The 18th Meeting of Japan CF-Research Society

JCF18 ABSTRACTS

November 24-25, 2017

Research Center for Electron Photon Science, Tohoku University

Japan CF-Research Society

Program of JCF18 Meeting Japan CF-Research Society

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Thee.	Tohoku University, Sendai, Japan	
Paper presentation:	Oral presentation 25 min. + Discussion 5 min.	
Language:	English or Japanese	
Book of Abstract:	Only available at JCF home page (http://jcfrs.org/)	

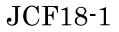
November 24 (Fri), 2017

 13:00-13:10 Opening Address Y. Iwamura (Tohoku University) Session 1 Chairman; K. Tsuchiya (NIT, Tokyo) 13:10-13:40 JCF18_01 K. Tanabe et al. (Kyoto U.) Direct Joule Heating of D-Loaded Pd Plates in Vacuum 13:40-14:10 JCF18_02 Y. Sato et al. (Iwate U.) Deuterium desorption experiments using Pd-Zr and Pd-Ni-Zr multi-layered samples 14:10-14:40 JCF18_03 H. Numata Search for characteristic microstructure of Pd rod formed during repeated cathodic and anodic electrolysis 14:40-15:00 Break Session 2 Chairman; S. Narita (Iwate U.) 15:00-15:30 JCF18_04 A. Kitamura et al. (Technova Inc.) Comparison of excess heat evolution from zirconia-supported Pd-Ni nanocomposite samples with different Pd/Ni ratio under exposure to hydrogen isotope gases 15:30-16:00 JCF18_05 Y. Iwamura et al. (Tohoku U.) Reproducibility on Anomalous Heat Generation by Metal Nanocomposites and Hydrogen Isotope Gas 16:00-16:30 JCF18_06 M. Kishida et al. (Kyushu U.) Measurement of Anomalous Heat Generation in Hydrogen Flow by Differential Scanning Calorimetry 	12:00-13:00	Registration		
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	16:00-16:30	JCF18_06 M. Kishida et al. (Kyushu U.)		
by Differential Scanning Calorimetry		Measurement of Anomalous Heat Generation in Hydrogen Flow		
		by Differential Scanning Calorimetry		

16:30-17:00	JCF18_07	T. Hioki et al. (Nagoya U.)	
	In-situ XRD and XAFS Analyses for Metal Nanocomposites		
	used in Anomalous Heat Generation Experiments		
17:00-17:10	Break		
17:10-17:30	JCF Annual M	eeting	
17:30-20:00	Reception		

November 25 (Sat), 2017

Session 3	Chairman; Y. Iwamura (Tohoku U.)		
9:30-10:00	JCF18_08	K. Tsuchiya (NIT, Tokyo)	
	Progress of density functional methods in LENR and their problems II		
10:00-10:30	JCF18_09	K. Tanabe (Kyoto U.)	
	Theoretical Investigation of Plasmonic Field Enhancement on Planar Metal Surfaces		
10:30-11:00	JCF18_10	K. Ooyama (Ooyama Power Inc.)	
	Nuclear Fusion	Mechanism in Crystal	
11:00-11:15	Break		
Session 4	Chairman; H. Numata		
11:15-11:45	JCF18_11	K. Tanabe (Kyoto U.)	
	Is the Heat Difference between D and H Really a Sign of Fusion?		
11:45-12:15	JCF18_12	H. Miura	
	Water Clusters	Related to OHMASA-GAS	
12:15	Adjourn		



Direct Joule Heating of D-Loaded Pd Plates in Vacuum

Yuta Kitagawa¹, Shunsuke Ono¹, Yusuke Hayashi¹, Eiichi Yamaguchi², and Katsuaki Tanabe^{1*} ¹Department of Chemical Engineering, Kyoto University ²Graduate School of Advanced Integrated Studies in Human Survivability, Kyoto University *tanabe@cheme.kyoto-u.ac.jp

A gas-phase experimental research in quest of condensed-matter fusion is underway by using multilayered deuterium-containing Pd plates. In our experiment, we in particular directly apply a bias voltage across the Pd sample to provide a current injection through Pd, to stimulate the nuclear reaction by Joule heating, also anticipating strong electrodiffusion or electromigration, in addition to the conventional deuterium diffusion induced by pressure/mass-concentration and thermal gradients.

