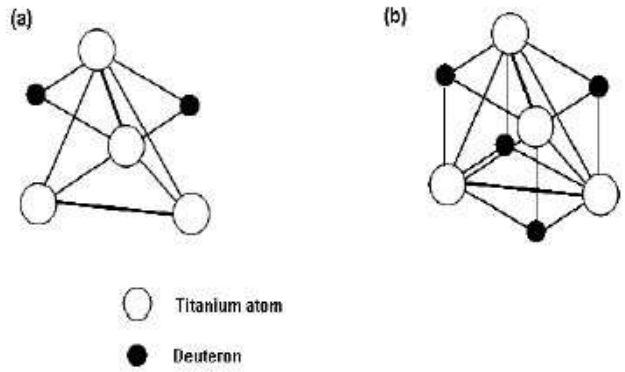

Figure 4. Ti cage models with two bridged deuterium atoms.

number of electrons outside the argon shell is far less than the preferred number of electrons to be stable, which is nine.

As a result, it seems that the electrons left from the deuterium atoms that entered the titanium metal will move toward the titanium orbits side. On the other hand, to get to a stable condition, deuterons will have a tendency to jointly own the electron with the titanium atoms.

As an example of diborane, Ti atom also is electron-deficient substance. So we can easily guess Ti atoms cause two deuterium atoms to have ligancy 2 as in the case of diborane. So it seems the adsorbed two deuterium atoms will also form ligancy 2. In this condition, it seems that two Ti atoms will prepare two bridged deuterium atoms indicated in Fig. 4a. If two orthogonal pairs of two Ti atoms in the T-site will prepare two bridged deuterium atoms per each Ti pair, the classical model will be indicated as in Fig. 4b.

This form is equivalent to the Tetrahedral Symmetric Condensate (TSC) model which is presented by Takahashi [9]. It seems that four electrons that have left from each deuterium atom may form bosonized pair [9] in the outer orbit of each Ti atom forming two orthogonal edges of the tetrahedron cage of which the edge is composed of two Ti atoms. According to hypothesis of Takahashi, it says that strong central squeezing force may happen by TSC plus four spin-regulated (bosonized) electrons. However, the author's model is a form of combined material produced just after deuterium atoms entered into Ti crystal. On the other hand, Takahashi's model is the form with very short life assuming when the reaction happens in transient state under the special condition. So, the author thinks that his model is different from the author's model, and is a model which is a work in progress.

4.1.2. *Geometrical relation of the deuterium atoms in the tetrahedron cage*

In the case of titanium, its crystal is in the form of a hcp structure including cages as mentioned above.

Assuming that one of the cages is a regular tetrahedron and the titanium atoms are sphere like shape, the diameter of the inscribed sphere, between the three spheres of titanium atoms and within the regular triangular surface formed by the centers of three titanium atoms, is approximately 0.502 Å indicated in Fig. 5a. As the diameter of a deuterium atom is approximately 1.06 Å, if the deuterium atom intends to enter the tetrahedron cage, it must not be as a deuterium atom (D) but as a deuteron (d) having lost an electron. In the case of deuterons, it seems that each of them will be able to pass through the inlet of the cage provided that Coulomb repulsion is shielded, as its diameter is approximately 10^{-4} Å.

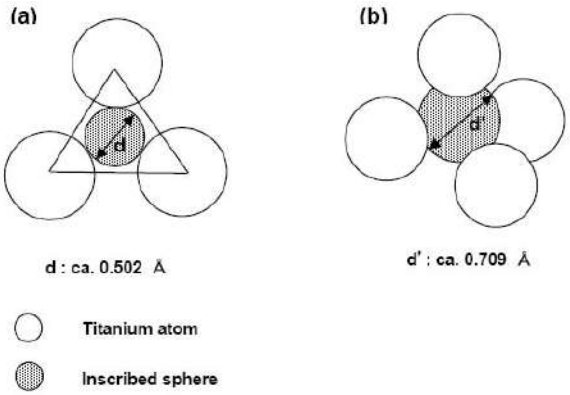

Figure 5. Conceptual figure of the tetrahedron cage in titanium crystal. (a) and (b): the diameter of the inscribed sphere.

