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# Energetics Of Defects And Strains In Palladium

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## Abstract

Pd employed as cathodes in cold fusion experiments contains various defects, each of which has an associated energy. In principle, some of the energy in Pd due to defects that exist before a cold fusion experiment could be released as apparent excess heat during the experiment. Energy densities were computed for high concentrations of vacancies, impurities (both substitutional and interstitial atoms), dislocations and grain boundaries, as well as for strains. It is concluded that pre-existing defects and strains cannot account for the energies released during cold fusion experiments. Nonetheless, defects may play other supporting or central roles in cold fusion.

## 1. Introduction

In cold fusion experiments, excess power  $P_x$  is defined as the difference between power emerging from the experiment (as measured by calorimetry) and the input electrical power (the product of the voltage and current). The time integral of  $P_x$  over the course of the experiment is  $Q_x$ , the excess energy (heat), that is,  $Q_x = \int P_x dt$ . The source of  $Q_x$  is the core problem in cold fusion. By now, there is abundant evidence that  $Q_x$  is the result of exothermic nuclear reactions. This evidence has three forms: (a) some of the excess heat values exceed 100 eV per metal atom in the experiment, that is, they are far beyond chemical energies, (b) higher concentrations of some elements are measured, and they correlate quantitatively with  $Q_x$  in several cases, and (c) energetic nuclear radiations are detected in many experiments.

Despite the diversity and amount of evidence that  $Q_x$  is of nuclear origin, uncertainties persist regarding the source of the energy, especially regarding the basic physical mechanisms(s) at work. The question of whether the electrolytic cells, and their relatively large electrodes in many cold fusion experiments, can function as energy storage devices, like springs or batteries, has hounded the field from its earliest days. As recently as April of this year, a letter to the editor of *New Scientist* asserted that there is a "simple and known explanation of the extra heat given off by metal hydrides, such as palladium deuteride. The extra energy comes from elastic relaxation." The letter was published under the heading "'Cold Fusion' Explained" (1).

The question of energy storage has two parts: (a) whether or not the annihilation of pre-existing defects or strains during an electrolysis experiment can release significant energy, and (b) whether or not energy stored in an electrode during hydriding (or deuteriding) can be released later, and be mistaken for excess power. The second part of the question has been answered by the experimental evidence referred to in the initial paragraph above. The purpose of this paper is to address the first part of the question by summarizing the energetics of palladium, which contains defects and strains prior to loading with a hydrogen isotope (which we will call hydriding to cover both protons and deuterons). Essentially, we ask if there is some significant mechanism for storing energy in advance of a cold fusion experiment, within the electrodes or other materials, whose release during an experiment would appear to be excess power.

We focus on palladium because of the importance of Pd-cathode experiments in the field. It has been used in many cold fusion experiments. Further, it is a reasonable representative of the metallic systems used in other cold fusion experiments. Also, values of the parameters that are needed for defect or strain energy estimates are known for Pd. We are concerned with all types of cold fusion experiments involving Pd,

including loading by thermodynamic, electrochemical and kinetic means. However, we will often make reference to the Pd cathodes in electrochemical experiments.

The energies stored in the starting material can be organized according to the dimensionality (D) of the defect structure, namely 0-D point defects (vacancies, or substitutional or interstitial impurities), 1-D line defects (dislocations), 2-D planar defects (grain boundaries, twin boundaries, stacking faults and surfaces) and 3-D elastic distortion (strains). For extreme concentrations of most of these defects, and a high isotropic linear elastic deformation, we computed the energy densities per cubic centimeter. The setup of each calculation, the parameters and conversion factors employed, and the results obtained for major types of defects are presented and discussed in the following sections.

## 2. Vacancies

Energy is required to create a vacancy in a material. The energy is that needed to break bonds with neighboring atoms. That is, the loss of binding energy between the missing atom and its surrounding atoms constitutes most of the vacancy creation energy. The lattice relaxation that occurs around a vacancy decreases the energy needed for creation of a vacancy.

