interstitial site of the crystal lattice. The host metal lattice expands through hydrogen storage, sometimes losing the high symmetry of the crystal lattice (Schlapbach and Züttel 2001). Hydrogen positions have already been described in the chapter on nuclear fusion. The loss of crystal symmetry would also affect the deuterium condensate in Pd.

9 Pd Crystal and Deutrium Condensation

The nuclear fusion phenomena produced in solid and liquid phases with deuterium have been found and attracted a great deal of attention. Naranjo reported an experiment using a pyroelectric power source using $LiTaO_3$ crystal (Figure 6) to achieve nuclear fusion in a desktop-like device (Naranjo, Gimzewski, and Putterman 2005). Other studies on nuclear fusion by muon catalysis were also reported. Although a plan for ITER has been developed and pushed forward, the ITER presents many engineering problems, and is extremely expensive. On the other hand, the nuclear fusion phenomena produced in solid and liquid phases with deuterium have attracted a great deal of attention. In general, nuclear fusion of hydrogen atoms occurs at high temperatures under high pressure. However, condensation fusion at close to room temperatures was reported, and various fundamental studies are still ongoing. Studies on nuclear fusion for hydrogen storage metallic alloys are currently in progress [7–14] (Takahashi et al. 1998; Takahashi and Yabuuchi 2007A; Takahashi 2007B, 2009; Heidenreich et al. 2006; Kayano et al. 1994; Konashi et al. 1996; Bom et al. 2003). Nuclear fusion in condensed matter is expected to have potential as a clean energy source because DD fusion produces only helium-4 and low radioactivity.

There are several characteristics of the condensation fusion:

- Smaller amount of neutrons detected in comparison to ordinary nuclear fusion.
- Few γ-rays detected.
- Deuterium is used for fusion.
- Occurrence of fusion in materials with fcc and hcp structures, and no fusion reaction for bcc structure.
- ^{4}He is the main element generated.
- Reproducibility of nucleus change.
- Excess heat of 0.1 ~ 1 W cm^{-2}.

The nuclear reaction in hydrogen storage metallic alloys and a cross section of DD nuclear fusion were summarized here. Metallic alloys for hydrogen storage such as palladium were selected for analysis. Using the results mentioned above, the possibility of nuclear fusion in the solid phase was discussed.

The atomic structure model of hydrogen (deuterium) storage Pd is shown in Figure 9(a) (Oku and Kitao 2015). The deuterium injection into the Pd crystal causes a temporal formation of D-cluster restricted by Platonic regular polyhedrons and tetrahedral symmetric condensate (TSC) (Takahashi and Yabuuchi 2007A; Takahashi

