Study of the motion of deuterium in the palladium deuteride lattice to investigate the validity of cold fusion

by

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ABSTRACT

The theoretical concepts of cold fusion is based on many assumptions. In this research, these assumptions are explored and investigations are proposed to determine whether they are justified.

The major part of this research examines the motion of deuterium in a palladium deuteride lattice, as we have postulated that the deuterium is free to move within a lattice cell. The motion of deuterium in the palladium deuteride lattice is subjected to three sets of electrostatic forces: a force field due to palladium atoms, one due to deuterium atoms and the attractive force from an adjacent hole. A computer program has been made to calculate these forces so as to investigate the validity of the assumption regarding the mobility of deuterium.

Results obtained from the program show that the maximum vibrational amplitude of a deuteron with a hole at its nearest neighbor is 26550 fm (0.266$\mathring{A}$). The activation energy of the deuteron was found out to be 4.62 eV.

In this research, we have also explored the palladium deuteride structure. Questions have been raised about this structure. The effect of electric field on this structure has been discussed. Also in this research two kinds of experiments have been suggested which will help to verify the assumptions made behind the theoretical concept of cold fusion.

CHAPTER 1. INTRODUCTION

Fusion, a Form of Nuclear Energy

It is commonly held today that the world's ultimate energy supplies will be provided either by the sun, by geothermal energy stored in the Earth's interior, by nuclear fuels found on the Earth, or by some combination of these sources. There are two main variants of nuclear energy to be considered: fission and fusion. In this study we consider fusion only.

Fusion denotes a class of nuclear reactions involving the nuclei of the lighter elements in the periodic table; in these reactions, which are accompanied by a net release of large amounts of energy, the light nuclides combine to form at least one heavy nuclide. A number of elements existing abundantly on earth can serve as nuclear fuels for fusion, enough to represent essentially inexhaustible sources of energy for the future. Under the proper conditions the low atomic number elements will react to convert mass to energy ($E = Mc^2$) via nuclear fusion. For example, the fusion of the hydrogen isotopes, deuterium(D) and tritium(T) according to the reaction

$$D + T \rightarrow {}^4He + n \qquad (Q = 17.6MeV) \tag{1.1}$$

produces 17.6 MeV of energy. The fusion of 1.0 gm of tritium together with 2/3 gm of deuterium produces $1.65E5$ Kw-hr of thermal energy. Deuterium exists as 0.0153%

of volume in sea water and is readily extractable, thus constituting an essentially infinite fuel source. Tritium undergoes beta decay with a half-life of 12.5 yr. Thus it must be produced artificially, for example, by neutron capture in lithium(Li). The tritium production reactions are :

$$n + {}^{6}Li \rightarrow T + {}^{4}He \tag{1.2}$$

$$n + {}^{7}Li \rightarrow T + {}^{4}He + {}^{1}n \tag{1.3}$$

The first reaction has a large cross section for thermal neutrons, while the second reaction is more probable with fast neutrons. When lithium is placed around the fusion chamber, the fusion neutrons can be used to produce tritium, introducing the possibility of a fusion reactor breeding its own fuel.

Another promising fusion reaction is :

$$D + D \rightarrow \begin{cases} T + H & (\mathrm{Q{=}4MeV}) \\ {}^{3}He + n & (\mathrm{Q{=}3.25MeV}) \end{cases} \tag{1.4}$$

This reaction has two branches of roughly equal probability. With this reaction the fusion fuel source is essentially inexhaustible, since the amount of recoverable deuterium in the world's water is enormous. A third possible fusion reaction is :

$$D + {}^{3}He \rightarrow {}^{4}He + H \qquad (\mathrm{Q{=}18.2\ MeV}) \tag{1.5}$$

There are many other reactions involving the low atomic number elements.

In order for a fusion reaction to take place, the two nuclei must have enough energy to overcome the repulsive coulomb force acting between the nuclei, and to approach each other sufficiently close that the short-range attractive nuclear force becomes dominant. Normally, this means that the fusion fuel must be heated to a high temperatures. For the D-T reaction, the temperature must exceed $5E7\ K^{\circ}$ before a significant fusion rate occurs. An even higher gas temperature is required for the other fusion reactions. At such temperatures the material exists as a macroscopically neutral collection of ions and unbound electrons which is called a plasma, that is, an ionized gas distinguished from ordinary gases by its ability to conduct electricity easily and to respond readily to electromagnetic forces.

Two main lines of approach towards developing a practical fusion reactor for civilian applications have evolved in the course of the past quarter of a century : the magnetic confinement approach and the inertial confinement approach.

Magnetic confinement

In a macroscopic sense, plasma behaves as if it were diamagnetic. Consequently, a properly designed magnetic field configuration will produce stresses to counterbalance the pressure of the plasma. In this manner the magnetic field can act as a container, confining the plasma material to a specific volume in space.

A magnetic field confines charged particles to small orbits in the plane of the normal to the field. In order to prevent them from leaking out along the field lines, one must use either a torroidal geometry in which the field lines form closed flux surfaces, or rely on magnetic mirrors or other end-stopping effects to reflect the particles. A fusion plasma cannot be maintained at thermonuclear temperatures if it is allowed to come in contact with the walls of the confinement chamber, because material erroded from the walls would quickly cool the plasma. Fortunately, properly designed magnetic fields can be used to confine plasma within a chamber without contact with the wall.

The basis for the magnetic confinement of a plasma is the fact that the charged particle spiral about magnetic field lines. The radius of the spiral, or gyroradius, is inversely proportional to the strength of the magnetic field, so that in a strong field charged particles move approximately along magnetic field lines.

Inertial confinement

Inertial confinement fusion takes a very different approach. A tiny pellet containing deuterium and tritium inside a thin heavy metal shell is suddenly struck with an intense laser or particle pulse that immediately vaporizes the outer layer of the solid and forms a plasma, which continues to absorb the laser radiation. The plasma itself is unconfined and it rapidly blows off or ablates, which (by Newton's third law) drives a compressional shock wave back into the remaining core of the pellet; this shock wave compresses and heats the core to the point at which thermonuclear ignition can occur at the highest density region near the center. The alpha (α) particles resulting from fusion rapidly lose their energy in collisions with ions in the dense fuel. This contributes additional heating, and the thermonuclear burn propagates outward, finally blowing the pellet apart and ending the reaction. Applying Lawson's criterion which estimates the minimum necessary product of ion density and confinement time (time until the pellet blows apart) for sustaining a fusion reaction, if the confinement time were as short as $E-8$ - $E-9$ s, we would need a density of at least $E30$ - $E31$ $/m^3$ of deuterium and tritium particles. To run an inertial confinement reactor at a net energy gain, we must exceed considerably the Lawson criterion.

Research on cold fusion is taking place simultaneously on many fronts, and while many magnetic confinement and inertial confinement devices are within the last order of magnitude of exceeding the Lawson criterion, there is as yet no single leading candidate for the basic design of a controlled fusion reactor. Despite the many technological problems, progress in the last decade has been considerable , and it may not be overly optimistic to extrapolate to the break-even point within the next decade or two.

Cold Fusion

On March 23, 1989, Fleischmann and Pons [1] announced their achievement of sustained, controlled fusion at room temperature in a Palladium (Pd), cathode of an electrolyte cell using heavy water (deuterium oxide) as the electrolyte. Fleischmann and Pon's results are particularly surprising to the scientific community because there had been no hint of fusion type reactions in deuterated compounds. However Fleischmann and Pons have not described the details of how their experiments were performed. Many scientist have tried to reproduce them but with ambiguous results. Ambient or cold fusion of deuterium occurs when two deuterium nuclei with ambient kinetic energy quantum mechanically tunnel through their mutual coulombic charge barrier. There are four essential ingredients, or processes, for sustained controlled nuclear fusion of either the hot or the cold variety: tunneling probability, collision frequency, fusion probability, and sustaining the reaction. The power delivered by nuclear fusion–the fusion rate–is proportional to the product of the first three processes. The fusion probability is dependent on processes that occur inside the nuclear well and determine the reaction products. The fourth process involves preventing the reaction from being terminated because certain isotopes have entered the reaction vessel and interfered with the process and ensuring that the fuels are replenished.

The ability to achieve fusion at low temperature appears to be related most likely to unexpectedly high tunneling probability and collision frequency. The fusion rate is extremely sensitive to the tunneling probability. Even small variations in the relevant variables can substantially change this coefficient, which in practical terms, is a measure of how atomic nuclei can overcome the barrier of their mutual electrical repulsion. Tunneling is a quantum mechanical phenomenon in which a particle whose energy is less than the potential energy of a barrier can nevertheless be found on the other side of the barrier. For fusion to occur, the deuterium nuclei must overcome the repulsive coulombic barrier. Once the barrier is overcome, the attractive nuclear force dominates, allowing the nuclei to fuse.

Description of the Problem

Our group consisting of Dr. Spinrad, Taher Al Jundi and the author are trying to determine whether or not cold fusion in an electrolytic cell is theoretically possible. In this thesis we are trying to model the behavior of D in Pd-D. The model is described in Chapter Three. We have assumed that the deuterons are highly mobile in the palladium deuteride lattice. In Chapter Four we will discuss the net force on the moving deuteron due to neighboring palladium and deuterium atoms, and also due to a hole at a neighboring lattice site, in order to find out the activation energy of the moving deuteron. From the deuterium behavior we can use quantum mechanical calculations to find the fusion rate. This is the subject of Taher Al Jundi's thesis. Finally, we explore in this thesis the implications of our model and suggest experiments that can test the validity of our model.