At any temperature, there is a thermodynamic equilibrium concentration of vacancies in a material. The higher temperature, the higher will be the vacancy concentration. Pd has  $6.8 \times 10^{22}$  atoms per  $\text{cm}^3$ . Assuming a high temperature of  $500^\circ\text{C}$ , the vacancy fraction in Pd is about  $10^{-10}$  (2). Hence, the number of vacancies is near  $6.8 \times 10^{12}$  per  $\text{cm}^3$ . The vacancy formation energy is about 1 eV (3). So, we arrive at:  $6.8 \times 10^{12}$  eV  $\times 1.6 \times 10^{-19}$  J/eV, or about  $10^{-6}$  J/ $\text{cm}^3$  for the energy density due to vacancies. Hence, vacancies can “store” only very small energies in Pd, even if the temperature is high compared to temperatures in most cold fusion experiments. At room temperature, the vacancy concentration is five orders of magnitude smaller than at  $500^\circ\text{C}$ .

We note that Fukai and his colleagues have shown that the vacancy concentrations in the Pd-H system can approach 20% under special conditions (4,5). They exposed Pd (and Ni) to hydrogen gas at a pressure of 5Gpa (about 50K atmospheres) and  $700\text{-}800^\circ\text{C}$ . Complexes of H and vacancies formed with high densities. When the H was removed, the vacancies remained in high concentrations. Whether or not these observations are germane to cold fusion experiments is unclear. The effective pressures in electrochemical loading experiments are very high. Commonly, more than 10 protons or deuterons pass through each Pd unit cell face on the cathode surface each second during loading. However, the ambient temperatures in cold fusion experiments are usually near room temperature ( $25^\circ\text{C}$ ). The *in situ* dynamic x-ray diffraction experiments employed by Fukai et al could be applied with great effect in cold fusion experiments.

The hydriding and dehydriding processes in cold fusion experiments cannot remove all the initial vacancies in a sample of Pd. Their presence is a thermodynamic imperative. However, even if vacancies could be made to disappear, it is clear that their annihilation during a cold fusion experiment cannot account for observed excess energies.

## 3. Substitutional and Interstitial Impurities

Atoms other than palladium can reside in a palladium lattice in two types of positions. They can occupy lattice sites in place of palladium atoms (substitutionals) or they can reside in locations between the normal lattice sites (interstitials). Each of these possibilities will be discussed in turn.

Putting larger atoms on lattice sites in place of Pd atoms requires energy due to the strain introduced into the lattice in the neighborhood of the substitutional. Conversely, small substitutional atoms permit some lattice relaxation in their region. In both cases, the electronic binding energies also change for most substitutionals. Despite these differences, the energy per substitutional is near 1 eV (6). We assume that 1 in 1000 atoms is a substitutional impurity, that is, the Pd is “3 9s” pure, or has 1000 ppm of substitutional impurities. This is a very high value for an impurity concentration. Hence, we have:  $6.8 \times 10^{22}$  Pd/ $\text{cm}^3 \times 10^{-3}$  substitutionals/Pd  $\times 1$  eV/substitutional  $\times 1.6 \times 10^{-19}$  J/eV, or about  $10$  J/ $\text{cm}^3$ . This energy density is significant, but the assumed substitutional impurity level is rather extreme.

Placing atoms of any elements above hydrogen into interstitial positional within a Pd lattice introduces strain into their neighborhood, and requires energy. Such dissolution also involves energy changes due to redistribution of the metallic bonding electrons near the impurity atom. However, similar to the case for substitutional atoms, the creation energy for interstitials is close to 1 eV per atom (7). If we again assume that the lattice has a high concentration of interstitial atoms, namely 1000 ppm, then the same arithmetic applies, and the energy density due to interstitials is about  $10$  J/ $\text{cm}^3$ .