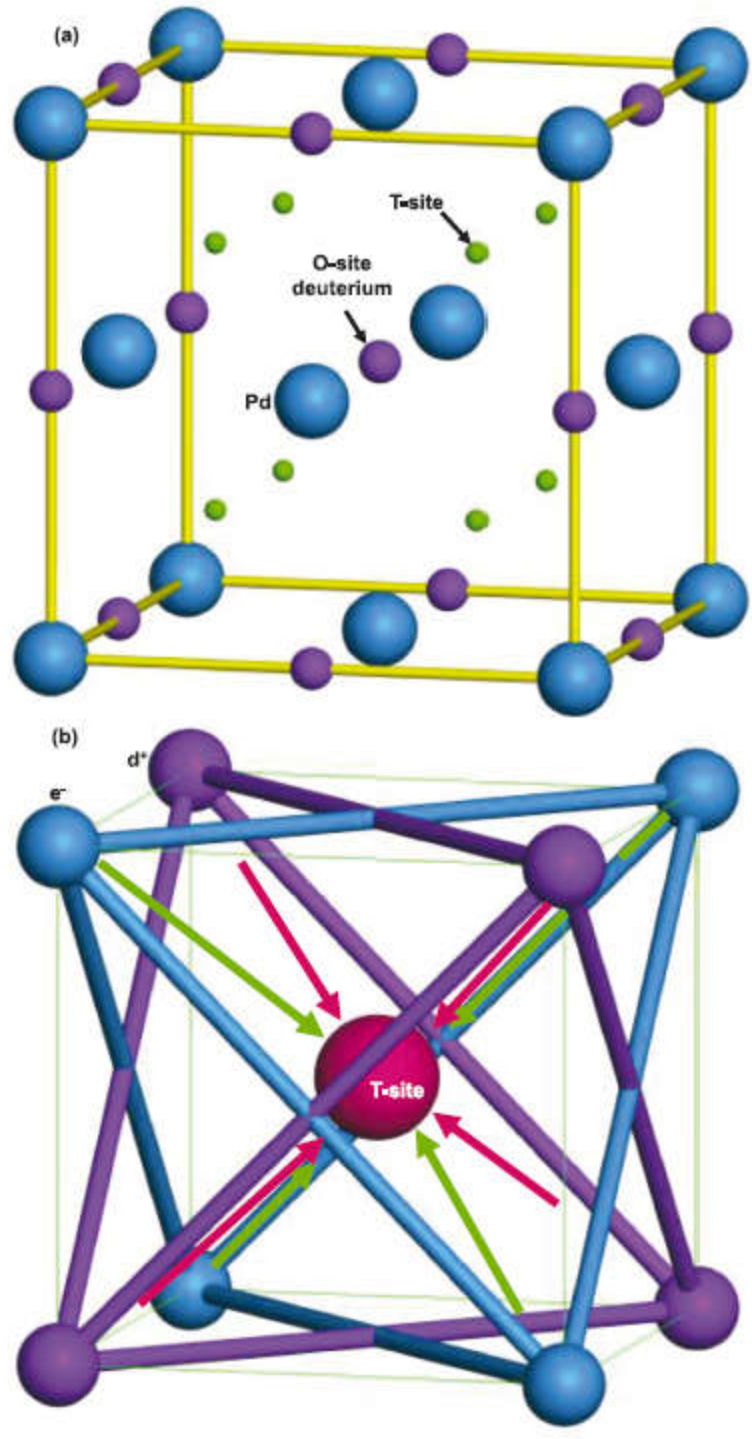

Figure 9: (a) Atomic structure model of PdD. Deuterium atoms are situated at octahedral sites (O-site). Tetrahedral sites (T-site) are also indicated. a = 0.389 nm. (b) Schematic illustration of tetrahedral symmetry condensate of four deuterium ions and four electrons around T-site.

2007B, 2009), as shown in Figure 9(b). Four deuterons and four electrons condensate at the T-site by background neutrons in nature, and these background neutrons play a role in promoting the condensation.

The time-dependent TSC-cluster trapping potential was calculated as eq. (11) from the Langevin equation for 4D/TSC based on the heavy mass electronic quasi-particle expansion theory calculation for barrier factors and the fusion rate (Takahashi and Yabuuchi 2007A; Takahashi 2007B, 2009), and the R_{dd} is expected value of D-D distance.

$$V_{\mathrm{TSC}}(R' : R_{\mathrm{dd}}(t)) = -\frac{11.85}{R_{\mathrm{dd}}(t)} + 6V_s(R_{\mathrm{dd}}(t);\, m, Z) + 2.2\frac{|R' - R_{\mathrm{dd}}(t)|^3}{[R_{\mathrm{dd}}(t)]^4} \tag{11}$$

The fusion rate was calculated by Fermi's golden rule, and the 4D fusion yield per TSC generation was also calculated (Takahashi 2009). The fusion yield and fusion products of deuterium condensate in PdD are summarized in Table 3 (Takahashi 2007A, 2007B, 2009). Although neutrons and tritium are produced by 2D and 3D condensation, respectively, the fusion yield is not higher than that of 4D condensation of TSC. Instead of TSC, an octahedral symmetric condensate (OSC) model has also been proposed. The calculation indicates that OSC is stable at R_{dd} = 40 pm as the ground states, and the potential was calculated to be *c.a.* −800 eV.

Table 3: Fusion reaction of deuterium condensate in PdD.