CHAPTER 2. LITERATURE REVIEW

Fleischmann and Pons [1] have reported that fusion seemed to occur in an eight inch long by three inch diameter glass electrolytic cell containing a platinum coiled wire anode and a palladium tube cathode with 6-8 volts applied to the cell. The electrolyte was deuterated water to which 0.1 M lithium hydroxide was added to aid electrolysis. Television pictures of cell in the operation reveal copious bubbles, which suggest that the current is of the order of an ampere, possibly more. The nuclear fusion events presumably occur at the cathode to which the deuterons are accelerated up to 8-eV energies.

Since the original work many improvements have been made in attempting to experimentally verify the Fleischmann - Pons phenomenon. Considerable attention has been paid to (1) reducing the probability of contamination in experiments in which tritium, a fusion product, was found; (2) reducing backgrounds and increasing efficiency in neutron counting; (3) improving calibration methods and reducing sensitivity to spatial variation of temperature in calorimetry; and (4) a using closed cell [2,3,4,5].

The three types of evidence used to identify cold fusion are detection of tritium, neutrons and heat production in the cell. Many experiments seeking to find this evidence have been conducted all over the world.

At Texas A & M University, Packham et al. have reported [6] that eleven electrolytic cells using a single source of palladium for cathodes and nickel for anodes produced tritium activity in amounts from 116.6 to 83300 Bq/ml ($10E6$ times background). At Las Alamos National Laboratory, Storms and Talcott [7] have reported that seven of nine new closed cells have produced tritium in amounts up to six times the background concentration in the electrolyte. Several groups at the Bhabha Atomic Energy Research Center (BARC) [2] have also reported the production of tritium. The measurement of tritium generation is the strongest of the three types of evidence for cold nuclear reactions.

In two hundred early experiments on twenty five electrolytic cells at Texas A & M university, statistically significant neutron emission from three separate experiments using the same piece of palladium was obtained by Wolf [8]. In more recent experiments, five different electrodes have given neutrons for about ten hours. Count rates were three to five times background corresponding to source strengths of 50 n/min . BARC [2] also reported neutron counting to be about two to five times the background. Menlove and Jones report [9] several hundred neutrons occurring from palladium electrolytic cells. The bursts are repeatable in a statistical sense. Although the quality of experiments claiming to measure neutrons is high at least at Texas A & M, LANL and BARC, the low counting rates at Texas A & M do not support high confidence in these results. The burst nature of neutrons at LANL are at rates well above background providing a clearer signal but, conceivably, the bursts could be due to micro - hot fusion. On both these bases the BARC results appear, perhaps, to be the more definitive. Therefore, the neutron evidence could be seen as less compelling then that from tritium.

Appleby et al. at Texas A & M University [10] have used a sensitive heat flow commercial calorimeter not dependent on temperature distribution and they claim excess power up to 50 mW in 0.5 mm palladium cathodes. Oriani et al. at the University of Minnesota [5] has used an open cell in a heat flow calorimeter not sensitive to temperature distribution. Total energy recorded was 0.075 MJ. Hutchinson at Oak Ridge National Laboratory [11] reported total integrated energy of 3 MJ. Bryne et al. at the University of Utah [12] has reported that up to 56 W excess power were generated in five open cells on several occasions in a calorimeter somewhat susceptible to non - uniformities of temperature distribution. According to Oregon State University scientists [13], five significant excess heat generation events have occurred, the cause of which remains unexplained as no evidence of the traditional deuterium - deuterium (D-D) products (tritium and neutrons) has been found despite a rigorous effort to ensure that all products were adequately monitored.

Protons must accompany tritium from D-D fusion whatever the mechanism or the net branching ratio is. Taniguchi et al. [14] claims to have observed protons in six out of twenty three experiments using a 10 μm palladium foil cathode as one side of an electrolytic cell.

Despite these advances no one has yet succeeded in producing a procedure that can lead to reproducible results. Futhermore, we see the positive results from research groups against a background of a large number of negative results from other research groups. In most cases, these latter groups are just as credible and experienced as those reporting positive results.

Table 2.1: Vibrational amplitudes of Pd-H and Pd-D systems

Elements	Sample	Vibrational Amplitudes (Å)
Pd	Pd	0.069
Pd	$PdH_{0.706}$	0.071
Pd	$PdD_{0.658}$	0.064
H	$PdH_{0.706}$	0.23
D	$PdH_{0.658}$	0.20

Palladium Deuteride Structure

Neutron diffraction investigations done by Worsham, Wilkinson and Shull [15] on the powdered samples have shown that at a low hydrogen and deuterium concentrations, the fcc α phase exists and has a lattice constant of $3.89\mathring{A}$. As the hydrogen or deuterium concentrations increases, it is claimed that a fcc β phase appears, in which the lattice is expanded to $4.02\mathring{A}$. According to them there are no intermediate values of the lattice constant. The diffraction pattern at relatively high H and D concentrations characteristic of β phase show that Pd-D and Pd-H systems have a NaCl type structure, in which the hydrogen and deuterium atoms have entered the octahedral positions about the palladium atoms as shown in Fig 2.1. The values of the hydrogen and deuterium root-mean-square vibrational amplitudes listed, in Table 2.1, are much larger than those for palladium, indicating that there is considerable motion of the hydrogen and deuterium atoms.

Worsham et al. also exhibited the actual neutron diffraction patterns for low concentrations of H and D in Pd (0.07 and 0.068 atom ratio respectively) but did not publish the patterns for more concentrated systems. Their published curves are

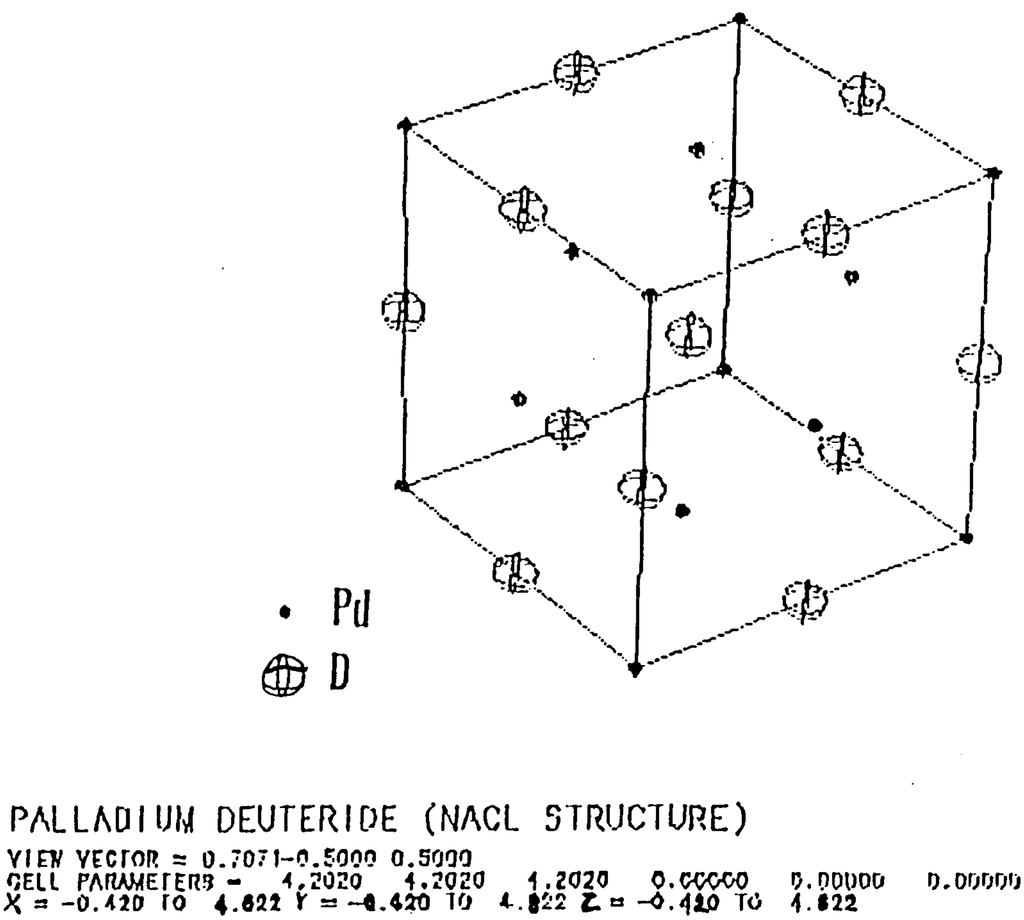

Figure 2.1: Palladium Deuteride

reproduced in Fig 2.2. The slight asymmetry of the large reflections was ascribed to small unresolved reflections as shown by the cross-hatched area on the small angle side of the reflections. These small reflections occur at the proper angle positions for reflections from the expanded β phase, and a comparison of the relative intensities of these reflections with those of known β phase indicated that, for both the hydride and deuteride, β phase contamination was present in the low concentration samples. According to Bergsma and Goedkoop [16] the root mean square displacements due to thermal motion of the palladium and hydrogen atoms at room temperature are found to be $0.1 \pm 0.01\AA$ and $0.24 \pm 0.02\AA$, respectively. Measurements of the total neutron scattering cross section as a function of neutron energy and energy distribution of 0.004 eV neutrons scattered at 90° are reported and interpreted in terms of an Einstein model for the proton vibrations with fundamental frequency corresponding to $0.056 \pm 0.002 eV$. From this the root mean square displacement of the protons relative to the palladium sublattice at room temperature is estimated to be $0.22 \pm 0.01\AA$, in aggrement with the values found by diffraction. The cold neutron scattering data also gives information about the heat motion of the palladium atoms. Interpreted on a Debye model they yield a Debye temperature of $300 \pm 25K^\circ$ and a root mean square displacement of $0.10 \pm 0.01\AA$.