It is important to note that extracting the energy, during a cold fusion experiment, that is due to the creation of substitutional or interstitial impurities in a Pd lattice *prior to* the experiment is possible only if the

impurities are removed in the course of the hydriding or dehydriding. And, the decrease in the entropy of the system would partially offset the decrement in the energy due to removal of impurities. If the impurities are not removed, their creation energy cannot appear as apparent excess power and energy. It is possible that the redistribution of impurity atoms during an experiment will relieve some lattice stress and release some energy, but that would be relatively small compared to the creation energies of impurities or the energies associated with dislocations or grain boundaries, which are given in the following sections. In short, the presence of substitutional or interstitial impurity atoms in a Pd lattice will not lead to significant apparent excess energies in cold fusion experiments.

Additional comments can be made regarding impurities in cold fusion experiments, aside from their potential role as an energy storage mechanism. These deal with the possibilities that impurities either (a) are involved in setting up the conditions conducive to nuclear reactions at low energies, or (b) actually participate in such reactions. The Appendix contains material on these additional potential roles for impurities.

#### 4. Dislocations

Dislocations are thought of as linear defects because their length greatly exceeds their width within a lattice. They are of two basic types, called edge and screw dislocations. For both, their creation can be conceptualized as beginning with a cut into a lattice. In the case of edge dislocations, an extra plane of atoms is inserted into the cut and the lattice closed. The name comes from the extra plane having an edge along the length of the dislocation. In the case of screw dislocations, the halves of the original lattice on the sides of the cut are translated parallel to the bottom of the cut and then rejoined. The name comes from the structure of the resulting lattice in which the atomic planes form a spiral, or screw, around the edge of the original cut. Both types of dislocation are classified by a vector, called the Burger's vector, which gives the direction and size of the lattice deformation that was needed to produce the dislocation. For an edge dislocation, the vector is perpendicular to the dislocation and usually equal to a lattice constant in length. Figure 1 shows a schematic cross section of an edge location, with its Burger's vector. For a screw dislocation, the Burger's vector is parallel to the dislocation and, again, commonly one lattice constant in length.

Since both types of dislocation involve significant local lattice deformations, they have energetic elastic strain fields associated with them. The deformations and associated strains account for the energies required to produce dislocations in a lattice. The energy per unit length for an edge dislocation is  $\mu b^2$  (9), where  $\mu$  = the shear modulus ( $8 \times 10^6$  psi in Pd) and  $b$  is the Burger's vector (about 0.2 nm for Pd). A very heavily cold-worked metal has about  $10^{16}$  m/m<sup>3</sup> or  $10^{10}$  m/cm<sup>3</sup> of dislocations (10). It is noted that this distance of 10 million kilometers of dislocation length in 1 cm<sup>3</sup> is remarkable. It is roughly 30 times the earth-to-moon distance. If the dislocations at this high density were arranged in three orthogonal arrays, one for each of the three directions in the lattice, this dislocation density implies that they are spaced by only about 100 lattice constants. This is certainly an extreme defect condition.

We assume the very high dislocation density of  $10^{10}$  m/cm<sup>3</sup> for the isolated dislocations. Using the conversion factors of 1 J = 0.74 ft-lbs and 1 m = 3.28 ft, along with the values for  $\mu$  and  $b$  given in the last paragraph, an energy of about 20 J/cm<sup>3</sup> results. This energy density value is comparable to those for impurity atoms. However, the case for dislocations differs from that for substitutional or interstitial impurities. While it is not clear that impurities will be removed from a lattice during a cold fusion experiment, it is possible that dislocations will be annihilated and their energy recovered. The effects on the dislocation structure and density initially within Pd or other metals due to hydriding to various concentrations and due to dehydriding are not known. In general, the energy associated with existing dislocations should decrease with hydriding and vice versa, even without changes in the dislocation density. Despite such uncertainties, the implication of the above estimate is clear, namely that dislocations cannot be a large source of released energy in cold fusion experiments.