Multibody deuterium	Fusion yield (fs^{-1} cm^{-3})	Fusion product (ns^{-1} cm^{-3})
2D	1.9	Neutron: 10
3D	1.6×10^{9}	Tritium: 8×10^{8}
4D	3.1×10^{11}	Helium: 3×10^{11}

On the other hand, the Langevan calculation indicates a lowest potential for TSC of −3500 eV for Rdd = 3 fm, as shown in Figure 10. The condensation time was calculated to be 1.4 fs (Takahashi 2009). For R_{dd}, the deuterons and electrons condensate into an intermediate ^{8}Be. After that, the ^{8}Be collapses into two ^{4}He. This indicates that the TSC model is more suitable for D-cluster condensation. For actual Pd crystals, the deuteron supply is required to preserve the continuous fusion reaction, and the diffusion mechanism of deuterium in the Pd crystal should be investigated.

The diffusion coefficient D of deuterium in the Pd crystal was investigated using the data reported in

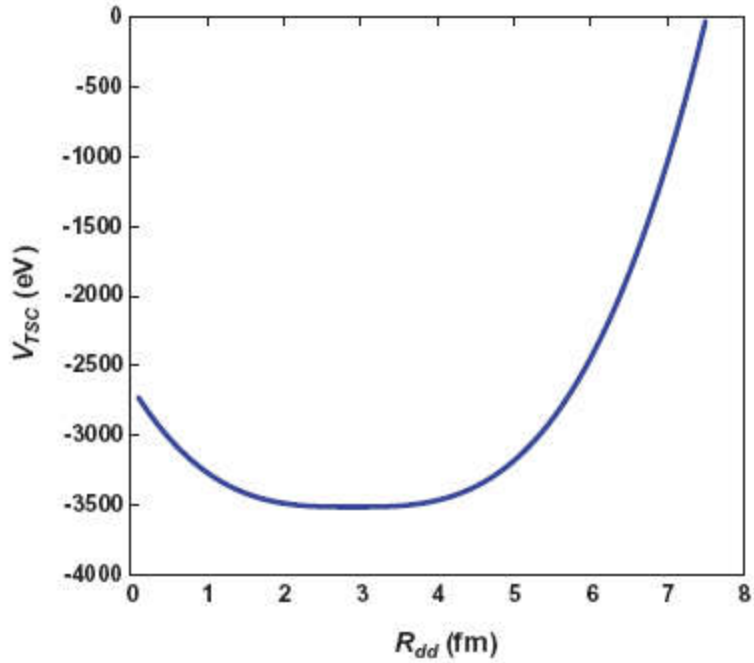

Figure 10: TSC trapping potential at the final stage (TSC-min) of condensation calculated by Langevin equation.

Table 4 and the eq. (12), where D: diffusion coefficient, D_0: constant, E_D: activation energy, k: Boltzmann constant and T: temperature.

$$D = D_0\, exp\left(\frac{-E_D}{kT}\right) \tag{12}$$

Table 4: Diffusion of deuterium atoms in fcc metals.

Metal-D	E_a (eV)	D_0 (10^{-7} m^2 s^{-1})	Temperature (K)
Pd-D	0.21	1.7	218–333
Ni-D	0.40	4.2	220–1273
Cu-D	0.38	7.3	723–1073

Although the reported data for the Pd-D system was obtained at around room temperature, deuteron diffusion at higher temperatures were estimated by the Flynn-Stoneham eq. (13) based on the thermally activated tunneling mechanism (Oku and Kitao 2015; Flynn and Stoneham 1970; Hirth 1980). The hopping probability W between the nearest deuterium atomic sites is calculated as follows, where the tunneling matrix element J value was estimated from the experimental data.

$$W = \left(\frac{J^2}{h}\right)\pi\sqrt{\left(\frac{\pi}{E_a kT}\right)}\, exp\left(-\frac{E_a}{kT}\right) \tag{13}$$

Then, the diffusion coefficients at higher temperatures are calculated from the following relation:

$$D = \frac{d^2 W}{6} \tag{14}$$

The nearest D-D distance (d) is equal to the distance of the nearest octahedral-sites, which is 0.2751 nm. The diffusion coefficients of deuterium atoms in Pd as a function of temperature are shown in Figure 11(a). The D values increase as the temperature increases. Figure 11(b) shows the diffusion time of deuterium atoms between the nearest O-sites in Pd, and the transport time of deuterium between the nearest neighboring D atoms in Pd crystal lattice is shown in Figure 12 as a function of temperature (Sugimoto 2006). The diffusion time decreases exponentially as the temperature increases, and then slowly decreases at higher temperatures near the melting point of Pd (1828 K). Therefore, the decrease in the diffusion time of deuteron caused by elevating the temperature is limited.