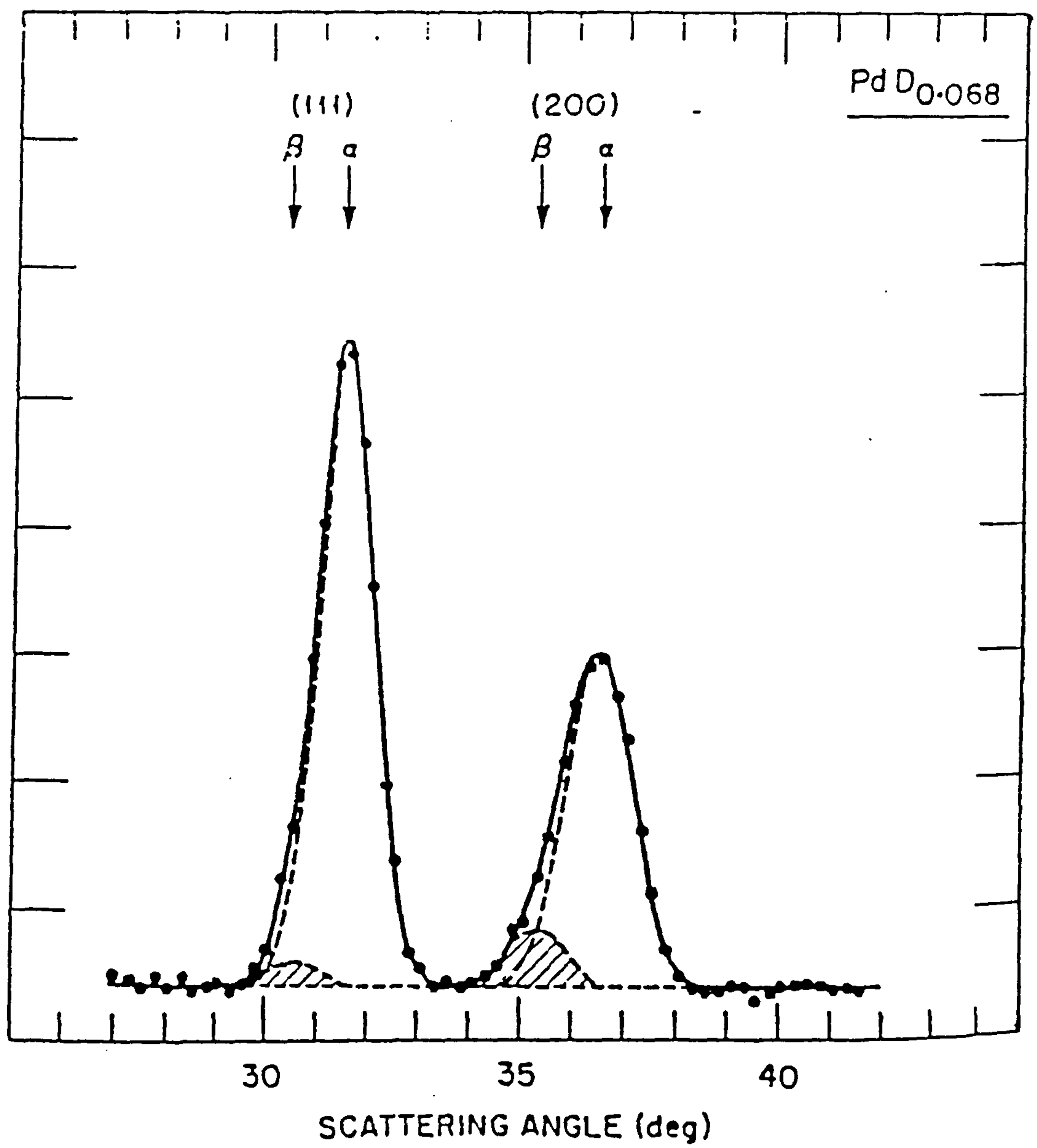

Figure 2.2: Partial neutron diffraction patterns for Pd-D

CHAPTER 3. ASPECTS OF THE MODEL

Palladium Deuteride Structure

Palladium metal forms a fcc crystal lattice at ambient conditions. Absorbed deuterium is very mobile in palladium and exhibits a large diffusion coefficient. When deuterium is absorbed in palladium it is currently believed to occur in two phases [15,16] (alpha and beta). Both phases are fcc with regard to the palladium. At low deuterium concentrations, the alpha phase exists with a lattice parameter of 3.88$\AA$. As additional deuterium is introduced into the palladium, the alpha and beta phases are believed to coexist in equilibrium until a D/Pd atom ratio of $\sim$ 0.7 is reached. Above this, the palladium system is believed to assume a pure beta phase. The lattice parameter increases with increasing deuterium absorption until it reaches a value of 4.02$\AA$.

In the beta phase, deuterium is located in the octahedral positions of the palladium lattice. The Pd-D structure, shown in Fig 2.1, is similar to the structure of NaCl. The small neutron cross section of deuterium in the Pd-D system, as measured in neutron diffraction studies, indicates that the deuterons are loosely held at these positions. The results of scattering amplitudes for Pd, Pd-H and Pd-D systems are given in Table 2.1 [2]. From Table 2.1, we can see that deuterium is much more mobile than Pd in the Pd-D system. We are not satisfied by the explanation of Worsham et al. [15] about the small diffraction pattern reflections are due to the phase mixing. We consider that this could be due to a high probability of deuterons jumping to empty lattice sites.

At this juncture, two questions can be raised regarding the structure.

(1) Does the deuterium occupy a fixed lattice site as in a true compound crystal or does the lattice site merely represent the most probable position of an atom that can move almost as freely as in a liquid?

(2) Are the alpha and beta really separate phases or does the palladium lattice simply expand (as it does when the temperature is raised) as deuterium is added?

In order to explore the first question we fit a model under the following assumptions. When we focus on a single hydrogen and its environment, planes of symmetry lead to an octahedral cell. The six Pd atoms closest to the hydrogen are situated at the apices, and the lines connecting closest neighboring Pd atoms outline the eight triangles that make up the octahedron. There are twelve such lines, and a transverse from the hydrogen at the center of the octahedron through the midpoint of each of these lines points directly to the nearest neighbor hydrogens. The volume of the octahedral cell is $2(2.01E5)^3 fm^3$ and it contains one Deuterium and six Palladiums, with each palladium shared by six cells. We are visualizing the deuterium at the center of the cell. The deuterium centered octahedron represents the volume within which we analyze possible D-D interactions.

It is generally assumed that Pd-D is metallic; that is, we consider the Pd and D to have lost their valence electrons, which latter form a virtual continuum through out the body of the material. Thus the octahedral Pd-D cell has four electrons, three electrons from Pd and one from D. These electrons are assumed to be approximately uniformly distributed in the cell; however, we have not been able to find a definite experiment to demonstrate this. According to quantum mechanics, electron density is greater in the vicinity of a foreign impurity than it would be in the vicinity of the normal ion in the lattice. Indeed, if we consider deuterium as an impurity in the palladium lattice, we would expect the free electrons to be more dense around the deuterons, providing shielding from electrostatic forces acting on them. These electrons could shield the deuterons from their mutual repulsion and allow them to approach each other more easily.

Consider a model of PdD with atomic ratio near unity. Now if we consider an empty lattice site in a deuterium position then the empty site behaves like a negative charge, drawing nearest neighbor deuterons to it. There will be occasions when two out of the twelve neighbors arrive almost simultaneously, and it is in the outcome of such an event that we are interested. Exactly once in eleven times when two deuterons arrive at the same hole, they will be traveling in opposite directions along a straight line. The deuterium pair would then form a vibrating, system. This observation arises from the fact that there are twelve nearest neighbors. When a hole is formed, and we find one deuteron that jumps to fill it, than eleven other nearest neighbor deuterons would be left. Out of these eleven deuteriums, when a second deuteron also enters the same subcell, all but one will come at angles to the first. Then the two particle system would be more likely to have an angular momentum, which will result in keeping them apart. One, however, will come from the direction exactly opposite from the first, and the pair will be much more likely to undergo close collision.

