Prelude

Despite the many hundreds experiments, producing excess heat, which is not explainable by chemical reaction, and measuring the produced ^4He nuclear product, which gives the correct magnitude for typical deuterium fusion reaction, low temperature nuclear fusion has not been accepted and even not considered as a legitimate science. This rejection is rooting in the vested interest of the current establishment. The detected low energy nuclear fusion requires changing the paradigm in the field of nuclear science. This paradigm shift would discredit the lifelong work of the majority of current researchers, which would not only heart they ego, but would also jeopardize their current and future funding. Please bear in mind blocking the development of any new paradigm is always the high interest of the establishment.

Physical Model for Lattice Assisted Nuclear Reactions

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Abstract

Atomic scale description of the electrochemically induced cold fusion is presented. The model consistent with the conditions required for successive experiments and offers physical explanation for the occurrence of nuclear fusion at low energies. Based on this atomic scale description, the vibrational frequency of the D_2 molecules in vacancy is calculated. The fundamental frequency of the vibrating Deuterium molecule in a cavity is 21.65 THz, which is almost identical with the observed "sweet spot" in the two laser experiments at 20.8 THz, indicating that this previously unidentified peak represents the self frequency of the Deuterium molecule in vacancy. The fundamental frequencies in vacancies for HD and H_2 molecules are also calculated. It is predicted that these frequencies in HD or H_2 systems should also activate the reaction and that the fundamental frequencies in cavities should remain unchanged regardless of the hosting lattice.

1. Introduction

Fleischmann and Pons [1, 2] reported electrochemically induced excess heat in palladium–deuterium system. No new chemical product have been detected in the experiments. The observed quantity of heat could not have been produced by any known chemical reaction. Fleischmann and Pons speculated that the excess heat might have been the result of nuclear reaction, what they called "cold fusion" of the deuterium. No appropriate technical description of the Fleischmann and Pons experiments were disclosed. The conducted subsequent experiments by other laboratories, had very low reproducibility. Based on the low reproducibility and lack of theoretical support mainstream science rejected cold fusion. In retrospect it is known that successful experiment requires high loading [3]. Out of the 217 publications reporting negative result in refereed journal only 3 had 0.9 or higher D/Pl loading ratio required for successful experiment. At the same time period 49 positive experiments were also reported [4].

Despite the problem with reproducibility in the past three decades many hundreds of successful experiments, producing electrochemically induced excess heat in palladium–deuterium system, have been conducted [5, 6]. Along with the excess heat, ^{4}He with qualitative correlation to the produced excess heat has been measured.[7-12]. The collected ^{4}He had the correct magnitude for typical deuterium fusion reaction, which yields ^{4}He as product [13]. The production of ^{4}He was conformed in many independent experiments, and the measured quantity of ^{4}He in many cases exceeded the content, present in air, excluding possible contamination [7, 14-16]. The production of ^{3}He or neutrons in these experiments has not been reported. Thus ^{3}He or neutrons has not been produced or the quantities were below the detection limits [8]. In sixty-one independent experiments the production of tritium above the background value has also been reported [5]. The quantity of Tritium was always too small to generate detectable heat, but sufficient to demonstrate an unexpected nuclear process [17].

The known and detected nuclear fusion processes of deuteriums in plasma and hot fusion reactors are [18]

1./ D + D ➞ T(1.01 MeV) + p (3.02 MeV) (50%),

2./ D + D ➞ ^{3}He (0.82 MeV) + n (2.45 MeV) (50%), and

3./ D + D ➞ ^{4}He (73.7 keV) + (23.8 MeV) (10^{-7}).

The two dominant reactions are the first two, 50-50 percent, and the occurrence of the third one is minor 10^{-7}. In the cold fusion experiments the detected fusion process is D + D ➞ ^{4}He (73.7 keV) + (23.8 MeV) (No gamma). The production of excess heat correlates with the measured amount of ^{4}He, however, no nuclear radiation has been observed and the produced ^{4}He is essentially at rest. In the follow up experiments, despite the already mentioned problem with low loading, the majority of the reported negative experiments did not measure excess heat or any nuclear product but rather looked for proton emission, characteristics of hot fusion. This misconception was also a significant contributing factor leading to the rejection of Fleischmann and Pons experimental results.

The energy of the electrolysis is very small. Thus x-ray radiation from the process is unexpected. However, X-ray emission from well focused point source has been detected [19]. The spectra of the emitted x-ray is consistent with the K-alpha radiations of the elements present on the surface of the cathode along with some Bremsstrahlung [20-22]. The radiation flux correlates with the produced heat [23, 24].