Our experimental setup is a stainless-steel-made, gas-phase reactor system including a deuterium-loading chamber, an electron-beam deposition chamber, and a reaction-analysis chamber [1,2]. A high-resolution small-amu quadrupole mass spectrometer, a gas proportional neutron detector, and a Geiger-Mueller detector for α , β , and γ rays are equipped to the facility. We first annealed a Pd plate with a dimension of $3 \text{ cm} \times 3 \text{ cm} \times 1 \text{ mm}$ at 1000°C for 10 hours in an external furnace in a nitrogen atmosphere to degrease the surface. Then we brought the Pd plate into the electron-beam deposition chamber via a pre-evacuation chamber. A Au film with a thickness of 1000 Å was deposited on one side of the Pd plate, as a low-contact-resistance electrode as well as a capping layer to induce single-directional deuterium diffusion and desorption for the ease of analyses. We then transferred the Pd plate to the deuterium-loading chamber. After filling the chamber with D_2 gas up to 760 Torr, we left the Pd plate for 5-10 hours at room temperature in order for the Pd plate to absorb deuterium asymptotically to the equilibrium. Finally, we transferred the Pd plate to the reaction-analysis chamber inside the cluster high-vacuum system with no ambient exposure. In the reaction-analysis chamber, a W needle electrode and a K-type thermocouple contacted the surface of Au-deposited side of the Pd plate. Electric current was then injected through the W needle to the Pd plate. We present our preliminary experimental results in the meeting.

We thank Hiroshi Sugiura for his support on the experimental equipment. We also thank for the technical advices by Kai Masuda, Tadahiko Mizuno (radial-ray detection), Yasuhiro Iwamura (Pd pretreatment), Akira Kitamura and Akito Takahashi (mass spectroscopy). This work was partially supported by the Thermal & Electric Energy Technology Foundation.

[1] E. Yamaguchi and H. Sugiura, Proc. ICCF-7, 420 (1998).

[2] H. Sugiura and E. Yamaguchi, Proc. ICCF-7, 366 (1998).

Deuterium desorption experiments using Pd-Zr and Pd-Ni-Zr multi-layered samples.

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Anomalous heat evolution has been observed in deuterium desorption experiment with Ni-based nano-composites supported by zirconia [1]. In the experiments, the phenomenon could be attributed to a specific property in deuterium diffusion with metal complexes as well as the nano-scaled fine-structure of the sample. Considering the specific conditions of the sample, we performed deuterium desorption experiment using multi-layered metal complex sample and investigated the thermal behavior in deuterium diffusion process.

We performed deuterium desorption experiments using various types of multi-layered complex samples such as Pd-Au, Pd-Ni, Pd-Ag, Pd-Ti, and investigated the deuterium diffusion associated with the thermal behavior. We also performed the multi-layered complex samples with fine-structured interface. In the experiment, these samples were fabricated by depositing thin metal layer onto a Pd foil substrate by Ar ion beam sputtering. After loading deuterium, the sample was set into an evacuated chamber (~10⁻⁴ Pa) and applied DC current to stimulate deuterium out-diffusion. During the experiment, the surface temperatures of the sample and the inside pressure of the chamber were recorded continuously for 24 h. We observed different thermal behavior in deuterium diffusion for the each of samples [2,3]. For the Pd-Ni and Pd-Ag with a fine-structured interface, we observed the short-period fluctuation in temperature which lasted 2–4 h at the beginning of the desorption experiment. Also, for the Pd-Ti, we observed a sudden temperature increase 1-2 h after beginning the experiment.

In the latest experiments, we have examined Pd-Zr, Pd-Ni-Zr complex samples. For the Pd-Zr, we observed a sudden temperature increase 1-2 h after beginning of desorption experiment. This phenomenon was similarly observed for Pd-Ti sample. For the Pd-Ni-Zr, we observed various temperature behaviors. It indicates that slight difference of structure or composition of Pd-Ni-Zr complex may significantly affect the deuterium diffusion behavior which results in the thermal one.