The basic process by which a vacancy moves from one lattice to another is, of course, by the jumping of an atom into the vacant lattice site. Consider a vacancy originally at B (Fig 3.1) in a PdD lattice. In Fig 3.1 the vacancy has moved from B to A by virtue of the atom originally at A having jumped into the site at B. When A moved to B, it had to pass through a saddle point O, i.e., the atom had to jump through a ring of atoms around O, for which it had to possess a minimum characteristic energy or activation energy. We must evaluate the force field and activation energy if we wish ultimately to calculate the rate at which jumps through the saddle point occurs.

To study this effect we calculated separately a net force field due to Pd atoms, one due to deuterium atoms and a negative charge placed at any one deuterium atom position, such that it behaves as a hole [Appendix A]. Based on these force formulas we wrote fortran programs to calculate net force and energy for these three cases [Appendix B].

A mystery remains in the kind of bonding between deuteriums and palladium. In this case, we have the deuterium ion passing through the palladium crystal. It might be considered that while doing so the deuteron would collide with the palladium atom and excite the atomic electrons of palladium to excited states. This energy would come from the deuteron. Sometimes enough energy is transferred to these atomic electrons that some of them are knocked out and join with electron sea, thus ionizing the palladium crystal. On using Bethe's formula [17] to calculate the rate of energy loss, or stopping power, [Appendix A], we find that the rate of energy loss by high energy ($\geq$ 100 eV) deuterium to the palladium lattice would be about $4.94E12eV/sec$ and the time in which this energy will be lost is about $1.088E - 16sec$. On such an argument, even a high energy deuteron would lose most of its energy to the lattice

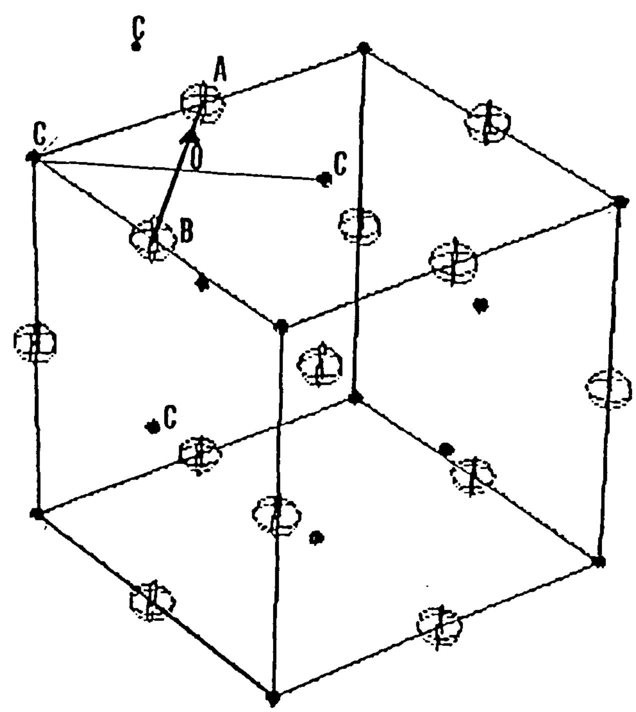

Figure 3.1: Vacancy Jump in Palladium Deuteride

before striking another deuteron. So if fusion is to be at all possible there must be some kind of focusing of deuteron motion such that deuterium will not collide with palladium lattice atoms. Then deuterium can be quite energetic and remain so for a longer time. Some of this focusing could be due to the electrostatic repulsion between deuterium and palladium ions.

Effect of electric field

The palladium can be brought to a high negative static potential, which amounts to putting many excess electrons into the system. By the laws of classical electrostatics, however, these extra electrons will be concentrated in the conducting skin at the surface of the system so long as the system is metallic. Deuterons in the outer layers of the palladium will be in a cell that is full of electrons. The electrons could shield the deuterons from their mutual repulsion and hence could increase the probability of fusion by quantum mechanical tunneling. This electron shielding behavior could also result in the decrease of the activation energy and hence increase the probability of jumping deuterons.

In Chapter Five, experiments are suggested to examine these possibilities.

CHAPTER 4. ELECTROSTATIC FORCES ON THE DEUTERON

Derivations of Forces Acting on the Moving Deuteron

We examine the motion of a deuteron in a PdD lattice subject to three sets of electrostatic forces: the force due to Pd lattice atoms, the force due to neighboring D atoms and the attractive force from an adjacent hole.

The force field from deuterium atoms can be written as:

$$F_D = e^2 \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} \frac{\frac{s}{\sqrt{2}}(\vec{x}+\vec{y}) - mt\vec{x} - nt\vec{y} - pt\vec{z}}{[(\frac{s}{\sqrt{2}} - mt)^2 + (\frac{s}{\sqrt{2}} - nt)^2 + (pt)^2]^{\frac{3}{2}}} \tag{4.1}$$

In this case m+n+p is even. We have excluded m=n=p=0 terms as this position is occupied by the moving deuteron itself.

Here:

F_D= Electrostatic force on a deuteron near (m,n,p) from neighboring D atoms = $\vec{O}$

s= Distance of deuteron from (0,0,0) in a channel direction; $\vec{s} = \frac{\vec{x}+\vec{y}}{\sqrt{2}}$

t= Half lattice constant of Pd lattice= 2.01E5 fm.

e^2= square of the charge due to electrons= 1.44E6 eV-fm

We introduce new indices i,j and q.

When m+n is even, then to make m+n+p even,

$m + n = 2i; m - n = 2j; p \rightarrow 2p$

$m = i + j; n = i - j$

When m+n is odd, then to make m+n+p even,

$m + n = 2i + 1; m - n = 2j + 1; p \rightarrow 2p + 1$

$m = i + j + 1; n = i - j$

On applying these new indices the above equation reduces to:

$$F_D = e^2 \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} \{ \frac{\frac{s}{\sqrt{2}}(\vec{x}+\vec{y}) - (i+j)t\vec{x} - (i-j)t\vec{y} - 2pt\vec{z}}{[(s^2 - 2\sqrt{2}ist + 2(it)^2) + 2(jt)^2 + (2pt)^2]^{\frac{3}{2}}} + \frac{\frac{s}{\sqrt{2}}(\vec{x}+\vec{y}) - (i+j+1)t\vec{x} - (i-j)t\vec{y} - (2p+1)t\vec{z}}{[(s^2 - 2\sqrt{2}(i+\frac{1}{2})st + 2(i+\frac{1}{2})^2t^2) + 2(j+\frac{1}{2})^2t^2 + (2p+1)^2t^2]^{\frac{3}{2}}} \} \quad (4.2)$$

$$F_D = e^2 \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} \{ \frac{(s - \sqrt{2}it)\vec{s} - jt(\vec{x}-\vec{y}) - 2pt\vec{z}}{[(s - \sqrt{2}it)^2 + 2(jt)^2 + (2pt)^2]^{\frac{3}{2}}} + \frac{(s - \sqrt{2}(i+\frac{1}{2})t)\vec{s} - (j+\frac{1}{2})t(\vec{x}-\vec{y}) - (2p+1)t\vec{z}}{[(s - \sqrt{2}(i+\frac{1}{2})t)^2 + 2(j+\frac{1}{2})^2t^2) + (2p+1)^2t^2]^{\frac{3}{2}}} \} \quad (4.3)$$

When one sums over j and p, each numerator term in $(\vec{x} - \vec{y})$ or $\vec{z}$ has a positive number exactly balanced by a negative number. Thus finally the above equation reduces to the following form:

$$F_D = e^2 \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} \frac{(s - \sqrt{2}it)(\vec{s})}{[(s - \sqrt{2}it)^2 + (2j^2 + [2p]^2)t^2]^{\frac{3}{2}}} + e^2 \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} \frac{(s - \sqrt{2}[i+\frac{1}{2}]t)\vec{s}}{[(s - \sqrt{2}[i+\frac{1}{2}]t)^2 + (2[j+\frac{1}{2}]^2 + [2p+1]^2)t^2]^{\frac{3}{2}}} \quad (4.4)$$

Similarly, the force field from palladium atoms can be written as:

$$F_{Pd} = 3e^2 \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} \frac{\frac{s}{\sqrt{2}}(\vec{x}+\vec{y}) - mt\vec{x} - nt\vec{y} - pt\vec{z}}{[(\frac{s}{\sqrt{2}} - mt)^2 + (\frac{s}{\sqrt{2}} - nt)^2 + (pt)^2]^{\frac{3}{2}}} \tag{4.5}$$

But in this case m+n+p is a odd sum.

Here:

F_{Pd}= Electrostatic force on a deuteron near (m,n,p) from the Pd atoms = $\vec{O}$

We introduce new indices i,j and q.