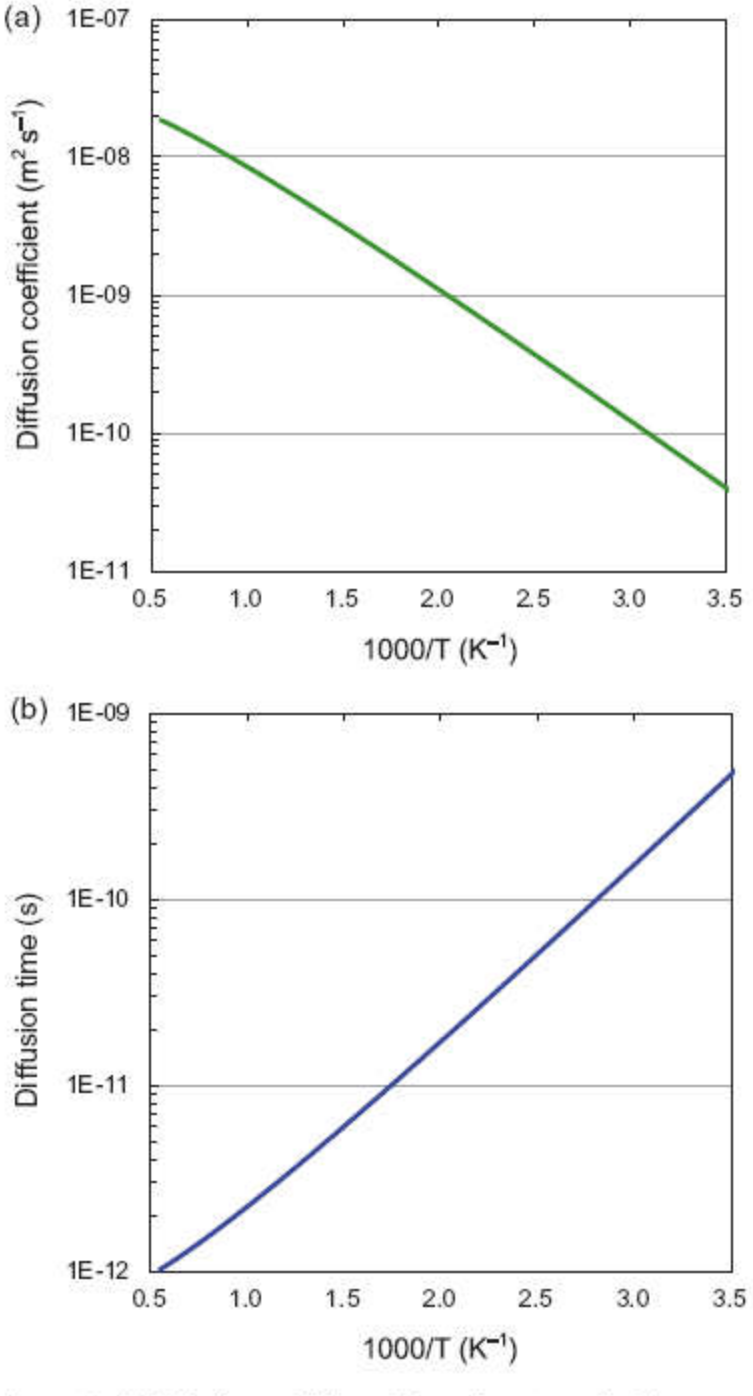

Figure 11: (a) Diffusion coefficient of deuterium atoms in Pd as a function of temperature. (b) Diffusion time of deuterium atoms between the nearest O-sites in Pd.