Based on the high number of successful experimental results, reporting the amount of excess heat, not explainable by chemical reactions, the production of new elements, such as tritium and helium four, the emission of x-ray, and the correlation of these independent measurements indicates that nuclear reaction at low temperatures can occur, eventhough the reproducibility is a problem and the expected high energy radiation is absent [25]. No viable theory for low temperature nuclear reactions is known. Here an attempt is made to present one.

2. Conditions for experimental success

Any theory must be consistent with experiments. In the past three decades the conditions required for successful experiment are mapped out almost completely for the palladium–deuterium system [17, 26]. Analyzing these previous successful experiments a comprehensive list of the reported conditions has been collected. The experimental conditions (E) reported from successful low energy nuclear reactions are:

E1./ very slow loading

[The diffusion of the deuterium into the palladium crystal structure introduce significant volume change. In order to accommodate this volume increase without damaging the crystal structure the loading should be very slow. The loaded palladium should be free of cracks. Otherwise the deuterium would live the metal.]

E2./ pure D_2O containing the least H_2O possible

E3./ higher than 0.85% loading of D/Pd [27]

E4./ presence of D_2 molecules in the palladium deuteride

[The interaction of the Deuterium atoms require the presence of D_2 molecules, which can be formed at higher loading than 0.85 in the presence of vacancies. Many experiments, with very high loading, produced no excess heat, indicating that the bulk PdD is not active. However, excess power had been reported immediately after Pd Co-deposition [19, 28], allowing D_2 molecules to be loaded.]

E5./ presence of mono-vacancies

[The formation of D_2 requires mono-vacancies because the electron density in PdD is too high for molecular D_2 formation. The D_2 molecule in the vacancy are stable only if all of the O-sites are occupied, which requires 0.85 or higher loading [29].]

E6./ higher than a trash hold current density

[The current density has to be above a critical trash hold value in order to start the reaction and to compensate for the loss of deuterium from the cathode.]

E7./ laser excitation and excitation by laser induced phonon vibration

[Optical phonon vibrations induced by laser/s can trigger the reaction under conditions where the cathode was below threshold for the excess power production. In the PdD system the called "sweet spots", where excess heat production were initiated, are 8.2, 15.1, and 20.8 THz [30, 31]. The observed 8.2 and 15.1 THz frequencies correlates well with the Γ and L point vibration of PdD respectively. Thus these vibrations can be associated with optical phonon frequencies of PdD with zero group velocities. There are no optical phonon modes in PdD, which would associate with the peak in the excess power spectrum at 20.8 THz. It has been speculated that the response at 20.8 THz is due to deuterium in vacancies in the gold coating, or due to hydrogen contamination [32].]

E8./ The reaction can be enhanced by increasing the current density [33], by increasing the temperature [34], and by the application of magnetic field.

[Even relatively small external magnetic fields can enhance the excess heat. The application of a large magnetic field results in substantial increase of excess heat.]

E9./ The laser induced phonon frequencies initiated heat production remains and continues despite the laser turned off.

[It has been speculated that this could be explained if the nuclear energy goes into optical phonon mode and maintains the reaction [35].]

E10./ The heat production is localized, like hot spots, which are associated with mini explosion [36].

The first two conditions (E1, and E2) are technical and has no relevance to theory. The experiments still have problem with reproducibility. Thus eventhough the conditions (E1-7) are satisfied the reaction might not be start. Based on the conditions (E3-10) it can be concluded that the low energy fusion reaction of deuterium requires the presence and the continuous supply of D_2 molecules to the vacancies and the excitation of these molecules above a certain activation energy. Thus the reaction occurs in the cavity or mono-vacancies and induced by vibration.

3. Theoretical expectations from a successful model

John Huizenga [37] wrote a book, with the viciously unscientific title, Cold Fusion: Scientific Fiasco of the Century. In this book he listed “three miracles”, which must be satisfactorily answered by any theory of cold fusion. The three miracles are

T1./ much enhanced tunneling through Coulomb barrier,
T2./ suppress p + t, and n + ^{3}He pathways to make ^{4}He + gamma,
T3./ disappearance of 24 MeV.

According to him these miracles are impossible. Analyzing the experimental observations of LENR, Edmund Storms [38] put together a list or facts, what any theory must be answered.

T4./ (Fact #1) Helium is generated without significant radiation
T5./ (Fact #2) The effects are occur either light hydrogen or deuterium
T6./ (Fact #3) Tritium is produced without significant neutrons or radiation
T7./ (Fact #4) Helium -3 is not produced as a primarily product - eliminating p + d fusion
T8./ (Fact #5) Transmutations occur with either light hydrogen of deuterium
T9./ (Fact #6) Reactions occur at special localized sites

Thus any successful theoretical model on one hand must be consistent with the required experimental conditions for successful reaction, and on the other hand must satisfactory explain or answer the theoretical obstacles raised by the current interpretation and understanding of the fusion process.

