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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" (2)

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Abstract

Following the previous study of the state of deuterium atoms in the titanium crystal (*J. Condensed Matter Nucl. Sci.* **5** (2011) 7), in this paper, the authors have analyzed the state of the deuterium atom in a tetrahedron cage, using the first principle molecular orbital calculation. In the simulation analysis of the tetrahedron cage, it is indicated that the titanium pair causes the deuterium atom to have ligancy 2 in the cage with two hydrogen atoms. If neutron generation occurs, we can deduce from the past experimental results that it occurs after a small increase of kinetic energy of deuterium atoms. This suggests that the quantity of neutron generated may increase if we can give kinetic energy to the adsorbed deuterium atoms in the titanium crystal by another means other than a temperature rise, at a suitable temperature and pressure. The authors propose a new experimental apparatus which appears to promote and increase the neutron generation.
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Keywords: Deuterium, Neutron generation, Proposed apparatus, Tetrahedron cage, Titanium

1. Introduction

In the previous paper [1], the author studied the experiment of neutron generation, using titanium shavings and deuterium gas packed in a cylinder [2,3], taking into account the factors which are related to it and the example of the first principle molecular orbital calculation.

Following the previous study of the state of deuterium atoms in the titanium crystal, the authors have here intended to study the state of deuterium atoms in the tetrahedron cage of titanium crystal and to analyze its mechanism mainly

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based on the first principle molecular orbital calculation. Furthermore, the method to promote the neutron generation is studied.

2. Assumed Tetrahedron Cage Model of Titanium Crystal with the Deuterium Atom

It is said that one of the locations where a deuterium atom is able to be located under suitable conditions is in the tetrahedral interstice. To study the state of the deuterium atom in the tetrahedron cage in detail, the electronic structure of the titanium–hydrogen (Ti–H) cluster models instead of titanium–deuterium (Ti–D) cluster models have been studied by the first principle molecular orbital calculation. It seems that the calculation results of both of these are almost the same and the convergence in the calculation of the former case is faster than that of the latter case.

Prepared cluster models are as follows.

The first is a regular tetrahedron cluster model (hereafter referred to as "model 1") indicated in Fig. 1 and the second is a cluster model which is composed of the tetrahedron cluster surrounded by minimum titanium atoms (hereafter referred to as "model 2") indicated in Fig. 2 (a).

The following explains why model 2 was prepared. The nearest distance from the deuterium atom to any titanium atom in model 1 is of equal distance apart, providing that the location of a deuterium atom is in the center of gravity. However, as there is the possibility of influence to the Ti–H cluster by the surrounding surplus titanium atoms, model 2 has been constructed.

If we calculate the parameters, such as Mulliken atomic charge, etc., indicating the combined state between the titanium atoms and the deuterium atom, the difference in numbers of total titanium atoms by adding titanium atoms to model 1 may be revealed in the simulation result. In the actual experiment, it seems that it is almost impossible for the deuterium atom in the cage to collide and react with another deuterium atom in the other tetrahedron cage, therefore we determined to analyze models 2 and 3.

Under the specified state, the combination between titanium atoms and hydrogen atoms may indicate stable ligancy 2 in the simulation. Under this assumption, the Mulliken atomic charge value based on the Mulliken density analysis and atom–atom overlap-weighted NAO bond order (hereafter referred to as "weighted bond order") [4] calculated are indicated in the development drawings of models 2 and 3. Model 3 is the modified model 2 with a hydrogen atom just outside of the tetrahedron cage in the center of it, see Figs. 3 and 4, respectively. In these figures, each circled number indicates the named number of each atom. In Fig. 3 for the cluster model 2 and in Fig. 4 for the cluster model 3.

Estimated results regarding model 2 are indicated in Fig. 3 by numerical value. Although it seems that the distance between the deuterium atom and the nearest titanium atoms in the assumed model 3 is equal to one another, the Mulliken atomic charge value based on Mulliken density analysis (hereafter referred to as "atomic charge value") for each titanium atom is not the same. These differences in combination are observed in the parameters indicated in Figs. 3 and 4.