When m+n is even, then to make m+n+p odd,

$m + n = 2i; m - n = 2j; p \rightarrow 2p + 1$

$m = i + j; n = i - j$

When m+n is odd, then to make m+n+p odd,

$m + n = 2i + 1; m - n = 2j + 1; p \rightarrow 2p$

$m = i + j + 1; n = i - j$

On applying these new indices the above equation reduces to:

$$\begin{aligned} F_{Pd} = {} & 3e^2 \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \sum_{p=-\infty}^{\infty} \\ & \{ \frac{\frac{s}{\sqrt{2}}(\vec{x}+\vec{y}) - (i+j)t\vec{x} - (i-j)t\vec{y} - (2p+1)t\vec{z}}{[(s^2 - 2\sqrt{2}ist + 2(it)^2) + 2(jt)^2 + (2p+1)^2t^2]^{\frac{3}{2}}} \\ & + \frac{\frac{s}{\sqrt{2}}(\vec{x}+\vec{y}) - (i+j+1)t\vec{x} - (i-j)t\vec{y} - (2p)t\vec{z}}{[(s^2 - 2\sqrt{2}(i+\frac{1}{2})st + 2(i+\frac{1}{2})^2t^2) + 2(j+\frac{1}{2})^2t^2 + (2pt)^2t]^{\frac{3}{2}}} \} \end{aligned} \tag{4.6}$$

$$F_{Pd} = 3e^2 \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \sum_{p=-\infty}^{\infty}$$

$$\{\frac{(s-\sqrt{2}it)\vec{s}-jt(\vec{x}-\vec{y})-(2p+1)t\vec{z}}{[(s-\sqrt{2}it)^2+2(jt)^2+(2p+1)^2t^2]^{\frac{3}{2}}}$$
$$+\frac{(s-\sqrt{2}(i+\frac{1}{2})t)\vec{s}-(j+\frac{1}{2})t(\vec{x}-\vec{y})-2pt\vec{z}}{[(s-\sqrt{2}(i+\frac{1}{2})t)^2+2(j+\frac{1}{2})^2t^2)+(2pt)^2]^{\frac{3}{2}}}\} \quad (4.7)$$

When one sums over j and p, each numerator term in $(\vec{x}-\vec{y})$ or $\vec{z}$ has a positive number exactly balanced by a negative number. Thus finally the above euation reduces to the following form:

$$F_{Pd} = 3e^2\sum_{i=-\infty}^{\infty}\sum_{j=-\infty}^{\infty}\sum_{p=-\infty}^{\infty}\frac{(s-\sqrt{2}it)\vec{s}}{[(s-\sqrt{2}it)^2+(2j^2+[2p+1]^2)t^2]^{\frac{3}{2}}}$$
$$+3e^2\sum_{i=-\infty}^{\infty}\sum_{j=-\infty}^{\infty}\sum_{p=-\infty}^{\infty}\frac{(s-\sqrt{2}[i+\frac{1}{2}]t)\vec{s}}{((s-\sqrt{2}[i+\frac{1}{2}]t)^2+(2[j+\frac{1}{2}]^2+[2p]^2)t^2]^{\frac{3}{2}}} \quad (4.8)$$

We made a fortran program to calculate these forces. For easy computation we did some simplifications [Appendix C] and reduced the force due to neighboring deuteriums and palladium atoms into two parts each.

$$F_{D1} = \frac{\vec{s}e^2}{t^2}[\sum_{l=2}^{10}a_l\frac{\frac{s}{t}}{(\frac{s^2}{t^2}+b_l)^{\frac{3}{2}}}-\sum_{l=1}^{10}\frac{\frac{9a_ls}{t}}{(\frac{81}{2}+b_l)^{\frac{3}{2}}}$$
$$-\sum_{l=1}^{10}a_l\sum_{i=1}^{4}(\frac{i\sqrt{2}-\frac{s}{t}}{([i\sqrt{2}-\frac{s}{t}]^2+b_l)^{\frac{3}{2}}}-\frac{i\sqrt{2}+\frac{s}{t}}{([i\sqrt{2}+\frac{s}{t}]^2+b_l)^{\frac{3}{2}}})] \quad (4.9)$$

where the value of l, a_l and b_l are as follows:

l	1	2	3	4	5	6	7	8	9	10
a_l	1	2	2	4	2	4	2	6	4	4
b_l	0	2	4	6	8	12	16	18	22	24

$$F_{D2} = -\frac{\vec{s}e^2}{t^2}[\sum_{L=1}^{5} a_L\{\frac{\frac{10s}{t}}{(50+b_L)^{\frac{3}{2}}} + \sum_{i=0}^{4}(\frac{\sqrt{2}(i+\frac{1}{2})-\frac{s}{t}}{((\sqrt{2}[i+\frac{1}{2}]-\frac{s}{t})^2+b_L)^{\frac{3}{2}}} - \frac{\sqrt{2}(i+\frac{1}{2})+\frac{s}{t}}{((\sqrt{2}[i+\frac{1}{2}]+\frac{s}{t})^2+b_L)^{\frac{3}{2}}})\}] \tag{4.10}$$

where the value of L,a_L and b_L are as follows:

L	1	2	3	4	5
a_L	4	4	4	8	4
b_L	$\frac{3}{2}$	$\frac{11}{2}$	$\frac{19}{2}$	$\frac{27}{2}$	$\frac{43}{2}$

The equation for the palladium force reduces to:

$$F_{Pd1} = \frac{\vec{s}6e^2}{t^2}\sum_{l=1}^{7} a_l[\frac{\frac{s}{t}}{(\frac{s^2}{t^2}+b_l)^{\frac{3}{2}}} - \frac{\frac{7s}{t}}{(\frac{49}{2}+b_l)^{\frac{3}{2}}} - \sum_{i=1}^{3}(\frac{i\sqrt{2}-\frac{s}{t}}{([i\sqrt{2}-\frac{s}{t}]^2+b_l)^{\frac{3}{2}}} - \frac{i\sqrt{2}+\frac{s}{t}}{([i\sqrt{2}+\frac{s}{t}]^2+b_l)^{\frac{3}{2}}})] \tag{4.11}$$

where the value of l, a_l and b_l are as follows:

l	1	2	3	4	5	6	7
a_l	1	2	3	2	2	2	1
b_l	1	3	9	11	17	19	25

$$F_{Pd2} = -\frac{\vec{s}6e^2}{t^2}\sum_{L=1}^{7} a_L[\frac{\frac{8s}{t}}{(32+b_L)^{\frac{3}{2}}} + \sum_{i=0}^{3}\{\frac{(i+\frac{1}{2})\sqrt{2}-\frac{s}{t}}{([(i+\frac{1}{2})\sqrt{2}-\frac{s}{t}]^2+b_l)^{\frac{3}{2}}} - \frac{(i+\frac{1}{2})\sqrt{2}+\frac{s}{t}}{([(i+\frac{1}{2})\sqrt{2}+\frac{s}{t}]^2+b_l)^{\frac{3}{2}}}\}] \quad (4.12)$$

where the values of L, a_L and b_L are as follows:

L	1	2	3	4	5	6	7
a_L	1	3	2	1	4	2	1
b_L	$\frac{1}{2}$	$\frac{9}{2}$	$\frac{17}{2}$	$\frac{25}{2}$	$\frac{33}{2}$	$\frac{41}{2}$	$\frac{49}{2}$

In our model we have considered that the deuteron is moving through a channel which is surrounded by tubes of spaced charges. At a distance of 5t or greater, these tubes will start behaving like unifomly charged tubes whose force on a charge moving along the channel will be zero.

The attractive force from an adjacent hole is given by:

$$F = \frac{e^2}{(\sqrt{2}t - s)^2} \quad (4.13)$$

Discussion Of Results Obtained From The Fortran Program

When the deuteron is at the (0,0,0) lattice site with a hole at its nearest neighbor position, the net electrostatic force on the moving deuteron is $0.18E-4eV/fm$ [Table 4.1]. At this position from Table 4.1, the contribution to the net force due to the palladium atoms is $2.66E-13eV/fm$, that due to the neighboring deuterium atoms is $-0.74E-12eV/fm$ and that from the hole is $0.18E-4eV/fm$. Thus the net force at (0,0,0) lattice position is entirely due to the attractive force from the hole. The net kinetic energy of the particle at this position is $0.0089eV$ [Table 4.2].

The vibrating deuteron would have maximum amplitude, when the kinetic energy goes to zero. Based on this concept, the maximum amplitude of the vibrating deuteron is $26550 fm$ ($0.266 \mathring{A}$), as reflected in the results of Table 4.2.

At the saddle point the net force on the deuteron goes to zero, due to balancing of the various components of the net force. From Table 4.1, at the saddle point (142000 fm), the net force is $-0.2E - 6eV/fm$. This small value could mean that the various components of the net force are balancing each other at the saddle point. The net energy at this point is -4.62 eV [Table 4.2]. From this we could conclude that the activation energy of the deuteron is 4.62 eV and some change in the site potential relative to the neighbouring site, effectively reducing the activation energy, would be needed to increase the fusion rate.

We plotted graphs from the output of the programs for energy versus displacement and force versus displacement [Figs. 4.1, 4.2, 4.3, 4.4, 4.5, 4.6, 4.7, 4.8].

In our program we calculated the energy using summation of the product of force and displacement, instead of integrating them. We think this will produce error only in the fourth decimal place position as the summation is done from 0 fm to 150000 fm with a step increment of 500 fm.