4. Proposed model for cold fusion

Based on the current understanding of the physical world low energy nuclear reaction should not occur. In the past thirty years many hundreds experiments verified the occurrence of LENR. Based on this accumulated experimental evidences the existence of LENR is undeniable. In order to understand the physics behind LENR requires a paradigm change in the field of nuclear science or in a broader sense in atom physics. It is suggested that the key ingredient in our understanding of LENR is the description of the electronic structures of the atoms. It has been suggested that the electron in the vicinity of the atom is not a point charge but rather a uniform surface charge forming an electron halo around the nucleus [39]. The only difference between this description and the current establishment is that not a point charge electron orbiting around the nucleus but rather the triggered vibrational wave propagates in the electron shell formed around the nucleus (Fig. 1). This electronic shell description of the elements were investigated for the Hydrogen atom [39]. Using the experimental data the velocity of the propagating wave on the surface of the electron shell was calculated. This velocity is identical with the velocity of the point charge electron calculated from the Bohr's model. Thus the electron halo model with propagating wave on its surface reproduces all the properties of the Hydrogen atom in the same manner as the previous descriptions. Additionally, the model explains the physics of emission and absorption of electromagnetic radiations of the atoms (Fig. 1), the uniformity and stability of the atoms, the physics of the particle-wave duality nature of the matter, gives the correct value for the ground state angular momentum and the ionization energy of Hydrogen atom. These features were not explained by the previous models. The model also consistent with classical electromagnetism and shows that there is no need to limit the extent of these laws at atomic scale. It will be investigated that how the proposed electronic structure description of the elements can satisfy the conditions set up for successful theoretical model of LENR.

T1./ "much enhanced tunneling through Coulomb barrier is required"
One of the strongest arguments against cold fusion is that the energies corresponding to room temperature reactions could not overcome on the strong Coulomb repulsion [37]. The electron shell structure of the Hydrogen atoms offers an explanation how two nucleus can get very close to each other without any repulsion. The positive nucleus are shielded by the electron shell allowing a very close encounter with no repulsion. Thus much much enhanced tunneling through Coulomb barrier is possible then in nucleus-nucleus interactions with no electron shell. The inclosed D_2 molecule in a cavity or mono-vacancy is excited by the vibration of the surrounding lattice, which can lead to the fusion of the two deuterium nucleus producing ^{4}He (Fig. 2). Edmund Storms introduced the nuclear active environment description and suggested that the reaction occurs on the surface of the metal in small nano meter sized cracks. This fusion mechanism is the same as the one described in vacancy. In a more general description of the fusion process, nano size cavity might be used instead of the mono-vacancy.

T2./ "suppress p + t, and n + ^{3}He pathways to make ^{4}He + gamma"
Huizenga assumed that high energy and low energy nuclear reaction should results in the same fusion products. At high energy collision of the nucleus, the energy is sufficient to detach either a proton or a neutron. Based on probability the chances are 50-50 percent for either proton or neutron will be detachment, which is consistent with the probabilities of reactions 1 and 2 in hot fusions. In few cases, even in hot fusions experiments, neither of the nucleons has enough energy to be detached and reaction 3 occurs. At low energy fusion the energy is not sufficient to detach any of the nucleons, therefore, reaction 3 becomes the dominant fusion process. This assumption is consistent with experiments, which reports 99.9% probability for the occurrence of reaction 3, which is D + D $\rightarrow$ ^{4}He (73.7 keV) + (23.8 MeV) [40, 41]. Thus suppressing p + t, and n + ^{3}He pathways to make ^{4}He + gamma does not require any miracle except the acknowledgement of the facts that high and low energies nuclear fusions are different physical processes.

T6./ "tritium is produced without significant neutrons or radiation"
The explanation of T6 is the same as T2. No high energy particle is present, which would result in proton emission. Thus tritium at LENR should not have been produced from two deuteriums. This prediction is consistent with experiments, which shows that the formation of tritium in low energy nuclear reactions requires the presence both deuterium and hydrogen [42]. Thus tritium forms from H + D, with no neutron radiation.

T7./ "Helium -3 is not produced as a primarily product - eliminating p + d fusion"
^{3}He is produced by p + d fusion. The energies in LENR are below the ionization energy of the Hydrogen (13.6 eV), therefore, no protons are formed. Thus p + d fusion should not occur at LENR. The lack of this reaction is consistent with LENR experiments.