Reference

[1] A.Kitamura et al., Proc of JCF16(2016)1.

[2] H.Kudo et al., Proc of JCF15 (2015) 20.

[3] S.Kataoka et al., Proc of JCF16 (2016)29.

Search for characteristic microstructure of Pd rod formed during repeated cathodic and anodic electrolysis

Hiroo NUMATA

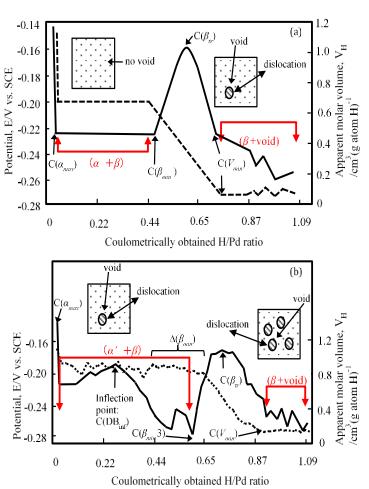
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Long-term electrolysis for well annealed thick Pd rod (9.0 mm diameter) in 0.1 *M* LiOD was performed ¹. Microscopic observation of the postelectrolysis Pd electrode surface showed the characteristic morphology of slip bands and doubly cross slip, while the cross sectional areas showed a peculiar morphology: ant-nest like voids, distributed not whole volume of the postelectrolysis Pd. The N-cycle model ² was proposed to understand the phenomena related with Cold fusion (CF); where the formation of reaction vessel was modeled as the first step. To understand the formation mechanism of such hypothetical vessel, we have investigated the physico-chemical properties of hydrogen dissolved in Pd by *in situ* potentiometric, resistance and dilatometric measurements during repeated hydrogen absorption/desorption electrolysis in glycerin and phosphoric acid ³. Figs. (a)- (b) below show a comparison of the potential (dotted line) and the apparent molar volume (solid line) as a function of Pd/H ratio during the first C mode electrolysis: (a) and the 2nd and 3rd repetitions: (b). In these diagrams for over the β phase (> β_{min}) the potential shifted with an increase in dilation, which suggests nonequilibrium PdH_{2-x} precipitation

followed by conversion to the β phase and void formation. Irrespective of the given physico-chemical properties, the insets reveal that an evolution of voids surrounded by highdefect density areas, which corresponds dislocations to and vacancies surrounding precipitates/matrix boundary 4).

In this study, estimation of stable micro void, with respect to hydrostatic pressure and hydrogen content will be conducted to strengthen the basis of the peculiar morphology observed during long term electrolysis. It will also be discussed that voids contain substances such as ions, electrons, atoms and molecules, which are analyzed in terms of the well-established plasma dynamics.

Refs. 1) H. Numata et al.: Conf. Proc. **Vol.33 of ACCF2**, "The Science of Cold Fusion", pp.71-79 (1991) 2) H. Numata and I. Ohno: **ICCF6**, Toya Japan, vol.1, pp.213 (1997) 3) H. Numata et al.: Fusion Technol., **38**, pp.206 (2000) 4) H. Numata: Proc. JCF17, (2017) to be published



Figs. (a)- (b) Schematics of the in situ measurements of potential (dotted line) and apparent molar volume (solid line) of 1st (a); and those of potential (dotted line) and apparent molar volume (solid line) of 3rd repetitions (b); as a function of x. $\Delta(\beta_{min})$ denotes (β_{min}) incremental charge between 2nd and 3rd repetition.

Comparison of excess heat evolution from zirconia-supported Pd-Ni nanocomposite samples with different Pd/Ni ratio under exposure to hydrogen isotope gases

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Hydrogen isotope absorption by palladium and nickel-based nanocomposite samples has been examined as a collaborative work using the experimental apparatuses installed at Kobe University and Tohoku University in order to share scientific understanding of the anomalous heat effects both at room temperature (RT) and elevated temperatures (ET). In the present paper we discuss D (or H) gas charging and heat release characteristics of PNZ6, PNZ6r and PNZ7k tested in Kobe.