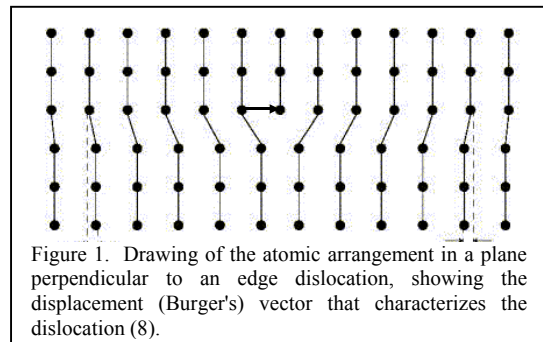


Figure 1. Drawing of the atomic arrangement in a plane perpendicular to an edge dislocation, showing the displacement (Burger's) vector that characterizes the dislocation (8).

## 5. Grain Boundaries

Grain boundaries are inter-granular defects that have two dimensions. Such interfacial defects separate regions of materials that have different structures or crystallographic orientations. Grains within materials are essentially single crystals that contain vacancies, and may also contain impurity atoms and dislocations. The boundaries between grains are collections of dislocations in sheets that may be planar or curved. Referring to Figure 1, if edge dislocations are one above another and parallel to each other, the lattices on the sides of the sheet of dislocations have an angle with respect to each other. That angle depends on the density (spacing) of dislocations. The strain fields of the individual dislocations interact, and the energies associated with individual dislocations add to constitute the formation energy of a grain boundary. If a material with small grains, that is, many dislocations, is annealed, the material attempts to minimize its total grain boundary area and energy by grain growth. Higher temperatures and longer annealing times promote growth of larger grains, as illustrated in Figure 2.

We model the grains in a cubic centimeter of Pd as small cubes bounded by three sets of parallel, equally-spaced planes, one set in each of the three orthogonal directions in the lattice. Take the cubic grains to be  $S$  mm on a side. The total area in  $1\text{ cm}^3$  is  $(10/S + 1)3$  planes  $\times 100\text{ mm}^2/\text{plane}$ . Clearly, when  $S$  is small, the total area of grain boundaries is large, and the energy associated with the grain boundaries is also large. Hence, we want to consider very small grains in order to make an estimate of total grain boundary energies that is in error on the side of being too high. To a good approximation, when  $S$  is small, the total grain boundary area is  $3000/S\text{ mm}^2$ . For  $S = 1\text{ }\mu\text{m} = 10^{-3}\text{ mm}$ , the area in  $1\text{ cm}^3$  is  $3 \times 10^6\text{ mm}^2$  or  $3\text{ m}^2$ . Grain boundary energies are generally about  $1\text{ J/m}^2$  (12), so the energy due to grain boundaries is about  $3\text{ J/cm}^3$ . Again, we arrive at a small energy density, despite the extreme assumption of micrometer-sized grains.

Because grain boundaries are made up of 2-D arrays of dislocations, it is possible to compare dislocation and grain boundary energies by using the energies per unit dislocation length (1-D) from the last section and the energy per unit grain boundary area (2-D) from this section. If an inter-granular angle  $\theta$  of  $0.1$  radian (about  $6^\circ$ ) is assumed, then the energies in  $1\text{ cm}^3$  are  $0.1\text{ mJ}$  for *both* the arrayed (but non-interacting) dislocations and for the arrayed (and interacting) dislocations in a grain boundary. Apparently, the overall strain field energy of dislocations is roughly independent of whether they are isolated or in an ordered array. However, it must be noted that grain boundary energies do depend on the inter-grain angle  $\theta$ . Maximum grain boundary energies occur for  $\theta$  near  $30^\circ$ , and near  $6^\circ$ , they have a value near 50% of the maximum. Taking this into account would make the computed energy for interacting dislocations in a grain boundary half of that for the same number and length of non-interacting dislocations. If the reverse were true, then grain boundaries would be unstable and they would tend to disassemble into separate dislocations.

As with dislocations, the effects on the grain structure initially within Pd or other metals due to hydriding to various concentrations and due to dehydriding are not known. However, again, grain boundaries cannot account for the excess energies seen in many cold fusion experiments, even if they were entirely destroyed during the experiment.