T5./ "The effects are occur either light hydrogen or deuterium"
T8./ "Transmutations occur with either light hydrogen of deuterium"
Both of these theoretical expectations requires an equivalency between H_2 and D_2 process. Based on the proposed physical process, the reaction is induced by the vibration of a molecule in the cavity of mono-vacancies of the host lattice. The enclosed molecule can be D_2, HD, or H_2, which changes only the fundamental frequencies of the molecules (explained later) but not the process itself.

T3./ "disappearance of 24 MeV"
T4./ "Helium is generated without significant radiation"
These two requirements (T3 and T4) raises the question how the produced 24 MeV energy of fusion can disappear. It should be stated that the energy produced by the fusion process D + D $\rightarrow$ ^{4}He (73.7 keV) does not disappear but rather transferred into the lattice as heat. The measured excess heat shows qualitative correlation with the produced ^{4}He [7-12]. Thus the requirements of T3 and T4 should be modified as follow. How does the produced energy in the nuclear fusion transferred to the lattice?

When two nucleus of the deuterium atoms fuses then the released energy burst the electron shells. This process might be responsible transferring the released nuclear energy to the lattice. Electron mediated radiation has been reported by many experiments [43, 44]. Theoretical models are also allow transferring the energy between nucleus and the lattice [45]. The nuclear energy transformation to the lattice not completely understood.

T9./ "Reactions occur at special localized sites"
The theoretical requirement T9 address the observations reported in E10. Experiments showed that the heat production is localized, like hot spots, which are associated with mini explosion [36]. This observation is consistent with the proposed cavity vibration of D_2 model. The reaction is a random event, occurring in isolated vacancies. These isolated events does not induce chain reaction. This might be the reason behind the reproduce-ability problem. The combined outcome of the isolated events is the production of extra heat, which can be a tool to enhance the reaction.

It is concluded that the presented simple electronic shell description of the atoms, along with the physical model, vibrating D_2 molecule in the cavity or mono-vacancy of Palladium, offers a feasible explanation for the LENR experiments (Fig. 2).

5. Predictions of the model

The origin of the third "sweet spot" detected in the two laser experiments [35] at 20.8 THz, triggering the reaction under conditions where the cathode was below threshold for the excess power production is unknown. If the presented model is correct then the reaction should be triggered by the self resonance frequency of the molecule (Fig. 3/a). This possibility is investigated. The usual way calculating the vibrational frequency of the diatomic Deuterium molecule is

$$G(v) = \omega_e\left(v+\frac{1}{2}\right) - \omega_e Xe\left(v+\frac{1}{2}\right)^2, \quad v = 0, 1, 2, 3 \ldots \qquad (1)$$

where ω_e, and $\omega_e X_e$ are the harmonic frequency and the first anharmonicity constant, respectively, and v is the vibrational quantum number with non negative integer values. The zero point energy (ZPE) of a diatomic molecule is then

$$ZPE = G(0) = \frac{1}{2}\omega_e - \frac{1}{4}\omega_e X_e. \qquad (2)$$

The experimental values of the vibrational ZPE energies for D_2, DH, and H_2 are 4.636×10^{13} Hz, 5.667×10^{13} Hz, and 6.533×10^{13} Hz respectively [46]. The zero point vibrational energy of D_2 (46.36 THz) is far off from the observed 20.8 THz triggering frequency. The possibility of beat frequency, with one of the observed lattice related vibrations is also unlikely. Thus the diatomic vibrational frequency of D_2 can not be the explanation for the observed "sweet spot" at 20.8 THz.

In accordance to the proposed fission model (Fig. 2) the vibration of the Deuterium molecule occurs in a cavity or vacancy. Investigating the vibration in the cavity it can be concluded that the constant bouncing of the molecule from the wall of the cavity prevents the development of diatomic vibration. It is suggested that the vibration of the Deuterium molecule in a cavity can be depicted by the vibration of one of the Deuterium atom, which has the mass of the molecule attached to its electron shell (Fig. 3/b). This "cavity vibration" is modeled in the following way. The electron shell is stretched out, like a string, and the mass of the Deuterium molecule in the middle is attached to this string (Fig. 3/b). The length of the stretched electron shell is equal with the circumference of the great circle of the sphere, and can be calculated as:

$$L = 2\pi a_o, \qquad (3)$$

where a_o is the Bohr's radius. It is assumed that the radius of the Deuterium is the same as the Hydrogen atom. This assumption has no significance because the radius falls out by simplifying the formula. The stretching tensile force is generated by the surface tension of the electron shell. It is assumed half of the total force acts on both sides. It is calculated as:

$$T_{shell} = \frac{1}{2} 2\pi a_o \sigma, \quad (4)$$

where σ is the uniform surface stress in the electron shell. Assuming that the surface stress of the electron halo in the Deuterium atom is the same as in the Hydrogen atom, the surface tension can be calculated [39] as:

$$\sigma = \frac{e^2}{16\pi^2 \varepsilon_o a_o^3}, \quad (5)$$

where e is the elementary charge, and ε_o is the permittivity of free space, which has the value $8.854187817...\times10^{-12}$ $C^2/N\cdot m^2$ [47]. The angular velocity (ω) of this vibrating system can be calculated then as:

$$\omega = \sqrt{\frac{2T_{shell}}{mL}}, \quad (6)$$

where m is the mass of the object, equal with the mass of the Deuterium molecule:

$$m = 2(m_e + m_p + m_N), \quad (7)$$

where m_e, m_p, and m_N are the masses of electron, proton and neutron respectively.
The frequency of the vibrating electron shell with the attached Deuterium molecule to its surface is:

$$f = \frac{1}{2\pi}\sqrt{\frac{2T_{shell}}{mL}} = \frac{1}{2\pi}\sqrt{\frac{\sigma}{m}}, \quad (8)$$

The calculated fundamental frequency of the vibrating Deuterium molecule in a cavity is 2.165×10^{13} Hz (21.65 THz). This frequency is almost identical with the observed sweet spot at 20.8 THz (Fig. 4). Based on this agreement it is suggested that the third sweet spot or triggering frequency measured by the two laser experiments represents or relates to the self frequency of the Deuterium molecule in a cavity. The self frequencies of HD and H2 in cavity are also calculated based on the same assumptions. The calculated frequencies of HD and H2 are 2.500×10^{13} Hz (25.0 THz), and 3.062×10^{13} Hz (30.62 THz) respectively.

The diatomic vibration and the vibration in cavity both have two degrees of freedom, which allows calculating the temperature (T) relating to the vibrational energy as:

$$T = \frac{hf}{k_B}, \quad (9)$$

where h is the Planck constant, and k_B is the Boltzmann constant. The temperatures relating to the cavity fundamental vibrational frequencies of D_2, HD, and H_2 are 1039, 1200, and 1470 Kelvin respectively. These temperatures should be the optimum values for stimulating the reactions. The calculated frequencies in cavity, the experimental vibrational ZPE energies, and the equivalent temperatures for D_2, DH, and H_2 are listed in Table 1.

If the vibrational frequency of Deuterium molecules in cavity represents the reported sweet spot at 20.8 THz as suggested, then this frequency should remain the same regardless of the lattice. Like in NiD system, the two lattice related peaks should be different, however, the 20.8

THz triggering frequency should remain the same. It can also be predicted that the calculated cavity frequencies for HD and H2 should trigger the reaction, and these frequencies should also be independent from the the vibration of the lattice.

6. Conclusions

Based on the many hundreds experiments reporting excess heat, which is beyond the quantity, which can be explained by chemical reaction, the measured ^4He fission product with the correct magnitude for typical deuterium fusion demonstrates that, despite the rejection of the majority of the scientific community, cold fusion is real, eventhough, the reproducibility is problem.
Based on the literature review, the conditions required for successful experiments in the Palladium, Deuterium system are high loading, presence of mono-vacancies, which are occupied by Deuterium molecules, continuous supply of D_2 above a threshold, and excitation or triggering by vibration. The experiments show that the vibrational energy of the deuterium molecule in the cavity or mono vacancy of the Palladium hydride is sufficient to overcome on the Coulomb barrier and form ^4He. The fusion process in LENR is $D + D \rightarrow {}^4He$ (73.7 keV) + (23.8 MeV) no gamma. By changing our perception on the electronic structure of the elements offers an explanation for the observed low energy nuclear reaction. It has been suggested that the fusion is possible because the electron forms uniform charge distribution around the nucleus, which shields the proton. Without this shielding effect, the fusion at the observed low temperatures, would be impossible. The proposed model is consistent with all the conditions required for successful experiment, and can answer all the theoretical requirements.

The fundamental vibrational frequency of the D_2 molecule in cavity had been calculated, and agrees reasonably well with the reported sweet spot frequency measured by the two laser experiments at 20.8 THz. Based on this agreement it is suggested that the detected sweet spot, or triggering frequency relates to fundamental vibrational frequency of Deuterium molecule in cavity. The fundamental vibrational frequencies of HD, and H_2 in cavity are 25.0 THz and 30.6 THz. These frequencies should trigger the reaction in HD, and H_2 systems. These predictions could be tested by experiments.