The simulation of the cluster model 2 indicates that the titanium atoms do not clearly cause the deuterium atom in the cage to have ligancy 2. The atomic charge values of each titanium atom in the cage become almost the same value except Ti(1) (Fig. 3). On the other hand, the atomic charge value of hydrogen is negative and its absolute value is small. It is observed that the hydrogen atom partially co-owns the electron of titanium atoms. However, in Fig. 4, as a hydrogen atom is added to the titanium atoms outside of the cage in cluster model 2, the atomic charge value of Ti(16) indicates higher values than that in Fig. 3. The atomic charge value of Ti(1) changes little and is almost equal to the value of Ti(16). As these titanium atoms cause the nearest hydrogen atoms to have ligancy 2, it seems that the atomic charge values of Ti(1) and Ti(16) will indicate higher values than those of Ti(4) and Ti(5).

Moreover, weighted bond orders, Ti(1)-H(31) and Ti(16)-H(31) become bigger compared to those indicated in Fig. 3. This suggests that the formation of the hydrogen bond in ligancy 2 is as described in our previous paper [1].

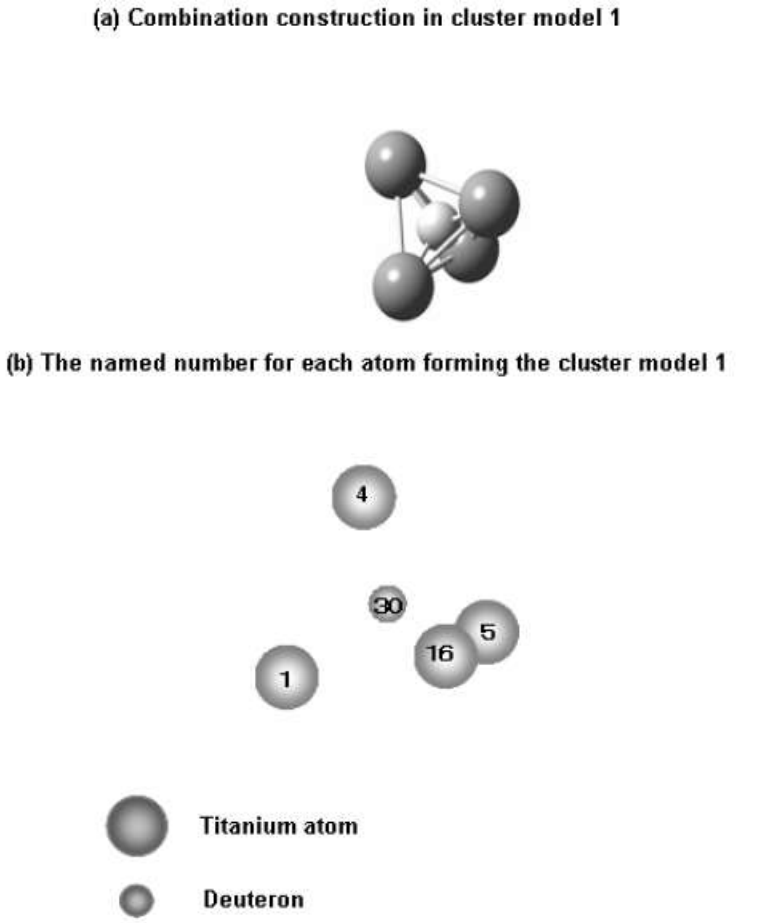

Figure 1. The cluster model 1, regular tetrahedron cage, (a) and (b).

3. The Study of the Experimental Apparatus to Cause Promotion of the Neutron Generation

From the result of the past experiments [2,3], it is observed that the conditions for neutron generation to occur are composed of the following items.

(1) Preparation of titanium shavings in the stainless steel cylinder which have fully adsorbed deuterium gas at a low temperature under a pressurized condition.
(2) About a 160–220 K temperature rise from liquid nitrogen under pressurized or evacuation condition in the above-mentioned cylinder.