## 6. Lattice Strains

Deformations can affect an entire three-dimensional object, such as the cathode in an electrochemical cell. There are two primary types of strains, plastic and elastic. Plastic strains are permanent in the sense that they remain after the applied forces that created them are removed. They are the result of the creation or multiplication of dislocations within the lattice of the material forming an object. Plastic strains can be very large, for example, when a rod is drawn (swaged) into a wire. Elastic strains are not permanent, but go away when the force that produced them is removed. Such strains are relatively small because the forces causing them have to be below the "elastic limit", above which plastic deformation occurs and the material can no longer spring back to its original shape.

The energy density computed in Section 4 for dislocations in a very highly deformed material *prior to* a cold fusion experiment are germane to plastic deformations that might be caused *during* an experiment.

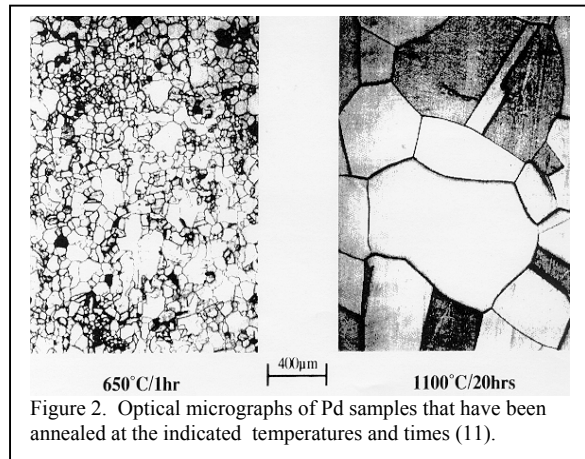


Figure 2. Optical micrographs of Pd samples that have been annealed at the indicated temperatures and times (11).

However, plastic deformation due to applied stresses does not generally occur during cold fusion experiments, so we limit our attention to elastic changes in the lattice.

The "elastic relaxation" mentioned in the letter from Stecki (1) is a change in the lattice parameter of Pd when it undergoes the *internal chemical change* of losing the hydrogen or deuterium, which had been loaded into the lattice. It is not the result of any *external mechanical change*. Since external mechanical forces are not commonly applied to the materials during cold fusion experiments, elastic deformation is usually not relevant to such experiments. However, the relatively few cold fusion experiments that have employed high pressures did strain the Pd or other involved materials. It is easy to estimate the energy density that can reside in the lattice strains during high-pressure cold fusion experiments.

Elastic deformation can be produced by two kinds of forces, (a) isotropic pressure in all directions simultaneously, which squeezes a lattice into a smaller volume, and (b) shear forces that act to deform a lattice in particular directions, without major changes in the volume of the deformed object. Applied shear forces are not relevant to cold fusion experiments. We consider isotropic pressure as indicative of the energetics of lattice strains, and most germane to pressurized cold fusion experiments.

Isotropic pressure can be expressed as  $P = K \times \Delta V/V$ , where the bulk modulus  $K = 180 \times 10^6$  Pa for Pd (14) and  $\Delta V/V$  is the relative volume change due to the pressure. We take a large elastic deformation of 1%, so  $\Delta d/d = 10^{-2}$  or  $\Delta V/V = 10^{-6}$ . The work per unit area is  $(F \Delta d / \text{Area}) = P/\text{area}$ . Considering the six faces of a cube 1 cm on a side, and using the conversion factors of  $1 \text{ Pa} = \text{N/m}^2$ ,  $1 \text{ N} = 0.225 \text{ lbs}$  and  $1 \text{ J} = 0.74 \text{ ft-lbs}$ , the elastic strain energy per  $\text{cm}^3$  is  $10^{-2} \text{ J}$ . This value is very small, entirely unable to explain the excess energy in cold fusion experiments.