These samples consist of Pd-Ni nanocomposites embedded in ZrO_2 particles that had been formed by milling of calcined amorphous ribbons of Pd, Ni and Zr mixture made by melt-spinning method. The calcination was performed in atmospheric air for 60 hours at 450 °C. The PNZ6r sample is a re-oxidized sample of PNZ6 after finishing a series of D(H) gas charging/calorification experimental runs at RT and ET with repeated sample baking. The PNZ6 and PNZ6r samples contain Pd and Ni with atomic ratio of Pd/Ni = 1/10, while the PNZ7k sample contains them with Pd/Ni = 1/7. About 100 gram of the sample containing about 20 gram of Ni was used in each case.

The samples have been characterized by XRD, SEM-EDX and TEM analyses to reveal existence of NiZr₂ phase and formation of NiZr₂D_x under exposure to D₂ gas. The samples have also been subjected to ERDA analyses to examine hydrogen isotope distribution in the near surface region. The results of the gas charging/calorification measurements are summarized as follows:

- (1) Similarly to other PNZ samples tested so far, in the initial phases at RT (#1-1) for virgin PNZ6 and PNZ7k samples, hydrogen absorption and heat evolution are characterized by large amount of the loading ratio $L_{\rm M} \equiv D/({\rm Pd}\cdot{\rm Ni}) \sim 3.4$ and the specific absorption energy $\eta_{\rm av} \sim 0.6 \,{\rm eV/D}$.
- (2) On the other hand, in #n-1 ($n \ge 2$) phases at RT for these samples after the cycle of RT-ET D(H)gas charging phases followed by vacuum baking between #(n-1) and #n runs, the values reduces to $L_M \equiv D/(Pd\cdot Ni) \sim 1.3$ and $\eta_{av} \sim 0.3 - 0.4 \text{ eV/D}$, to which formation of PdD/NiD and NiZr₂D_x contributes.
- (3) In the ET phases, the excess power W_{ex} continuing for several weeks with the maximum reaching 24 W and slowly decreasing to around 10 W has been recorded for PNZ6, while $W_{ex} \sim 7 8$ W for PNZ6r, and 3 4 W for PNZ7k.
- (4) The fact that the samples with Pd/Ni = 1/10 showed much higher excess power than the sample with Pd/Ni = 1/7 suggests that the atomic ratio is one of the key factors to improve the COP.
- (5) The maximum integrated excess energy amounts to 40 MJ/mol-Ni or 200 MJ/mol-H without any observable change in the sample composition, which cannot be explained by any chemical process.

Reproducibility on Anomalous Heat Generation by Metal Nanocomposites and Hydrogen Isotope Gas

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Anomalous heat generation experiments using metal nanocomposites and hydrogen isotope gas based on Kitamura and Takahashi paper [1] have been performed at Kobe University and Tohoku University as a collaborative work in order to confirm the existence of the anomalous heat effects. As a result, amount of anomalous heat generation per hydrogen or deuterium exceeded 10eV/H or D at least. The released energy is supposed to be very difficult to explain by known chemical processes only [2].

In this paper, we describe reproducibility on obtained experimental results with CNZ $(Cu_{0.044}Ni_{0.31}Zr_{0.65})$ and PNZ $(Pd_{0.044}Ni_{0.31}Zr_{0.65})$ samples.

For samples preparation, amorphous mixture of metal elements (Pd, Ni, Zr and Cu) were prepared by the melt spinning method at a Sendai company. By annealing the mixture in air at a temperature of 723K for 60 hr at Kobe University or Nissan Motor Co., Ltd., preferential oxidation of Zr to ZrO2 was expected with a consequent formation of binary-nanoparticles of Pd/Ni or Cu/Ni embedded in it.

As to CNZ samples, we performed two experiments using CNZ5s and CNZ6s with the same composition at Tohoku University. Anomalous excess heat generations were observed for the the samples at elevated temperature (150°C-300°C). Generated excess energies per absorbed H for CNZ5s and CNZ6s were 68 eV/H and 55eV/H, respectively. They cannot be explained by any known chemical process. Coincident burst-like increase events of the pressure of reaction chamber and gas temperature, which suggested sudden energy releases in the reaction chamber, were observed for both experiments using CNZ5s and CNZ6s samples.