Item (2) mentioned above, appears to trigger the process of neutron generation. It means an increase of kinetic energy of the deuterium atoms in the titanium crystal.

If the nuclear fusion occurs by the collision of deuterium atoms in the cage of titanium crystal, the increase of kinetic energy of the deuterium atoms adsorbed in the titanium crystal may be able to promote it and thus increase the

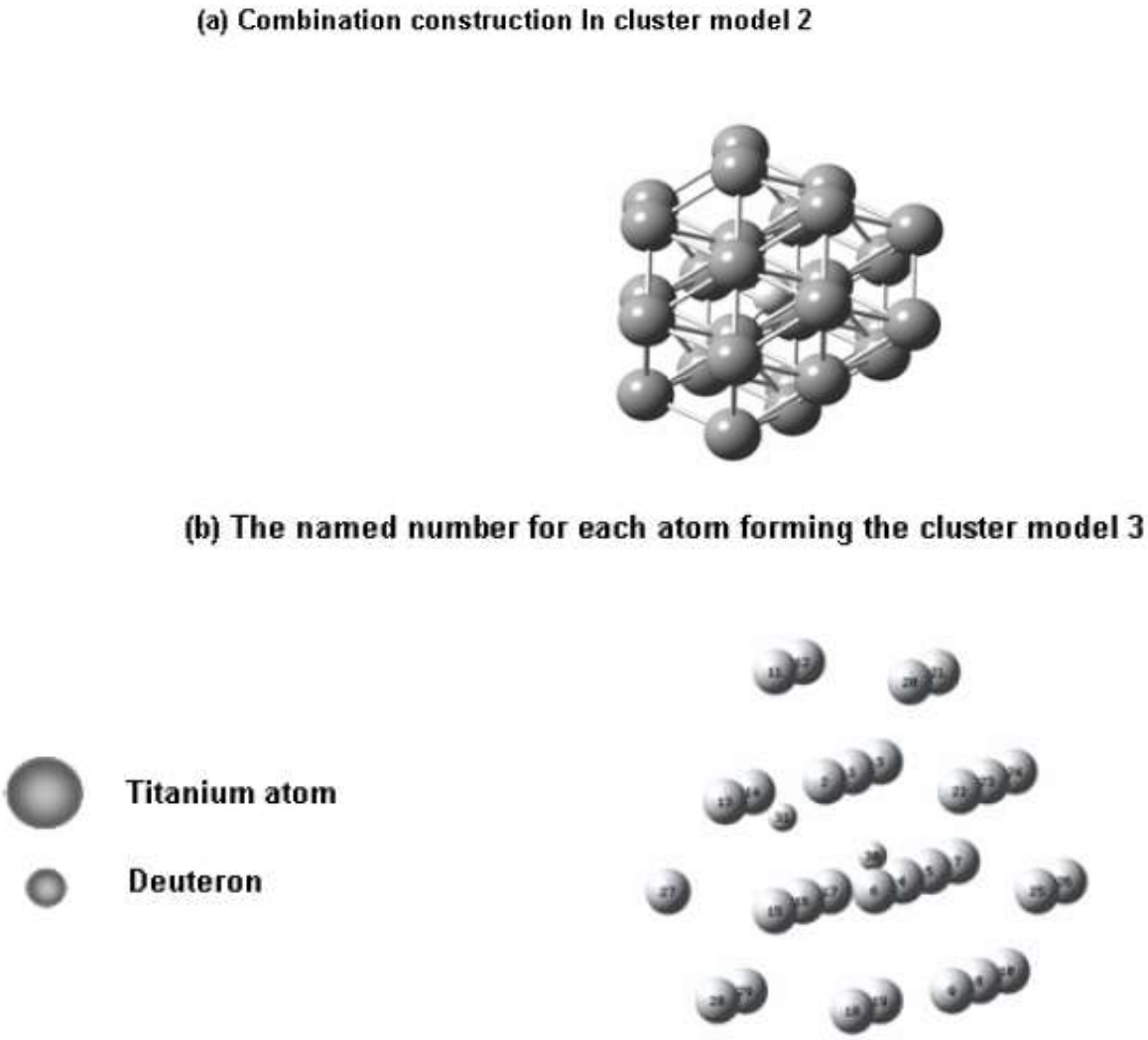

Figure 2. The cluster models 2 and 3, model 2 is the tetrahedron cage with surrounding minimum titanium atoms and a deuterium atom in it. Model 3 is the modified model 2 with a deuterium atom outside the cage, (a) and (b).

neutron generation. We intend to study the reason of neutron generation in accordance with the analogical principle compared to chemical reaction. In the chemical reaction, it is said that the factors influencing the reaction condition are temperature, pressure and the catalytic function to promote the reaction.

Regarding temperature and pressure in the experiments [2,5], the conditions of both of them are almost the same, although the operational conditions are different. The only difference between these experiments is that one occurs in the active period run by depressurizing (at desorption phase from liquid nitrogen temperature warming to room temperature) and the other occurs at warming to room temperature with pressurized condition after thawing terms and

cooling cycles.

The notable condition is that the neutron generation in both experiments always occurs at the warming term in the process after enough adsorption of deuterium gas to titanium shavings. Regarding temperature change, it is approximately a 160–220 K temperature rise from liquid nitrogen temperature, mentioned above. Also, the kinetic energy of a free deuterium atom at 80 and 300 K are 6.9 and 25.9 meV, respectively.