Table 4.1: Results from the Fortran programs for the displacement versus various forces

Displacement (fm)	Palladium Force (eV/fm)	Deuterium Force (eV/fm)	Force from the Hole (eV/fm)	Net Force (eV/fm)
0	2.66E-13	-0.74E-12	0.18E-4	0.18E-4
5000	-5.59E-6	-0.18E-5	0.19E-4	0.11E-4
10000	-1.12E-5	-0.37E-5	0.20E-4	0.43E-5
15000	-1.17E-5	-0.56E-5	0.21E-4	-0.24E-5
20000	-2.20E-5	-0.75E-5	0.22E-4	-0.89E-5
25000	-2.73E-5	-0.93E-5	0.22E-4	-0.15E-4
30000	-3.23E-5	-0.11E-4	0.23E-4	-0.21E-4
35000	-3.72E-5	-0.13E-4	0.24E-4	-0.27E-4
40000	-4.17E-5	-0.15E-4	0.25E-4	-0.33E-4
45000	-4.59E-5	-0.17E-4	0.26E-4	-0.38E-4
50000	-4.98E-5	-0.19E-4	0.27E-4	-0.42E-4
55000	-5.31E-5	-0.21E-4	0.29E-4	-0.46E-4
60000	-5.60E-5	-0.23E-4	0.30E-4	-0.50E-4
65000	-5.83E-5	-0.25E-4	0.31E-4	-0.53E-4
70000	-5.99E-5	-0.27E-4	0.32E-4	-0.55E-4
75000	-6.08E-5	-0.29E-4	0.33E-4	-0.57E-4
80000	-6.11E-5	-0.31E-4	0.35E-4	-0.58E-4
85000	-6.05E-5	-0.33E-4	0.36E-4	-0.58E-4
90000	-5.91E-5	-0.36E-4	0.38E-4	-0.57E-4
95000	-5.68E-5	-0.38E-4	0.40E-4	-0.55E-4
100000	-5.36E-5	-0.41E-4	0.42E-4	-0.52E-4
105000	-4.97E-5	-0.43E-4	0.44E-4	-0.48E-4
110000	-4.49E-5	-0.46E-4	0.47E-4	-0.44E-4
115000	-3.93E-5	-0.49E-4	0.50E-4	-0.38E-4
120000	-3.31E-5	-0.53E-4	0.53E-4	-0.32E-4
125000	-2.62E-5	-0.56E-4	0.57E-4	-0.26E-4
130000	-1.89E-5	-0.60E-4	0.61E-4	-0.19E-4
135000	-1.13E-5	-0.64E-4	0.65E-4	-0.11E-4
140000	-3.38E-6	-0.69E-4	0.69E-4	-0.33E-5
145000	4.56E-6	-0.74E-4	0.74E-4	0.45E-5
150000	1.24E-5	-0.80E-4	0.80E-4	0.12E-4

Table 4.2: Results from the Fortran programs for displacement versus various energies

Displacement (fm)	Energy due to Palladium(eV)	Energy due to Deuterium (eV)	Energy due to the Hole (eV)	Net Energy (eV)
0	1.33E-1	-0.37E-9	0.89E-2	0.89E-2
5000	-1.54E-2	-0.51E-2	0.99E-1	0.79E-1
10000	-5.87E-2	-0.20E-1	0.19	0.12
15000	-1.30E-1	-0.43E-1	0.29	0.12
20000	-2.28E-1	-0.76E-1	0.39	0.89E-1
25000	-3.52E-1	-0.12	0.50	0.27E-1
30000	-5.03E-1	-0.17	0.60	-0.66E-1
35000	-6.78E-1	-0.23	0.72	-0.19
40000	-8.76E-1	-0.30	0.84	-0.34
45000	-1.09	-0.38	0.96	-0.52
50000	-1.34	-0.47	1.09	-0.72
55000	-1.60	-0.57	1.23	-0.94
60000	-1.87	-0.68	1.37	-1.18
65000	-2.16	-0.80	1.51	-1.44
70000	-2.45	-0.93	1.67	-1.71
75000	-2.75	-1.07	1.83	-1.99
80000	-3.06	-1.22	2.00	-2.28
85000	-3.36	-1.38	2.17	-2.57
90000	-3.66	-1.55	2.36	-2.86
95000	-3.95	-1.74	2.56	-3.13
100000	-4.23	-1.94	2.76	-3.40
105000	-4.48	-2.15	2.98	-3.65
110000	-4.72	-2.37	3.21	-3.88
115000	-4.93	-2.61	3.46	-4.08
120000	-5.11	-2.87	3.72	-4.26
125000	-5.26	-3.14	3.99	-4.40
130000	-5.37	-3.43	4.29	-4.51
135000	-5.44	-3.74	4.60	-4.58
140000	-5.48	-4.08	4.94	-4.62
145000	-5.47	-4.44	5.30	-4.61
150000	-5.43	-4.83	5.68	-4.57