PNZ7k and PNZ7s samples had the same composition. They were derived from a PNZ ($Pd_{0.044}Ni_{0.31}Zr_{0.65}$) material. Two independent excess heat experiments at Kobe and Tohoku Universities using PNZ7k and PNZ7s were conducted, respectively. Qualitative reproducibility between Kobe and Tohoku experiments was fairly good.

Reference

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Measurement of Anomalous Heat Generation in Hydrogen Flow by Differential Scanning Calorimetry

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When hydrogen or deuterium gas is in contact with some metal alloys at a temperature of $200-300^{\circ}$ C, excess heat except hydrogen absorption heat is detected, and the excess heat generation is maintained for more than 10 days. Total amount of the excess heat observed is enormous and cannot be explained by only chemical reaction. Such anomalous heat generation has been reported in a series of collaborative work [1,2]. The heat generation experiments have been carried out using precise flow calorimetry system and a lot of metal alloy powder (> 100 g) at Kobe University and Tohoku University in order to increase the heat measurement accuracy. However, the use of much metal powder needs a long-time observation which make it difficult to carry out a variety of experiments under different conditions. The abundance of powder also leads to a wide temperature distribution in the measurement vessel which makes it difficult to reveal the temperature dependence of anomalous heat generation.

In this work, using differential scanning calorimetry (DSC) and a small amount of palladium-nickel-zirconium (PNZ) alloy powder (40 - 100 mg), anomalous heat generation was observed in hydrogen flow. The powder sample was heated at 5 °C/min up to a predetermined temperature, and then the temperature was kept at a constant for 2 h - 8 h. The heat flow from the sample was measured in both hydrogen flow and helium flow. The difference in the heat flow between the hydrogen and helium flow was determined as the heat generation due to contact between metal and hydrogen.

The heat generation due to hydrogen absorption was observed for PNZ sample at around 200 °C during the elevated temperature process. During holding temperature process, some reference samples such as silver, magnetite, and zirconia showed no heat generation while PNZ sample exhibited a heat generation of 20-70 mW/g and the heat generation was maintained for more than 8 h. These results were similar to those obtained at Kobe University and Tohoku University.

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In-situ XRD and XAFS Analyses for Metal Nanocomposites Used in Anomalous Heat Generation Experiments

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Reproducible anomalous heat generation has been reported in a series of collaborative experiments performed at elevated temperatures $200 \sim 300^{\circ}$ C using metal nanocomposites and hydrogen isotope gas [1 - 4]. Using an active material PNZ6 of 124g, a generation of excess heat exceeding 10W was observed for about 45days [4]. The accumulated amount of excess heat exceeded 45MJ, which could not be explained by any known chemical reactions [4].

In this paper, structural changes of PNZ6 with increasing temperature under hydrogen atmosphere were studied by in-situ XRD (X-ray diffraction) and XAFS (X ray absorption fine structure) analyses using facilities of Aichi Synchrotron Radiation Center. The analysed material was the same with that used for the heat evolution experiments at Kobe University [4]. The in-situ XRD analyses were performed at 15keV under hydrogen of 0.4MPa, while raising temperature from room temperature (RT) to 600°C. The K-shell XAFS profiles of both Ni and Zr were taken under flowing hydrogen at 100 cc/min, while raising temperature from RT to 600 °C.

By the XRD analyses, following results were obtained: i) before hydrogen exposure, PNZ6 dominantly consisted of NiZr₂ and ZrO₂; ii) after hydrogen exposure, at 120°C the peak from NiZr₂ was divided into two peaks, suggesting the formation of two hydride phases NiZr₂H_x (x = x₁, x₂, [x₂ \gg x₁]); iii) at 200 ~ 300 °C, PNZ6 dominantly consisted of NiZr₂H_{x2} and ZrO₂; iv) at 400°C, the formation of ZrH₂ started, v) at temperatures higher than 500°C, ZrH₂ formed and NiZr₂ disappeared. The XAFS data were qualitatively consistent with the XRD results.

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Progress of density functional methods in LENR and their problems II

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It is well known that hydrogen and deuterium are easily absorbed into some materials. In these cases, they exists as positively charged ions. However, it is impossible to regard them as point charges, because they are the lightest ions. Therefore, many-body problems in quantum mechanics should be considered for LENR.