If such a small energy change by temperature rise makes nuclear fusion occur, we conclude that titanium atoms surrounding deuterium atoms act as an effective catalyst for nuclear fusion. Judging from the result of the first principle molecular orbital calculation indicated in Figs. 3 and 4, it seems that the combination of titanium and deuterium atoms locally form a kind of polar compound. Although titanium atoms combined to the deuterium atom can not move freely, they form local dipole (hereafter referred to as "Ti-d p-compound").

If titanium and deuterium atoms locally form a polar compound, then one of the methods to consider for utilizing the electromagnetic wave, is to increase the kinetic energy of the deuterium atoms combined to the titanium atoms in the crystal. If titanium and adsorbed deuterium atoms in titanium crystal form the local polar compound, even if it is in local portion, it seems that we can utilize the characteristics of a polar compound, therefore we can utilize the electromagnetic wave to give it the energy.

If the Ti–d p-compound is positioned in an alternating electromagnetic field, the polarization of it will occur and the deuterium atom will move following the frequency change. It seems that some portion of deuterium atoms in the combined state of ligancy 2, vibrate as if they were the swing of a pendulum in the vicinity of the axis with the two titanium atoms at both ends. Some of these atoms may then be able to enter into the cage and collide with the deuterium atom in the cage.

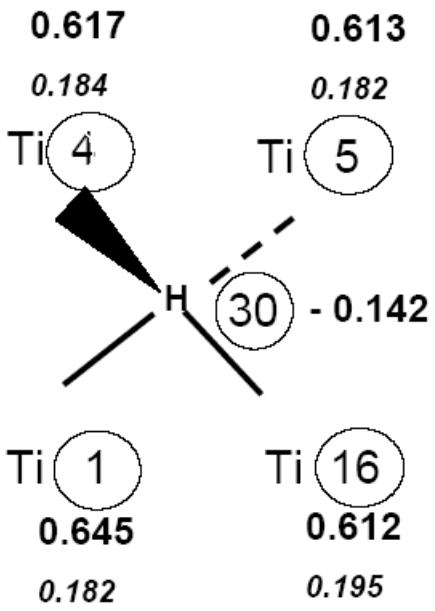

Figure 3. Atomic charge value (*bold*) and weighted bond order (*italic*) in the cluster model 2 are indicated in the development drawing of cluster model 2.