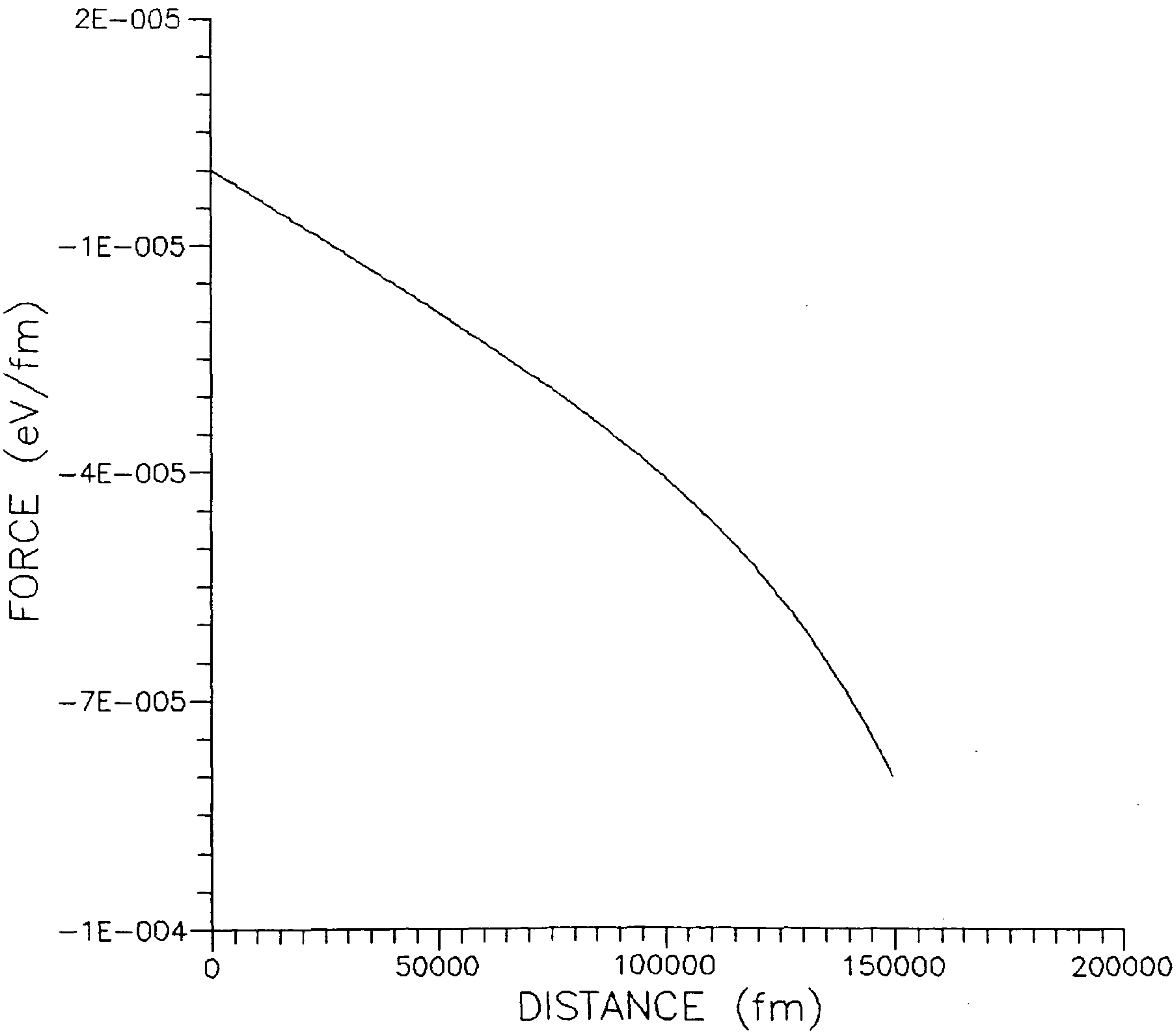

Figure 4.1: Force versus displacement for deuterium force

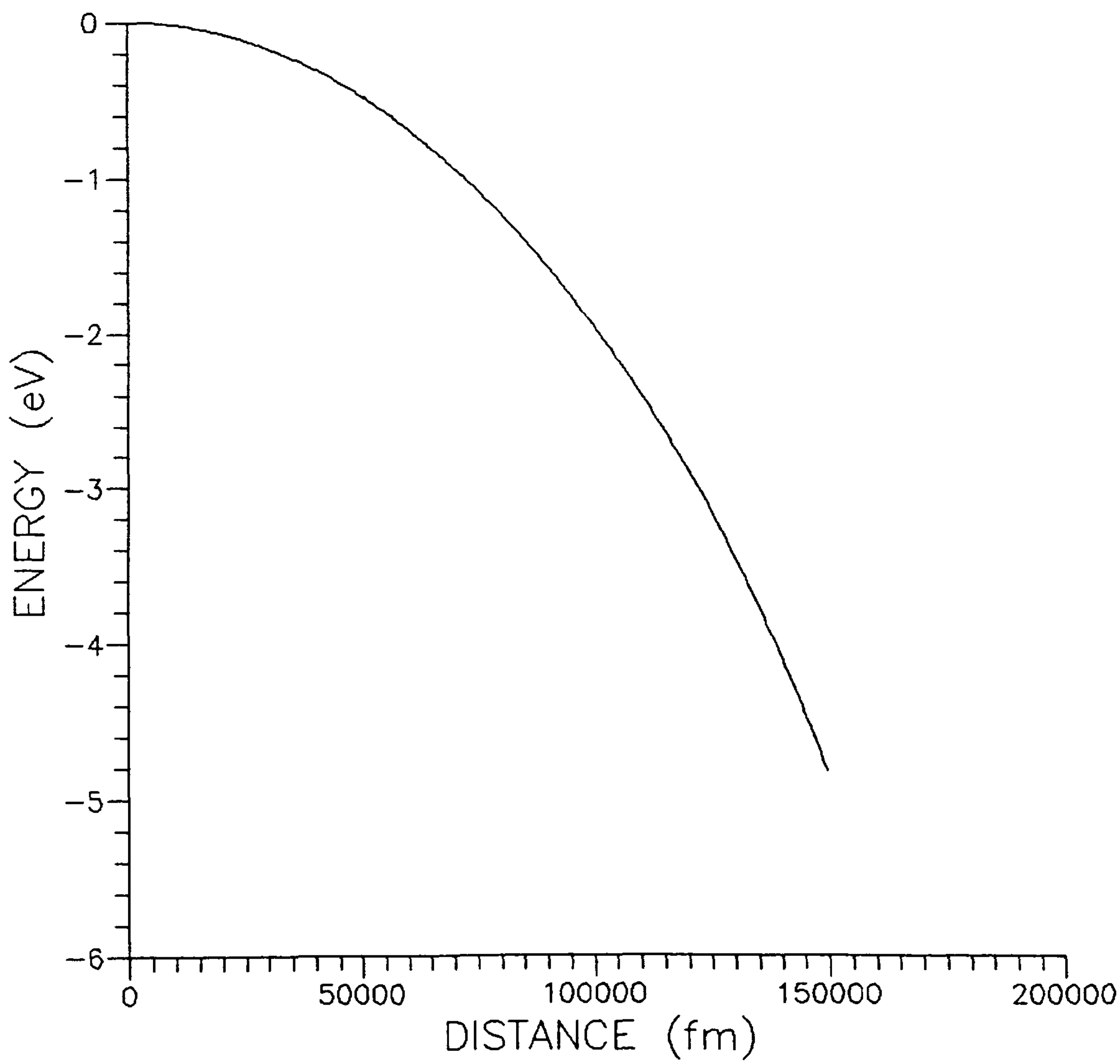

Figure 4.2: Energy versus displacement for deuterium force

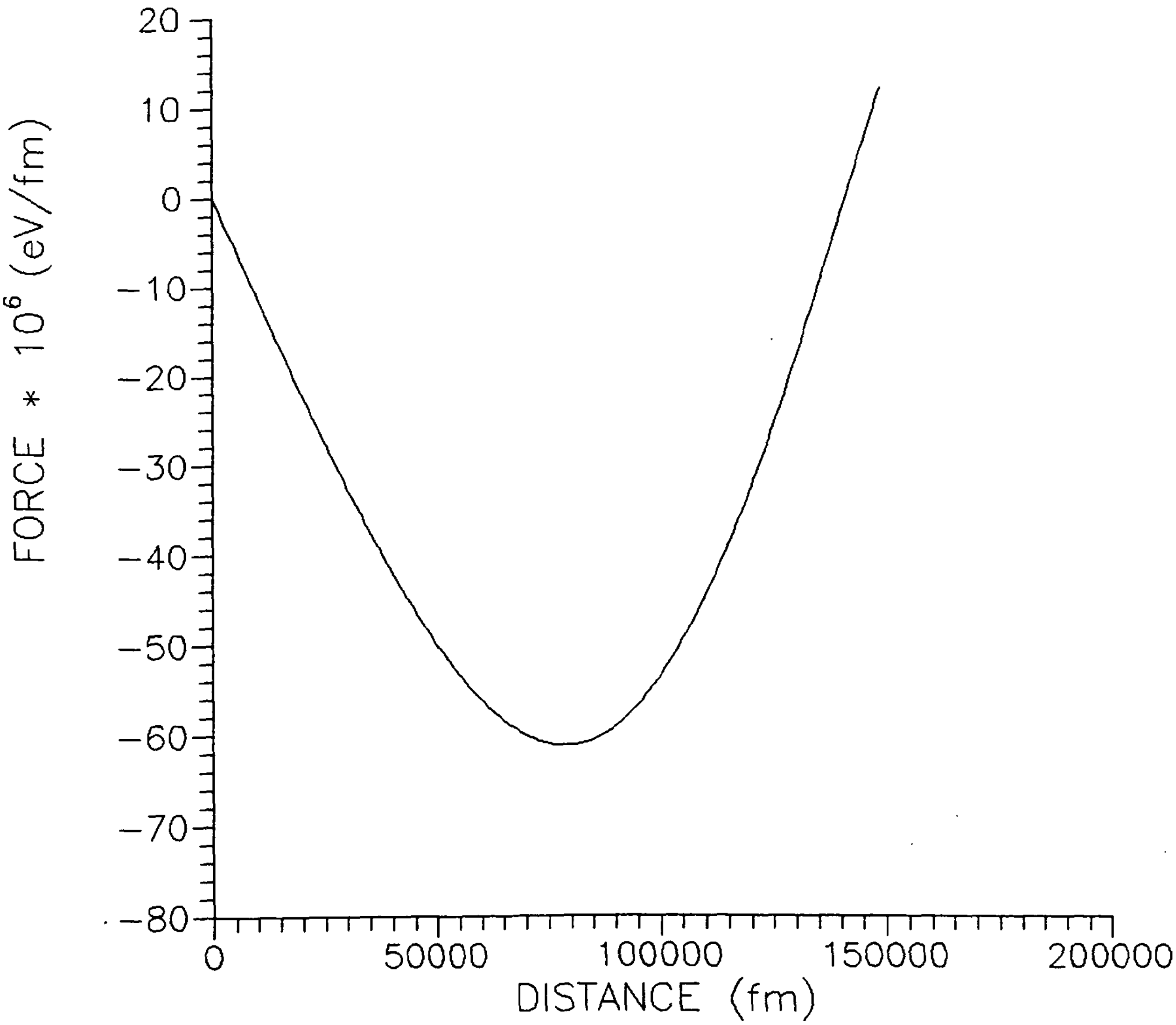

Figure 4.3: Force versus displacement for palladium force