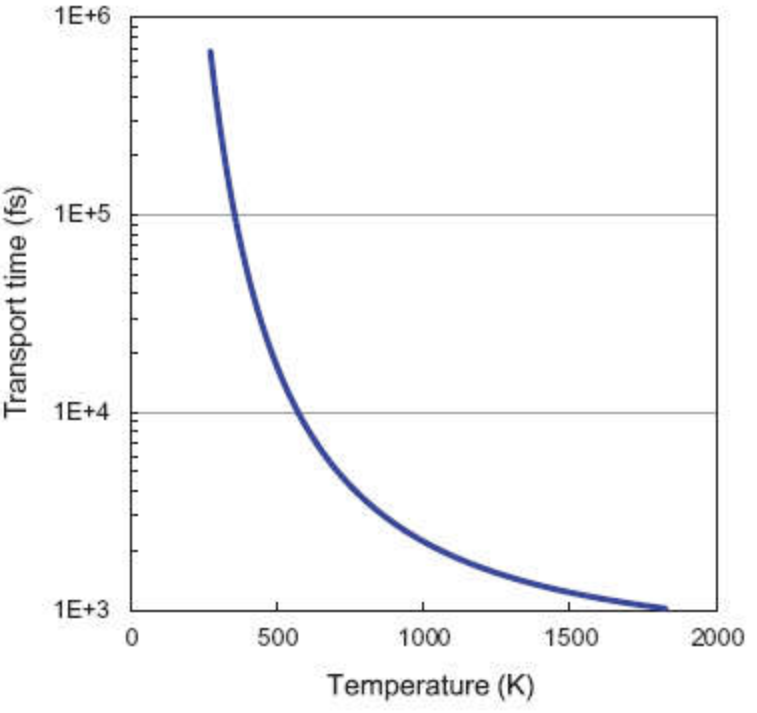

Figure 12: Transport time of deuterium between the nearest neighboring D atoms in Pd crystal lattice as a function of temperature.

To reduce the diffusion time, several approaches can be considered: reducing the activation energy, particle mass m and distance d. If the other elements are introduced into the Pd crystal, a reduction of the barrier energy of deuteron diffusion or an increase in the tunneling probability may be expected. Here, silver (Ag) was introduced into the Pd crystal, and the diffusion coefficients and diffusion time were calculated based on the proposed data (Ozawa et al. 2007), which indicated almost the same values as for the non-Ag doped Pd. Continuous fusion reaction of deuterium was reported for Pd-ZrO_2 nanocomposite materials (Kitamura et al. 2009), and further studies on the other elements or other methods might be examined (Grochala and Edwards 2004; Horinouchi et al. 2006; Mitsui et al. 2003; Kusada et al. 2014).

A schematic illustration of tetrahedral symmetric condensate and deuteron diffusion is summarized in Figure 13 (Takahashi 2007B, 2009). At the beginning of the condensation process, tetrahedral clusters of $4d^+$ and $4e^-$ are formed. After 1.4 fs, an intermediate nucleus ^{8}Be forms from the smallest TSC. Then, the ^{8}Be collapses into two ^{4}He. In order to continue the TSC, the deuterium should be supplied at the deuterium site in the Pd lattice. The diffusion time of deuterium is fairly long (~ 1000 fs) in comparison to