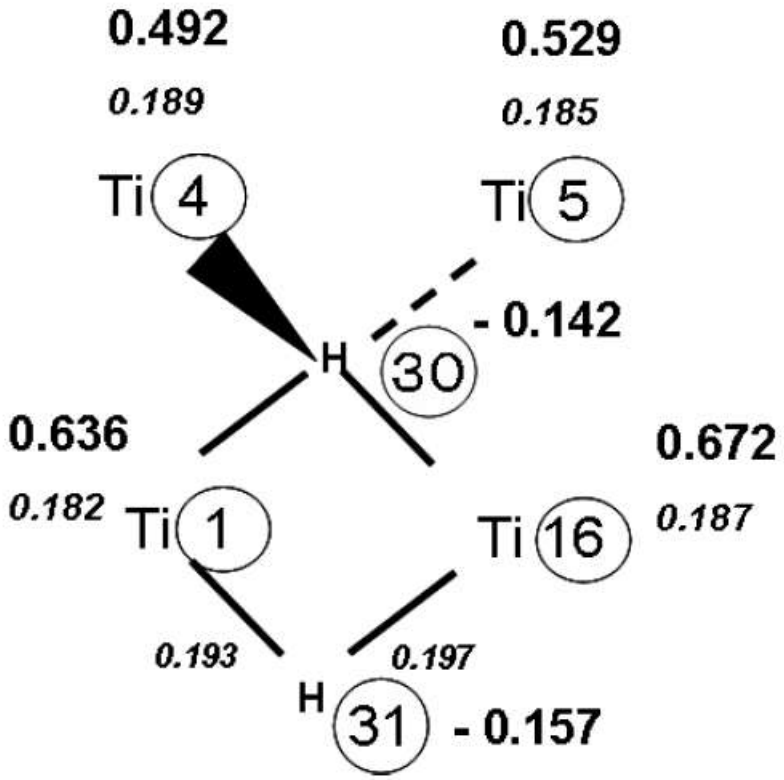

Figure 4. Atomic charge value (*bold*) and weighted bond order (*italic*) in the cluster model 3, are indicated in the development drawing of the cluster model 3. Two hydrogen atoms are located inside and outside the cage, respectively.

For example, if the direction of the electromagnetic wave is equal to the locus line from D(31) to D(30) indicated in Fig. 5, D(31) will be able to have a chance to enter into the tetrahedron cage.

The direct objective of the irradiation of the electromagnetic wave to the cylinder is not to heat the Ti–d p-compound but to increase the kinetic energy of deuterium atoms combined to titanium atoms. So the experiment by this apparatus should be executed in keeping with the planned suitable pressure and temperature condition so as not to decompose the deuterium bonds in ligancy 2. In Japan, two kinds of frequency are thought to be in accordance with the difference in the number of frequency when utilizing the electromagnetic wave. One is mainly for the use of small energy and its frequency is 2450 MHz, and the other is 915 MHz mainly for industrial use. If the deuterium atoms in Ti–d p-compound can move in the same way as hydrogen atoms in water molecules in food in microwave ovens i.e. following an alternating electromagnetic fields, we can expect an increase of kinetic energy of the deuterium atoms combined to the titanium atoms.

Although titanium atom in Ti–d p-compound cannot move as freely as that of oxygen and hydrogen atoms in a water molecule, we think that the microwave heating device mentioned above is applicable in the irradiation in the experiment, providing that the local polarization occurs in Ti–d p-compound and deuterium atoms will be able to move as hydrogen atoms in the water molecule. In treating hydrogen and deuterium gas, we think that it is important to take