The equivalent temperature of the vibrational frequencies are calculated for D_2, HD, and H_2. These are the optimum temperatures for enhancing the reaction. Further outcome of the proposed model is that the fundamental vibrational frequencies of molecule remains the same regardless of the hosting lattice. This predictions can also be tested by experiments.

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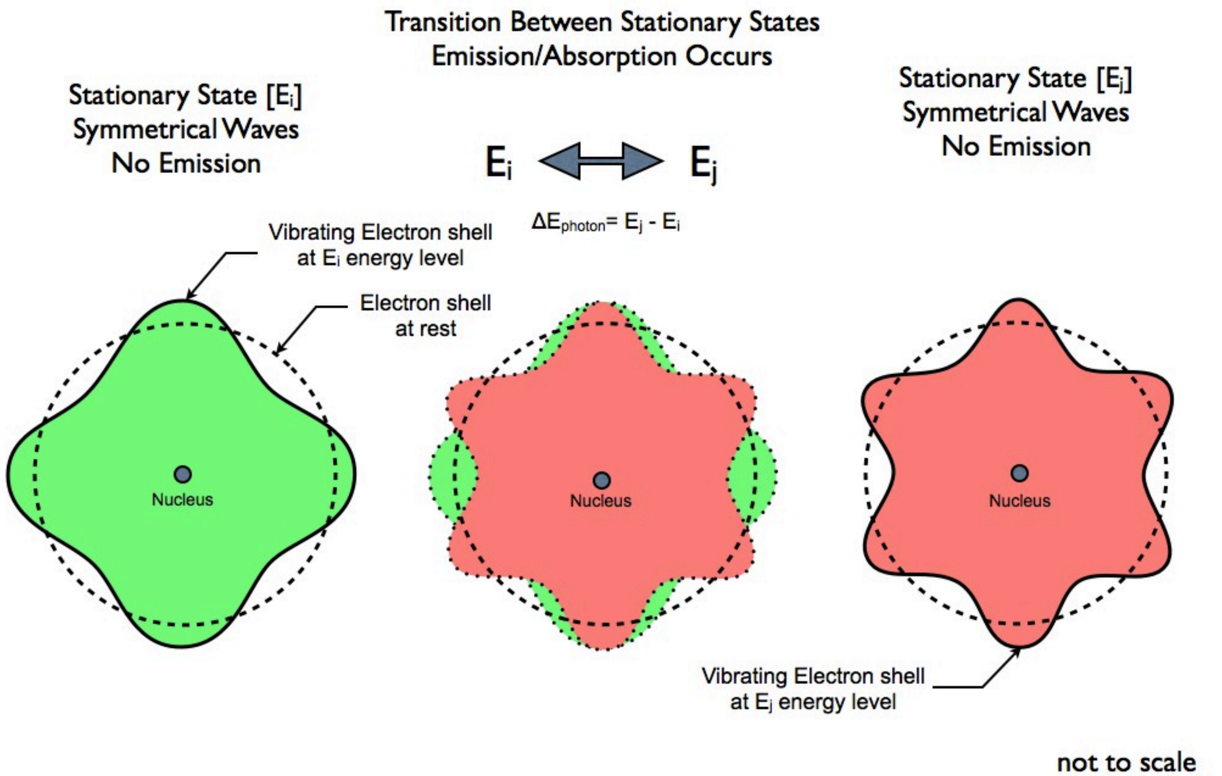

Figure 1 Schematic 2D figure of the uniformly distributed electron shell model showing the transition between two states. As long as the vibration of the electron halo around the nucleus is symmetrical, stationary energy levels, no emission occurs resulting from destructive interference. However, when transition occurs between one symmetrical vibration state to the another symmetric one then the vibration in the transition is asymmetrical resulting in electromagnetic radiation. The electromagnetic radiation can be either emitted or absorbed depending on the energy state of the states. The uniform surface charge distribution of the electrons explains the emission and absorption of photons without violating classical laws, which remains valid at atomic scale.