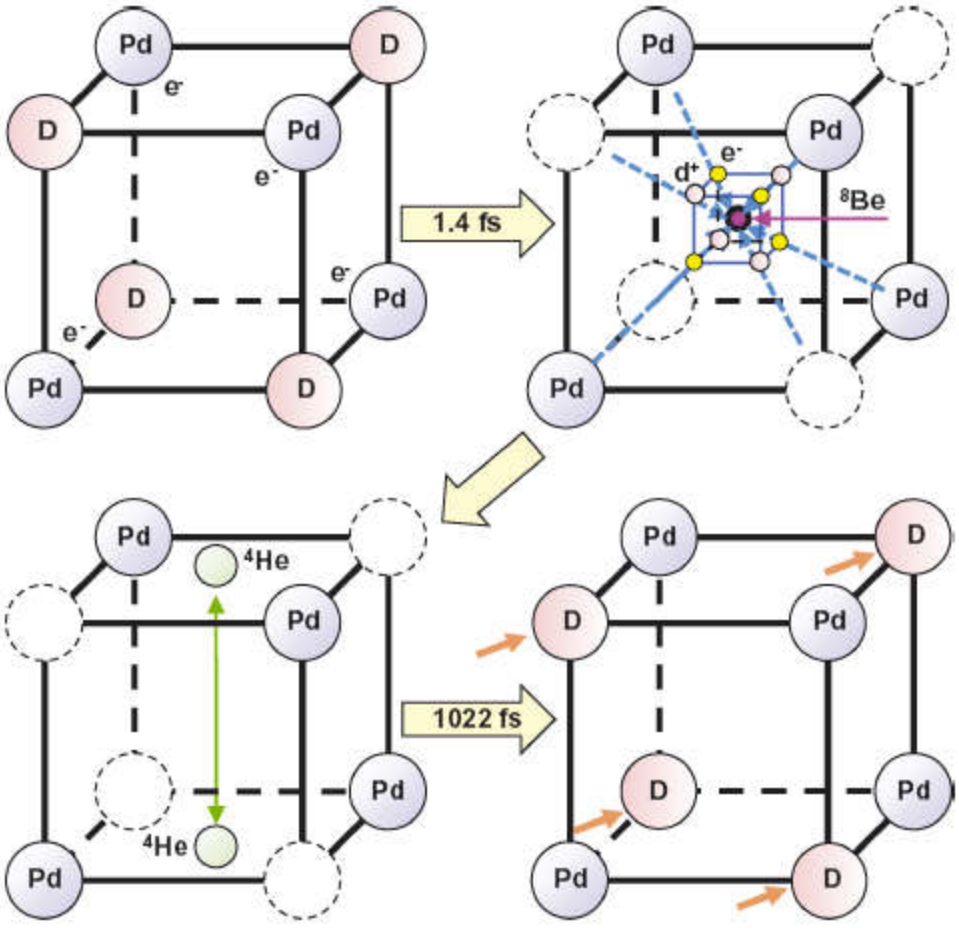

Figure 13: TSC and diffusion model for deuterons in Pd.

the fusion time for the 4D/TSC (1.4 fs), and a continuous fusion reaction may be difficult. Another method should be introduced to promote deuterium diffusion in the Pd crystal for the fusion reaction. Although the Pd element was selected for an analysis of continuous tetrahedral symmetric condensation of deuterium clusters, palladium has the material problem of being scarce and its cost is consequently high. Other hydrogen storage compounds should be investigated in further considering hydrogen diffusion in hydrogen storage materials (Bowman and Brent 2002).

The above 4D-TSC model predicted the transitory Bose-Einstein condensate (BEC) and ^{4}He production in microscopic space in hydrogen crystals with high symmetry. When the deuterons are introduced into the Pd lattice, the crystal lattice could expand and lose its tetrahedral symmetry, which might cause a decrease in the deuterium condensates in Pd. Although other theoretical predictions on the BEC condensate and deuteron fusion have been reported (Kim 2009, 2011; Widom and Larsen 2006).

The possibility of hydrogen storage in Pd was studied using a diffusion calculation and a potential calculation on 4D fusion. The nuclear fusion model for the 4D/TSC and diffusion of deuterium in Pd alloys was investigated. The diffusion time of deuterium is fairly long in comparison to the fusion time for 4D/TSC and creating a continuous fusion reaction may be difficult. The diffusion time of deuterium at the Pd-Ag alloy surface was almost the same as that of Pd. Enhancing deuterium diffusion in Pd alloys will be key in developing potential future methods for continuous nuclear fusion or for hydrogen gas storage.

10 Fusion Reactor Materials

Both excellent erosion resistance to high heat loading from plasma and high resistance to radiation damage by high-energy neutrons are required for the plasma facing components used in fusion reactors such as ITER. Although carbon materials have been extensively used for plasma facing components because of carbon's low atomic number and comparatively high thermal conductivity, its thermal conductivity is quite low at high temperatures such as those that occur during the operation of fusion reactors (Burchell and Oku 1994). Carbon/copper (C/Cu) composite materials have been produced because of the high thermal conductivity of Cu. The thermal conductivity of C/Cu composites was measured and examined at up to 1400 K for fusion applications (Oku, Hiraoka, and Kuroda 1995; Oku et al. 1998), and these measurements showed some improvement in the composites' thermal conductivity in comparison to C.