## 7. Other Defects

The defects discussed above are not the only defects that can occur in the materials in cold fusion experiments. Notably, a few other types of 2-D defects, besides grain boundaries, are known. In some crystals, twins can form. These are essentially lattices that are mirror images of each other across a "twin boundary". Such boundaries have low energies relative to grain boundaries. For example, a grain boundary in copper has an interfacial surface energy of about  $646 \text{ mJ/m}^2$ , while the energy of a twin boundary in Cu is only about  $44 \text{ mJ/m}^2$  (15). Stacking faults are 2-D defects in the arrangement of adjacent planes of atoms in a lattice. They also have much lower energies than grain boundaries. The stacking fault energy for Pd is  $180 \text{ mJ/m}^2$  (15). The overall area of twin boundaries and stacking faults are small compared to the grain boundary area we employed in Sections 5. Hence, the energies associated with twin boundaries and stacking faults are not important energy reservoirs in cold fusion experiments.

It is possible, in principle, that very energetic states can exist on the 2-D exterior surfaces of materials that go into cold fusion experiments. However, the fact that materials are introduced into cold fusion experiments in ordinary laboratory air militates against the importance of such energetic surfaces. That is, the presence of oxygen, humidity and other constituents of air, or an electrolyte liquid, would relieve energetic surface states through physical adsorption or chemical absorption onto the surfaces involved. In any event, the surface energies of clean materials are in the range of  $1\text{--}3 \text{ J/m}^2$ , so a cathode with  $10 \text{ cm}^2$  would have only a few mJ of surface energy (15).

Cracks can be considered as a 2.5 dimensional defect. That is, they are essentially planar, but do have some extent in the directions perpendicular to the plane of the crack. There are two kinds of energy associated with cracks, surface energies and lattice deformation or strain energies in the region of a crack tip. It is known that the presence of cracks in cathodes in cold fusion experiments makes it impossible to reach the high loading (ratio of deuterons to Pd atoms) that are prerequisite to the observation of excess heat. That is, cathodes with cracks are not important in cold fusion experiments, so we ignore such defects.

Voids are hollow regions within materials and can, in principle, exist within cold fusion materials. They might be produced by either the presence of bubbles in a casting or by coalescence of vacancies. Voids in Pd are rare, so the energy associated with their surfaces can also be ignored.

It appears that only some of the defects considered in the sections above are potentially germane to the energetics of cold fusion experiments.

## 8. Summary and Discussion

The following table summarizes the defect energy densities, given in  $\text{J}/\text{cm}^3$ , that were presented in Sections 2 through 6, for extreme assumptions of defect densities and uniform deformation.

Defect or Condition	Assumption	$\text{J}/\text{cm}^3$
Vacancies	$T = 500^\circ \text{C}$ , so Vacancy Fraction = $10 \exp(-10)$	$\sim 10^{-6}$
Substitutionals	Part per thousand impurity, i. e., "3 9s" pure.	$\sim 10$
Interstitials	Part per thousand impurity, i. e., "3 9s" pure.	$\sim 10$
Dislocations	Heavy Cold Work = $10 \exp(16)\text{m}$ per $\text{m} \exp(3)$	$\sim 20$
Grain Boundaries	Very Small (micrometer size) Grains	$\sim 3$
Isotropic Deformation	1% linear deformation in the lattice constant	$\sim 10^{-2}$

The values in the table show that total annihilation of the initial defects in a cold fusion experiment would yield, at most, less than 50 J of apparent excess energy. If that energy were entirely released, this would produce an apparent excess power of 50 W for 1 sec, 5 W for 10 sec, 500 mW for 100 sec, 50 mW for 1000 sec or 5 mW for 10Ksec from a Pd cathode  $1 \text{ cm}^3$  in volume.

As already stated, the release of all energy from point defects (vacancies, and both substitutional and interstitial impurities) is highly unlikely. The dislocation density assumed to make the energy estimate for 1-D defects is very extreme, probably at least a few orders of magnitude too large. Similarly, the assumed grain size for the 2-D defects is very small, and the computed grain boundary energy may also be orders of magnitude high. Hence, more realistic potentially available energies and powers are very much smaller than those cited in the previous paragraph.