In JCF17, we showed the progress of density functional methods in LENR and their problems by using our previous results for density functional calculations [1,2,3]. In JCF18, we show further considerations for the convergence aspects in the iterative calculations and guess the interactions between them including quantum mechanical many-body effects.

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Theoretical Investigation of Plasmonic Field Enhancement on Planar Metal Surfaces

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The power density supplied to deuterium-metal systems is a key to initiate the nuclear reaction. We previously proposed and analyzed the electromagnetic energy focusing effect around metal nanoparticles and nanoshells to significantly increase the reaction probability [1]. In the present work, we show that such a plasmonic field enhancement occurs also on planar metal surfaces. Removing the noble-metal approximation in Ref. 2, we have fully calculated the maximum field enhancement for the metals commonly used in the community (Fig. 1). The main formula to represent the field enhancement factor, defined by the ratio of the spatial electromagnetic energy densities with and without the metal object, is summarized as:

$$\eta = \frac{\left|\vec{E}_{SP}(0^{+})\right|^{2}}{\left|\vec{E}_{0}\right|^{2}} = \frac{c(\left|q_{1}\right|^{2} + \left|k_{SP}\right|^{2})\cos\theta(1-R)}{c\varepsilon_{1}^{1/2}k_{SP}^{1}\operatorname{Re}\left\{\frac{k_{SP}(\varepsilon_{1}q_{1} + \varepsilon_{2}q_{2}^{1})}{\varepsilon_{2}q_{1}^{1}q_{2}^{1}}\right\}}$$

where we followed a set of common notations in electrodynamics and the subscripts *1* and *2* denote the surrounding medium and the metal, respectively. The theory, assumptions, and calculation scheme we used will be presented in detail at the meeting. It should be noted that our calculation is only based on the Maxwell equations and involves nothing exotic or physically novel. We have thus found that a certain degree of enhancement is available on the metal-surface regions, implicating that this electromagnetic boosting effect had been unconsciously exerted in the experiments reported so far, particularly for the electrolysis-type ones. Importantly, this plasmonic enhancement occurs for the case of an optical-power incidence as well as an electric-bias application. It is therefore important to design and optimize the experimental systems, including the materials choice, structures, and operation conditions, additionally accounting for the plasmonic energy enhancement effect around the gas (vacuum)/liquid-metal interfaces.

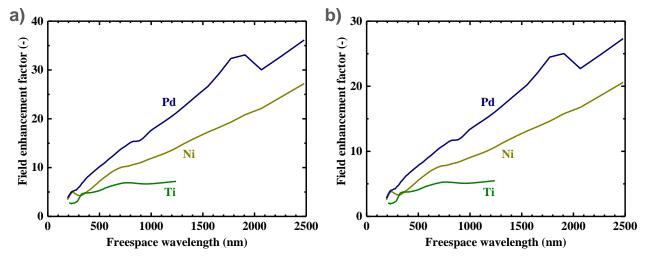


Fig. 1 Electromagnetic field enhancement factors on planar Pd, Ni, and Ti surfaces in (a) D₂/vacuum and (b) D₂O.

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Nuclear Fusion Mechanism in Crystal

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The author selected "Transmutation experiments induced by deuterium permeation" by Iwamura et al.[1] as an experiment in which nuclear reaction has definitely occurred, and considered the nuclear fusion mechanism in the crystal by finding the common point between this experiment and the experiment of "generation of excess heat of Pd cathode by electrolysis of heavy water" by Fleischmann and Ponds.

In these experiments, Pd are divided into two phases, an a phase with low deuterium concentration and an a' phase with high deuterium concentration, and internal stress are generated. Therefore, migration of edge dislocation occurs in the a' phase, abnormal accumulation of D nucleus which does not occur in static state occurs, and D-D nuclear fusion due to tunnel effect occurs. If the ion beams generated at this time reached the a phase with few crystal defects, there are led to the D nucleus accurately due to the channeling phenomenon, and secondary nuclear reactions are caused with a high probability. Furthermore, newly generated ion beams are led to another D nucleus, and nuclear reactions occur one after another.