4.1.3. *Deuterons able to exist in the tetrahedron cage*

Inside of the tetrahedron cage, the diameter of the inscribed sphere is approximately 0.709 Å indicated in Fig. 5b. So the distance from the center of this inscribed sphere to the center of the titanium atom is approximately 1.81 Å. On the other hand, using the average covalent radius of hydrogen, 0.3 Å [10], the estimated Ti–D distance is approximately 1.78 Å, assuming that both Ti–D and Ti–H distances are equal. Regarding the bridged Ti–D(-Ti) distance, it may slightly be longer than that of a single bond of Ti–D which is similar to the example of the distance of B–H (Ca. 1.19 Å) and bridged B–H(-B) (Ca. 1.33 Å) of diborane [6]. Anyhow, the estimated Ti–D distance coincides well with the distance from the center of the inscribed sphere to the center of the contacting spheres, Ti atoms.

4.1.4. *Plausible behavior and possibility of collision of deuterons in the tetrahedron cage*

As it is said, in the case of the tetrahedron cage, the location where a deuterium atom or deuteron is able to locate is in the cage.

As previously mentioned, we can infer that combined material as indicated in Fig. 4 will be formed. After that, as there is a stable location in the cage, it seems that the deuterium atom or deuteron in the state may intend to get to the stable location as indicated in Fig. 6 if the condition of nonequilibrium state occurs, such as changing of deuterium

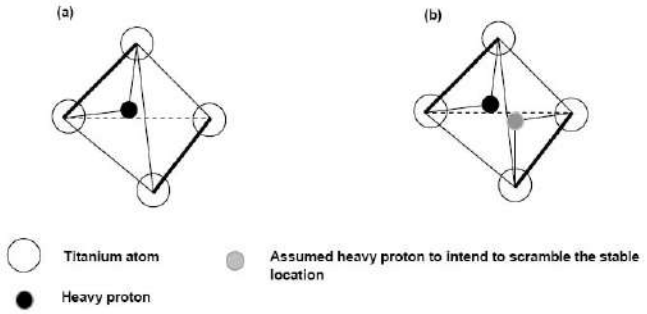

Figure 6. Ti cage models with the bridged deuterium atom in the T-site.

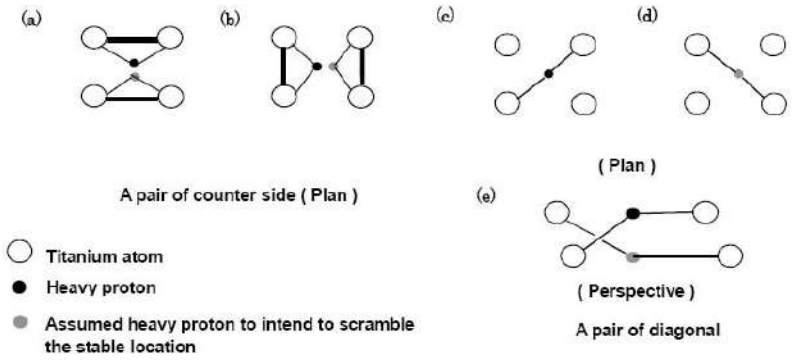

Figure 7. The heavy protons model in the O-site. (a), (b): a pair of counter side (plan), and (c), (d): a pair of diagonal side (plan), (e): a pair of diagonal side (perspective).

pressure and/or temperature in the cylinder.

If plural deuterium atoms or deuterons will enter the cage, collision may occur in the cage.

The constrained two deuterium atoms at the edge of the cage without a strong Coulomb repulsion by the bridging bond of ligancy 2 are electrically neutral. It may be that under this condition, deuterons do not need an enormous amount of energy to collide.

If we estimate the kinetic energy of a free deuterium atom at 80 and 300 K, the energy of each is 6.9 and 25.9 meV, respectively.