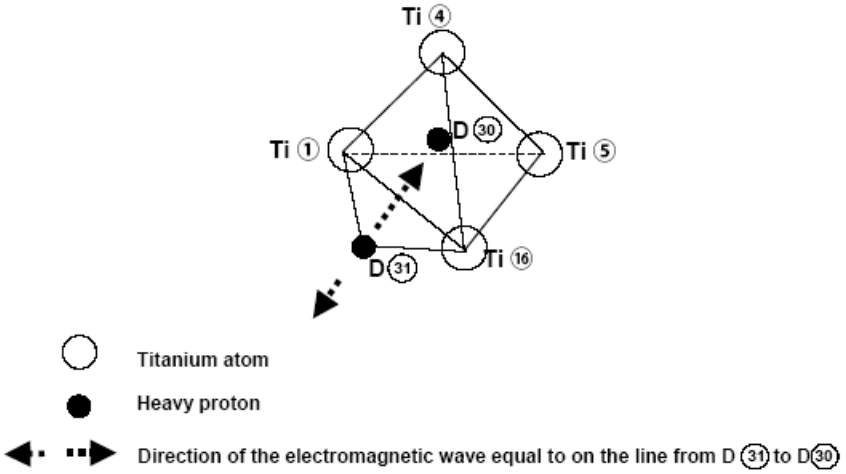

Figure 5. Preferable irradiation direction model of the electromagnetic wave.

into account of these characteristics. At low temperature, it is observed that the state of temperature equilibrium of deuterium is para form as same as that of normal hydrogen.

At temperatures below 100 K, essentially all ortho-hydrogen molecules are in the lowest ortho-rotational energy state (J: rotational quantum number, $J = 1$) and all para-hydrogen molecules are in the lowest rotational energy state ($J = 0$). The lowest ortho-state is associated with approximately 337 cal./mol more than the lowest para-state [6].

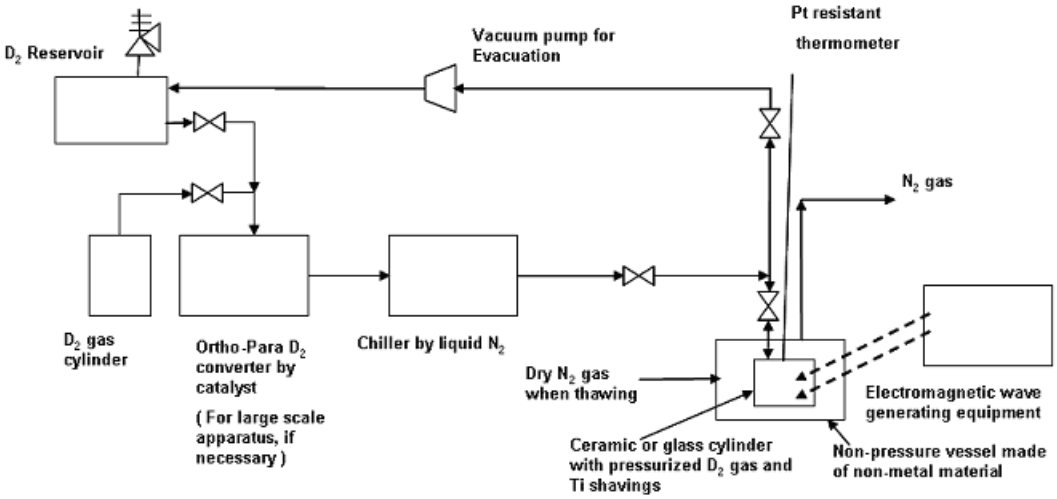

Figure 6. Block diagram of proposed neutron generation experimental apparatus.

This means that, at cryogenic temperature, this amount of energy is released as a result of the conversion of 1 mol of ortho-hydrogen to the para-form. So, to avoid the cold loss by the change of ortho–para equilibrium and to maintain the para-form, it is better to equip the ortho–para deuterium converter in the flow of a large scale apparatus. Referring to the deuterium separation apparatus by liquefied hydrogen distillation in the past, the ortho–para deuterium converter had also been equipped in the apparatus [7,8]. Taking the above into consideration, the block diagram of the proposed neutron generation experimental apparatus to increase kinetic energy of deuterium atoms is indicated in Fig. 6.