The author searched for chain reactions that could explain excessive heat and nuclide transformation and did not generate radiation with high penetrating power, and red the reaction equation presuming the existence of long-lived excited α -nuclei. However, there is a doubt about the existence of this excited α -nucleus, and since the energy of the ions observed in the experiment by Kasagi et al.[2] take values which are somewhat different from the energy of the ion generated by the chain reaction, the author predicts the existence of two D ion beams in a binary star state.

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Is the Heat Difference between D and H Really a Sign of Fusion?

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There have been reports on experiments comparing the cases with deuterium and hydrogen, claiming the realization of fusion reaction verified by larger heat generation from deuterium [1,2]. In this brief communication, we take a survey on the thermodynamics in D/H-Pd systems to examine whether this sort of claim stands or not.

For bulk Pd, the dissolution heat (in the unit of J/mol-gas) of D into Pd is known to be smaller than that of H [3,4]. The equilibrium solubility (mol-gas/mol-Pd) of D in Pd is moreover lower than that of H [4]. Consequently, the heat generation in D absorption is smaller than that of H. In this context, the claim above sounds valid because any larger heat generation from a deuterium system has to stem from some additional phenomena beyond the conventional physical chemistry.

It has however recently been found that the heat generation in D absorption is, oppositely, larger than that of H for Pd nanoparticles [5]. The principle of this experimental result has not been understood yet, but it may be related with the strain/distortion-induced modification of the potential energy surface for D/H atoms particularly in the subsurface region of Pd nanoparticles. The D/H solubility, for instance, is higher in smaller Pd particles [6] presumably due to the subsurface lattice expansion [7]. We may also need to account for the fact that the lattice-constant difference between the α and β phases becomes smaller as the Pd particle size decreases [8]. Some difference of the D/H-incorporation Pd lattice sites was also observed; the D/H atoms enter only the octahedral sites in the Pd lattice for bulk Pd, while entering also the subsurface tetrahedral sites as well as the octahedral for Pd nanoparticles [9,10]. The larger heat for D might be thus explained if the enthalpy change in the tetrahedral sites is larger for D than for H. More details will be discussed in the meeting.

In the field, an atomic-level understanding of hydrogen absorption has not yet been established, represented by the on-going argument for the penetration mechanism, quantum tunneling or a multiatomic concerted process [11]. All in all, we at this point cannot conclude that the higher heat generation from deuterium experiments than that for hydrogen controls can be a reliable proof of nuclear reaction, and more careful analyses of the data are necessary particularly for nanostructured Pd.

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Water Clusters Related to OHMASA-GAS

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OHMASA-GAS (Oxygen-Hydrogen Mixing Atomic Symmetrized Aeration-Gas), which is one of the hydrogen-including oxy-hydrogen gases, is obtained through the electrolysis of water under vibratory agitation by vibration blades and can be stored as the hydrogen (H) and oxygen (O) mixture gas. This gas has many practically useful properties such as titanium (Ti), tantalum (Ta), tungsten (W) metal or glassy carbon (C) melts instantly as if it vaporizes at about 3000°C or more when it comes into contact with the flame of burning gas at about from 600 to 700°C. Moreover some noticeable phenomena related to the generation of this gas have been reported that various elements are generated under vibratory agitation of the electrolytic solutions with alkali or alkaline-earth metal ions such as magnesium (Mg), calcium (Ca) or cesium (Cs).

In order to investigate these properties and phenomena, we supposed that OHMASA-GAS would be generated as water cage clusters which are made by division of large water tube clusters and encapsulate H atoms, and the generation of various elements under vibratory agitation would be caused by the collapse of a part of the large water tube clusters. In the last study, we have simulated the large tube water clusters with or without Mg atom and the small water cage clusters which encapsulated H atoms, by use of a computer simulation program MOPAC based on the semi-empirical molecular orbital method on a personal computer. In this study, we confirmed the some results of MOPAC by use of another first principles electronic state computer simulation program Quantum ESPRESSO based on Density Functional Theory on a personal computer. We are now investigating the properties of the small water cage clusters which encapsulate H atoms (OHMASA-GAS), and the strongly compressed states of a part of the large tube clusters.