4.1.5. *The state of the deuterium atoms combined with the octahedron cage formed by titanium atoms*

As in the case of the tetrahedron cage, it is said that there is a location where a deuterium atom or a deuteron is able to locate in the octahedron cage.

If we take out a quadrilateral pyramid cross section from the octahedron cage that is formed by titanium atoms, and set our eyes to the square part composed of two titanium atoms and a summit atom, both the diameters of the inscribed sphere within the top half pyramid and the inscribed sphere within the square cross section are Ca. 1.27 Å. So if the deuterium or deuteron is located in these locations of O-site, there is more space than in that of the T-site. As it is said, if the heavy proton is located in the center of the O-site, the location is that of the latter of the case mentioned above. In this cross section of the square area formed by four titanium atoms, two titanium atoms must be selected to get to the stable condition of deuterium atoms by forming the bridging bond of ligancy 2. Geometrically, there is a total of six possible independent Ti pairs of chemical combinations with a bridged deuterium atom in this part. These pairs are selected from the side parts and diagonal line parts in the square which is formed by Ti atoms indicated in Fig. 7.

If we assume the two heavy protons are constrained by two diagonally opposite titanium atom pairs indicated in Fig. 7c–e, both heavy protons in the cage will be localized along the centerline of the square, and move near the center point of the square. If the collision of caged heavy protons occurs, chances are that it will occur by the heavy protons constrained by two diagonally opposite titanium atom pairs of the different diagonal. However, the length of the diagonal is Ca. 4.18 Å and it is slightly longer than two times the estimated Ti–d distance, 3.56Å.

It seems that it is difficult to more precisely estimate the condition for the deuterium to locate by only the theory of chemical bond.

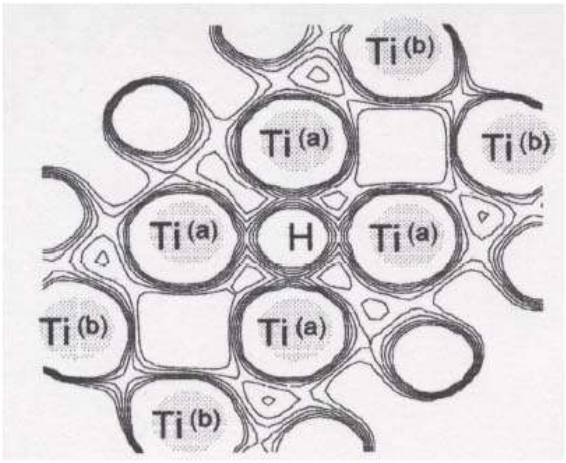

Figure 8. The distribution of charge density for (2–203) plane of Ti H3 (7.69 at.% H) cluster [11].

4.1.6. *The state of the deuterium atoms on the c-axis of titanium crystal*

The *c*-axis length of titanium crystal is Ca. 4.74 Å and it is said that two deuterium atoms can be located on the *c*-axis between titanium atoms [5]. The nearest titanium atom from the deuterium atom is at the end of this axis. If a deuterium atom combines with a titanium atom, it will be the titanium atom located at the end of the *c*-axis. Under this condition, we cannot find special condition for deuterium atoms to collide.

4.2. Analysis based on the first principle molecular orbital calculation

At present, there are not only the analysis based on the theory of chemical bond but on the first principles calculations. By comparison an analysis basing on a different stand point, it seems that we will be able to deduce a more precise state of deuterium in titanium crystal.

As there is the research of electronic structure of the Ti–H solid solution by a first principle molecular orbital calculation, the author cites in Figs. 8 and 9 [11]. Figure 8 shows the distribution of charge density around a hydrogen atom on Ti–H solid solution cluster.

Essentially, both the distance and the bonding force between Ti atom and H atom in the symmetrical location can be the same as each other. The bond between the second nearest Ti atoms ($Ti^{(b)}$) from the H atom in the center is strongly formed with each other. However, there is clear difference in the bond between the first nearest Ti atoms ($Ti^{(a)}$) and $Ti^{(b)}$. In diagonally face side Ti atom pairs surrounding H atom, there is a slight difference in the distribution of charge density between vertical and horizontal bonds of Ti and H atom in Fig. 8. It seems that there is a possibility the horizontal 2 face side Ti atoms pair may cause the hydrogen to have ligancy 2, although, of course, the resonance will occur between these pairs .