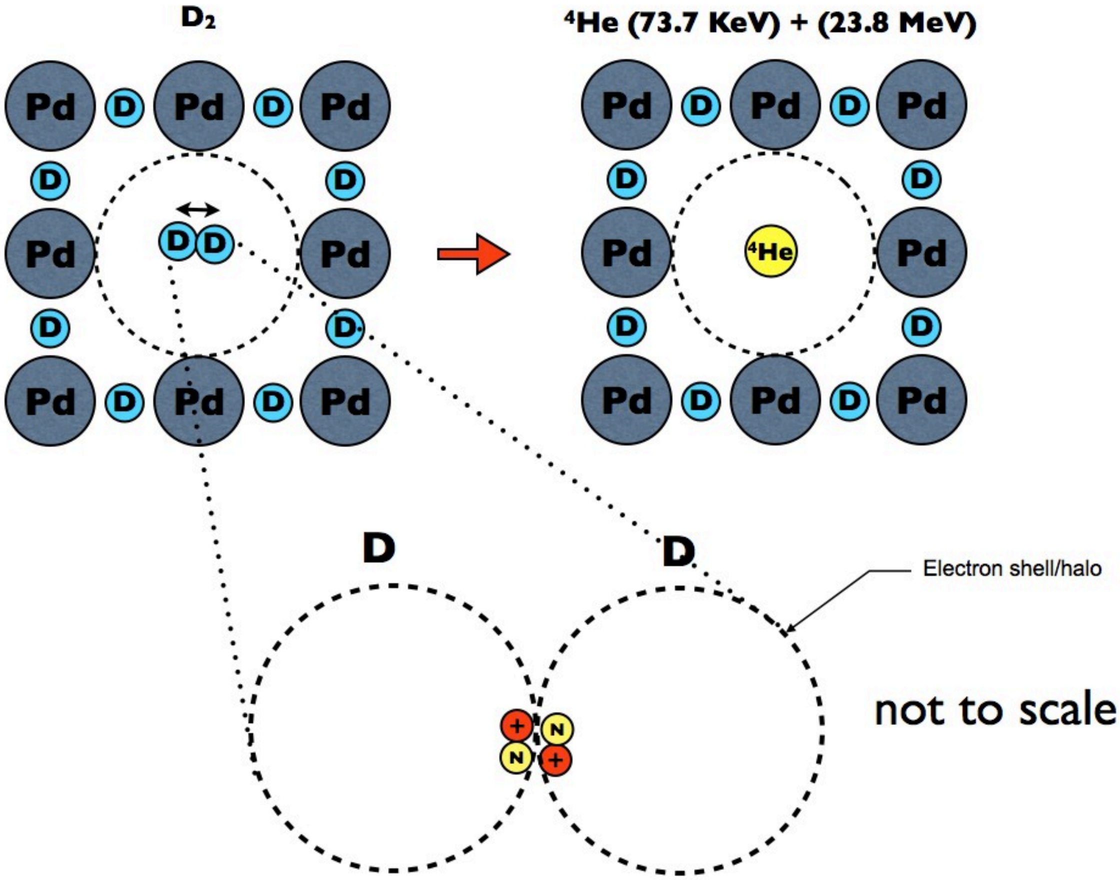

Figure 2 Schematic figure of the reaction. The Deuterium molecule is in a mono-vacancy. The loading of the surrounding Palladium is 0.9 or higher preventing diffusion. The vibration of the lattice triggers the vibration of the deuterium molecule. Close encounter of the two deuterium nucleus can result in fusion, producing 4He. The energy of the fission produces electromagnetic radiation, which dissipates in the lattice.