Many cold fusion experiments have cathodes with volumes well below  $1 \text{ cm}^3$ . Correspondingly smaller energies or powers would possibly be available from defects or strains in such cases. Hence, the energies stored in defects within the starting material are generally insufficient to account for observed excess energies in many cold fusion experiments, even if those energies could be entirely released by defect destruction during the processes of hydriding or deuteriding. We note that, because defect energies in Ni are generally similar to those in Pd, the rough estimates made above for Pd also apply to Ni in cold fusion experiments.

Interestingly,  $1 \text{ J per cm}^3$  corresponds to an average of only  $10^{-4} \text{ eV}$  per atom in Pd. This is quite a low energy density, which can be appreciated by comparing it with the heat (vibrational) energy of Pd near "room temperature". We use  $3/2kT$  as an estimate of vibrational energy in a solid like Pd, with Boltzman's constant  $k = 1.38 \times 10^{-23} \text{ J per degree Kelvin}$ . For a temperature of  $300^\circ \text{K}$ , the vibrational energy per atom is  $3.9 \times 10^{-2} \text{ eV}$ , which is about 400 times the energy density corresponding to  $1 \text{ J per cm}^3$ . For comparison, the electron affinity, heat of formation, binding energy and ionization energy for Pd are all on the scale of 1 or more eV per atom. If every Pd atom had about 1 eV of additional energy, the material would be a plasma with a temperature above 10,000 K. The defect energies we estimated, averaged over the Pd atoms in one cubic centimeter, give only very small volumetric energy densities, and, hence, small possible apparent excess energies.

Many questions about the dynamics of defects in Pd and other metals during hydriding and dehydriding remain unanswered. Research to determine the variation in vacancy concentrations and spatial distributions during and after hydrogen isotope dynamics in Pd is clearly needed, if vacancies play a role in cold fusion. Similarly, the effects of hydriding and dehydriding on any of the many possible substitutional and interstitial atom types, concentrations and distributions appear to be unknown and possibly relevant to the field of cold fusion. The changes in dislocations and grain boundaries, for different types and concentration of both these defects, with the type, concentration and dynamics of hydrogen isotopes, are other areas of ignorance. The interactions of these various types of defects might also be important, for example, the creation or annihilation of vacancies, dislocations and grain boundaries as they intersect each other. Further, the segregation of substitutional and interstitial impurities in the stress fields around dislocations and grain boundaries could play a role in creating the conditions needed for nuclear reactions at low energies in metallic lattices. In short, relatively little is known about the mechanisms and rates of the dynamics of defects and hydrogen isotopes in materials.

## Acknowledgement

Michael Staker provided references to the work of Fukai. We appreciate his assistance.

## Appendix: The Role of Impurities in Cold Fusion Experiments.

The possibility that substitutional or interstitial impurity atoms in Pd could store energy, which would be released during a cold fusion experiment and appear to be excess power, was discussed in Section 3. Here, we are concerned with two other roles that impurities might play in experiments that appear to produce nuclear reactions at low energies in solid materials. Lattice impurities can be of potential importance, either in (a) creating conditions conducive to nuclear reactions not involving them (such as reactions between two deuterons), or (b) actually participating in low energy nuclear reactions (most likely with isotopes of hydrogen). Because of these possibilities, there should be significant attention given to the impurities present in the materials in cold fusion experiments.

The occurrence of nuclear reactions at low temperatures in condensed matter must require quite special environmental conditions. If that were not the case, it is likely that such reactions would have been observed, studied and understood long ago. Storms called such special locations nuclear active regions or environments (16,17). It is conceivable that such active regions merely involve some combination(s) of chemical species and atomic structure, with the only defects being the inevitable thermodynamic vacancies. However, it seems more likely that impurity atoms, dislocations or grain boundaries would also play a role in forming the special conditions.