4. Discussion and Conclusion

Following the previous paper, we have simulated and intended to confirm the possibility of the existence of assumed cluster models, applying the first principle molecular orbital calculation. As a result, the cluster model 3 which has a hydrogen atom inside and outside of the cage respectively, has indicated that a titanium atom pair causes the hydrogen atom outside of the cage to have ligancy 2. In this connection, the estimated distance H(30)-H(31) in Fig. 4 is about 2.09 Å.

If the collision occurs in the tetrahedron cage, the driving force for deuterium atoms to collide may be the kinetic energy by vibration of polarized deuterium atoms in Ti–d p-compound. If the concept of room temperature nuclear fusion is correct, the observed phenomenon will also occur in an experiment from the liquid nitrogen temperature to the warming process of the deuterium adsorbed metal, which is electron deficient. It has suitable crystal construction and has adsorbed sufficient deuterium atoms.

As previously mentioned, the kinetic energy of a free deuterium atom at 300 K, the energy is about 25.9 meV. If we get the same energy quantity above mentioned by the radiation of ray, the wave length estimated by the formula based on Planck's law ($E = h\nu$) is about 48 μm. This wave length is within the range of infrared ray (0.8–1000 μm). So if we intend to utilize the electromagnetic wave in the experiment, it is preferable that its wave length should be shorter than 48 μm. By this selection of wave length, if the Ti–d p-compound is positioned in an alternating electromagnetic field, we presume that we will be able to expect from the result of past experiments both the necessary energy for the deuterium atom to collide each other and its vibration as the swing of a pendulum.

If we can give the kinetic energy under the specified low temperature and high pressure without decomposing the deuterium bonds in ligancy 2, for example by the irradiation of the electromagnetic wave, the vibration energy of the deuterium atoms combined with titanium atom in the crystal may increase and the chance of their collision in the crystal will also increase. As a result, it should make the quantity of neutron generation increase. For reference, it is necessary to take into account when irradiating in an experiment, that the efficiency of the microwave heating device to input electric energy is about 15%.

At present, we cannot theoretically estimate the necessary equivalent electromagnetic energy to generate the neutron per unit deuterium gas quantity in the specified condition. However, we deduce that the condition to generate neutrons is as follows. First, we should make the repulsion barrier around the deuterium nuclei thin by the nearer influence of the outer surrounding electrons under the low temperature and high pressure without destroying the titanium crystal lattice and deuterium bonds in ligancy 2.

Secondly, to prepare the condition of a non-equilibrium state by giving energy from the outer side. We think that one of the more effective means to prepare this condition than simple warming, is to irradiate the electromagnetic waves under the low temperature and high pressure and the reproducibility of the neutron generation in the experiment will be also improved. The authors would like to further analyze other suitable cluster models for nuclear fusion reaction.

Addendum

In the preparation of titanium shavings, it is preferable to shave the titanium bar or plate using a sharp-edged tool in a glove-box sealed by argon gas. The prepared titanium shavings should be packed in a ceramic or special glass cylinder without ever contacting air. This is to prevent titanium oxide from forming on the surface of the titanium shavings. According to the author's experience of titanium plate welding, there are major workmanship differences in the standard of welded seams between shaved plate surfaces and unshaved plate surfaces. Please note that the cylinder packed with titanium shavings should be made of ceramic or special glass when we irradiate the electromagnetic wave to the cylinder in the experiment, as a metal plate reflects the electromagnetic wave.

It is preferable to use nonmagnetic materials in the fabrication of all the equipment and apparatus. This is to prevent the converted para-deuterium form from changing to the ortho-deuterium form. It is also preferable that the design pressure of all the parts of the experimental apparatus is designed in a maximum working pressure. This is to simplify the flow of apparatus and to be able to decrease the total number of fittings.

If we intend to prepare the experimental apparatus, we think that there are several ideas in planning the part of the electromagnetic wave irradiation. In the other simple experiment, there is the example in which the simply altered microwave oven on the market is used for the irradiation of microwave [9].

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