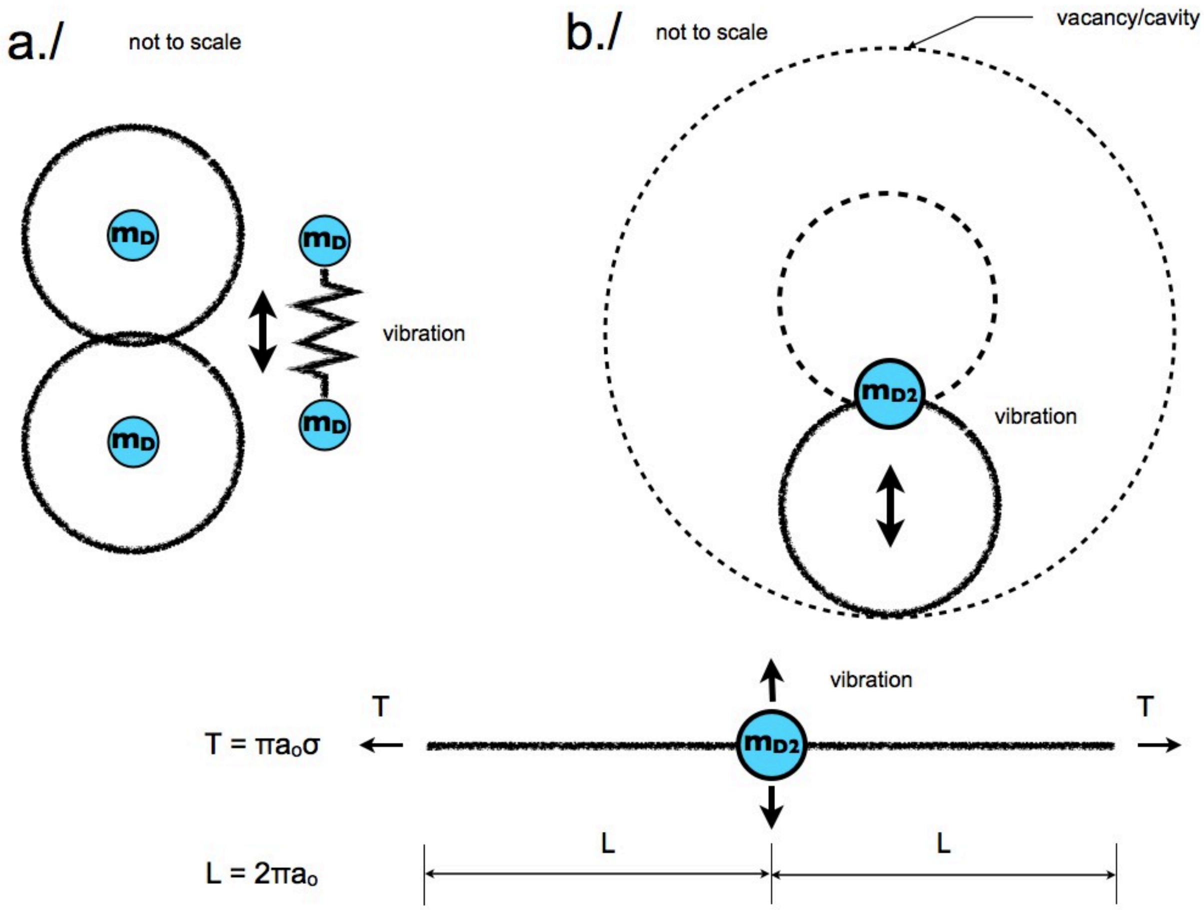

Figure 3 The vibration of the deuterium molecule. a.) diatomic vibration b.) vibration in the cavity.

Inside the cavity the molecule bouncing back and force from the wall, which prevents the development of diatomic molecular vibration. The vibration of the molecule can be depicted as the vibration of the electron shell of one atom with a mass equivalent with the mass of the molecule attached into its surface. This vibration is depicted by assuming that the electron shell acts as a string, and the mass of the molecule is attached to this string.

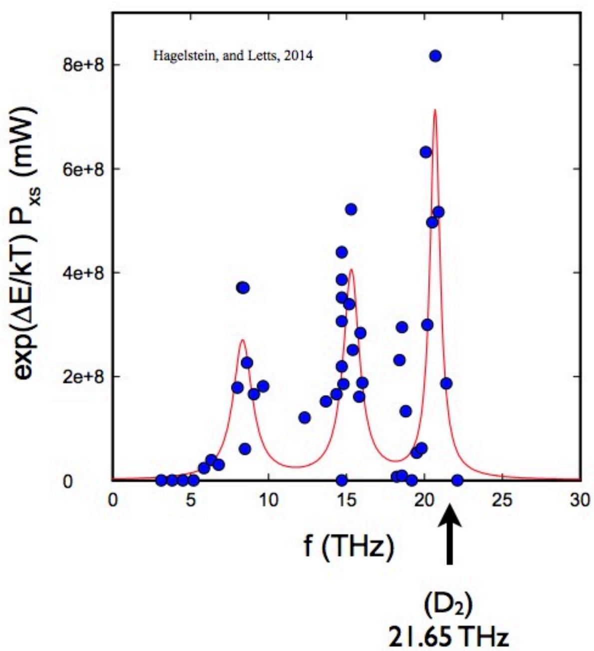

Figure 4 The calculated fundamental frequency of the vibrating deuterium molecule in vacancy is 21.65 THz. The detected sweet spots (triggering frequencies) of the two laser experiments are shown [48].

Table 1 The fundamental vibrational frequencies in cavity, the zero point energy of the diatomic vibration [46], and the equivalent temperatures of these vibrations for D_2, HD, and H_2 are shown.

vibration in vacancy	**D_2**	**HD**	**H_2**
frequency (THz)	21.65	25.00	30.62
wave number (cm^{-1})	722	834	1,021
temperature (K)	1,039	1,200	1,470
diatomic vibration	**D_2**	**HD**	**H_2**
ZPE frequency (Hz) [46]	46.36	56.67	65.33
ZPE wave number (cm^{-1})	1546.50(8)	1890.3(2)	2179.3(1)
ZPE temperature (K)	2,225	2,720	3,135