Impurities and other defects in nuclear active regions may perform a catalytic role without participating in the nuclear reactions. However, the critical environment might still be changed due to thermal effects following an exothermic nuclear reaction. There is a growing body of evidence that small crystallites are important for the production of excess heat. If 1 MeV is released into a nano-crystalline cube of Pd measuring 100 nm on a side and the energy distributed uniformly, the resulting temperature rise can be estimated two ways. Using  $3k\Delta T/2$  as the increase in atomic vibrational energy,  $\Delta T = 380$  K results. With the specific heat for Pd, namely 26.0 J/Kmole (14),  $\Delta T = 55$  K is obtained. This agreement is actually satisfactory, given the approximate nature of the vibrational calculation (an over estimate), and the fact that the temperature variation of the specific heat was ignored. Halving the nano-crystallite dimension to 50 nm would give  $\Delta T$  values 8 times higher. Similarly, if 24 MeV were released into a Pd nano-crystallite, substantially higher temperatures would result. Such temperatures are roughly consistent with the IR emission from hot spots on cathode surfaces (18). They might lead to diffusional modification of the defect structures in the nuclear active regions, although the time for which a small region would be very hot is short due to thermal diffusion to the surrounding material.

The second additional role for impurities is the possibility that, if impurities actually participate in nuclear reactions, relatively low concentrations and "burn rates" would yield energies that are relevant to cold fusion (19). Excess powers on the order of 1 Watt appear in many cold fusion experiments.  $1\text{ W} = 1\text{ J/sec}$  or about  $6 \times 10^{12}$  MeV/sec, again using the conversion factor of  $1.6 \times 10^{-19}$  J/eV. Hence, if each nuclear reaction gives 1 MeV,  $6 \times 10^{12}$  reactions/sec are needed to produce 1 W. In Pd, 1 ppm is about  $7 \times 10^{16}$  atoms/cm<sup>3</sup>, so there are about  $7 \times 10^{16}$  nuclei of 1 ppm impurities in 1 cm<sup>3</sup>. Hence, reactions of  $10^4$ /sec of a 1 ppm impurity would give 1 Watt, if each reaction gave 1 MeV. This means that total consumption, by 1 MeV exothermic nuclear reactions, of a 1 ppm impurity could yield 1 W for  $10^4$  sec, or about 3 hours. Higher powers could be available for shorter times for the assumed 1 ppm impurity level, or for similar or longer times for correspondingly higher impurity concentrations. If greater energies were released per nuclear reaction, then higher powers for similar times, or similar powers for longer times, would be possible. The point is that participation of low levels of impurities in nuclear reactions could account for the levels and durations of excess powers measured in many of the reported cold fusion experiments.

Given the multiple potential roles of impurities, it is desirable to have a rather complete inventory of the impurities within materials involved in cold fusion experiments both before and after the experiments. Having such data during experiments would also be of interest, but obtaining it is difficult, at best. Analysis for different elements in Pd at trace concentrations requires a variety of analytical techniques, most of which consume the sample. That is, most impurity concentration measurements require the use of materials from the same lot as the samples that actually go into a cold fusion experiment. This inevitably raises questions about variations of impurity types and concentrations within a lot of materials. Analysis of impurities after a cold fusion experiment has the same challenges, including sacrificing of the cathode or other material for the analysis by many quantitative methods.

There are two other general problems with impurity analyses. The first is simply cost. The determination of trace concentrations usually requires sophisticated equipment in the hands of an experienced operator. The second is the non-uniform spatial distribution of the impurities, especially in post-run samples. This requires sectioning of the relevant materials into numerous small samples and their analysis, again at significant costs.

A review of the experimental literature on low energy nuclear reactions shows that impurity analyses have rarely been thorough. Sometimes, the analysis provided by the supplier of Pd or other materials is

available. Less often, the experimenters have samples of materials analyzed before experiments. Post-run analyses are also done sometimes. Analyses, both before and after experiments, have only been done routinely in experiments aimed at detecting the growth in elemental concentrations, that is, transmutation rates (20,21). In short, there is a significant need in future cold fusion experiments for more and better analyses of impurities, both before and after experiments.

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