Figure 9 [11] shows the density of states of solid solution. In Fig. 9, density of state of 3d orbital of titanium decreases with increasing of hydrogen content and that of 4s orbital of titanium also slightly decreases with increasing of hydrogen content. It means that the electrons of 3d orbital of metallic bond is used for bonding between Ti atoms and the hydrogen atom.

In a regular octahedron cage, each orthogonal plane including the center line and the diagonal line of the square to (2–203) plane also has two diagonally face side Ti atom pairs. So it means that another Ti pair in the other planes

can cause hydrogen to have ligancy 2 if there is a hydrogen atom between them. On the other hand, there is only one location where H is stable is in the octahedron cage.

So, in a condition of nonequilibrium state inside and/or outside Ti metal, such as changing deuterium pressure and/or temperature, if deuterium atoms or deuterons scramble the location of each other, collision may occur near the center of octahedron cage.

As another inference of this analysis, in Ti metal composed of dense crystal, it seems that it may be difficult for two deuterium atoms in ligancy 2 to exist as indicated in Fig. 4. except Ti atom pair at cleavage plane and/or metal surface.

In other chance, the author would like to also analyze the tetrahedron cage, from both the theory of chemical bond and the first principles calculations.

5. Discussion and Conclusion

To clarify the mechanism of neutron generation experiment, the author analyzed the site and state of adsorbed deuterium into titanium metal, basing on both the theory of chemical bond and the first principle molecular orbital calculation.

As a result, it seems that the titanium atoms forming the cage cause the deuterium atom to have ligancy 2, especially at diagonally 2 face side Ti atoms in octahedron cage, from both the theory of chemical bond and the first principle molecular orbital calculation.

If two bridged deuterium atoms combine with two Ti atoms as "combined material", as same as that of diborane and bosonized electrons are produced in the orthogonal Ti pairs of the tetrahedron cage, its form is equivalent to TSC form presented by Takahashi. However, their images of each concept are different from each other.

On the other hand, taking into account of the result of the first principle molecular orbital calculation, it seems that the driving force for deuterium to collide may be scrambling force to get to the stable location by the deuterium atoms between different diagonally two face side Ti atom pairs in the octahedron cage. This situation may occur in a condition of nonequilibrium state, such as the change of temperature and/or pressure.

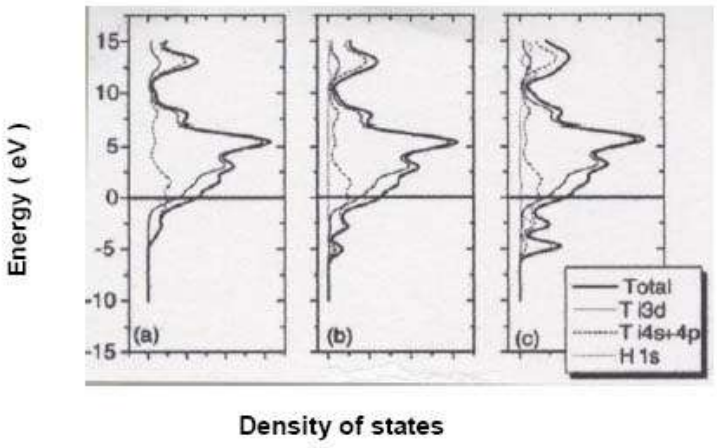

Figure 9. Density of states from (a) Ti, (b) TiH1 (2.70 at.% H), and (c) TiH2 (5.26 at.% H) cluster [11].

If the above-mentioned concept on the room temperature nuclear fusion is right, the observed phenomenon may also occur in an experiment under the condition of nonequilibrium state, such as changing pressure and/or temperature even with another element which is electron deficient, has suitable crystal construction and adsorbs the deuterium.

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