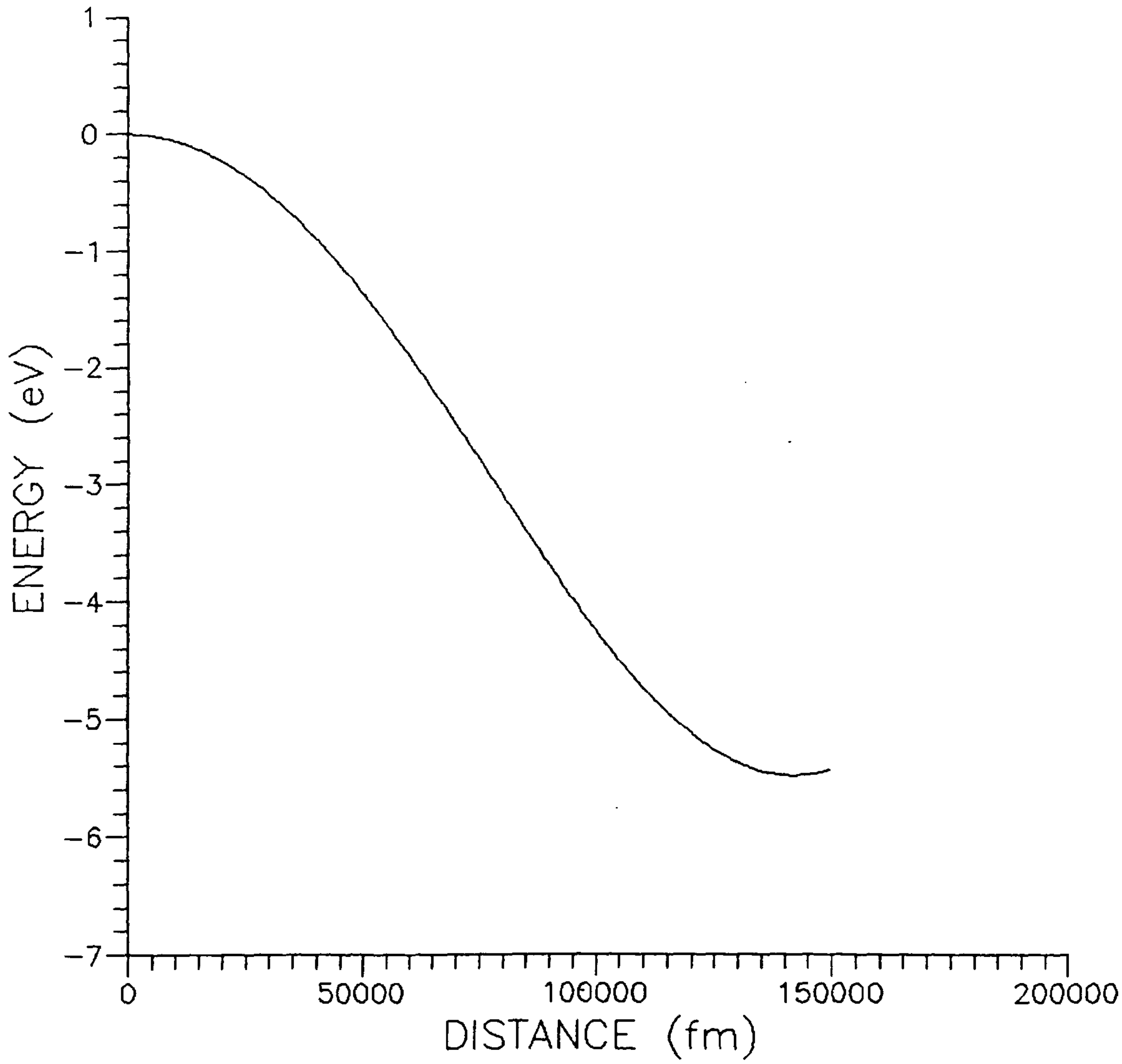

Figure 4.4: Energy versus displacement for palladium force

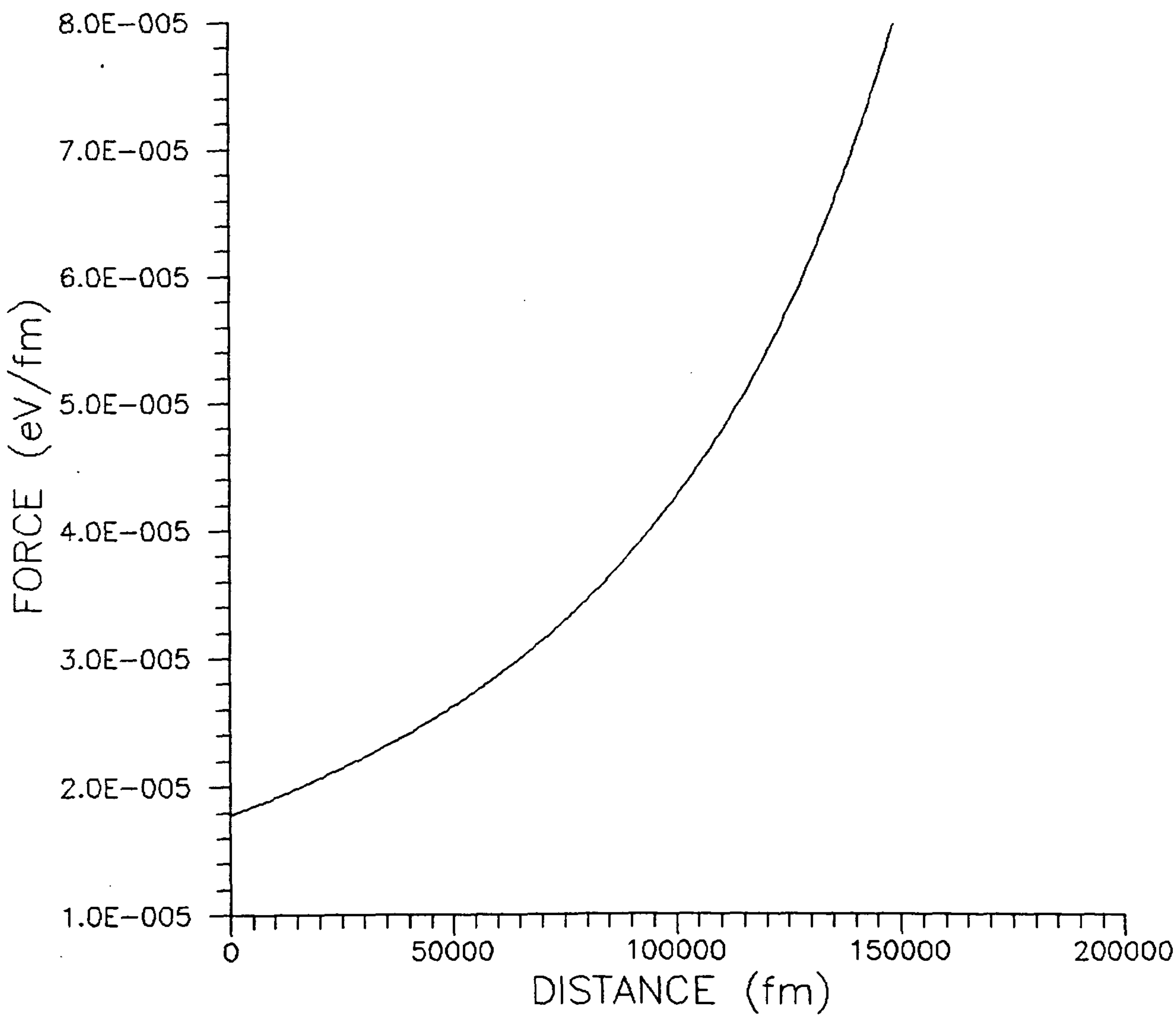

Figure 4.5: Force versus displacement for hole

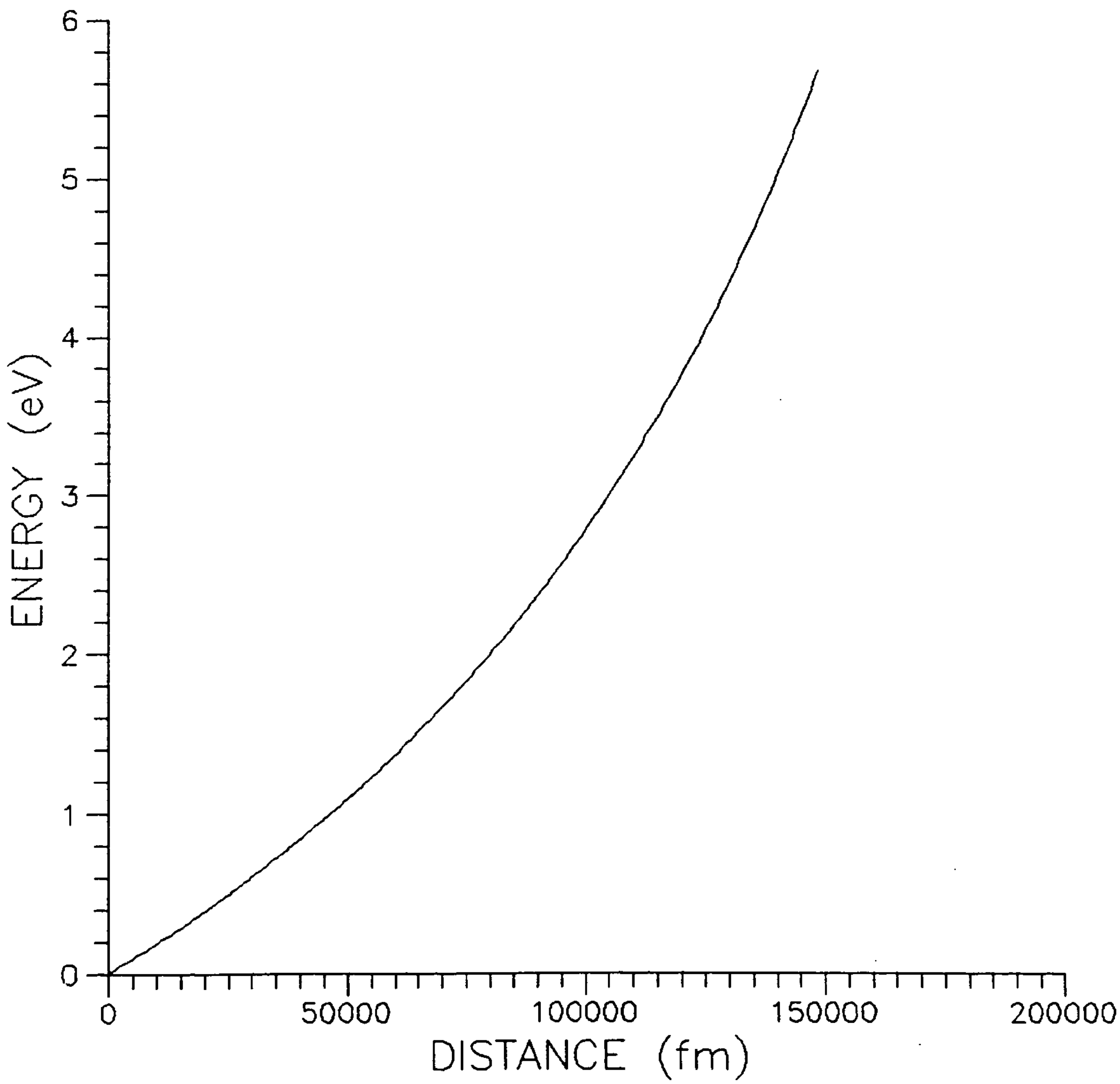

Figure 4.6: Energy versus displacement for hole

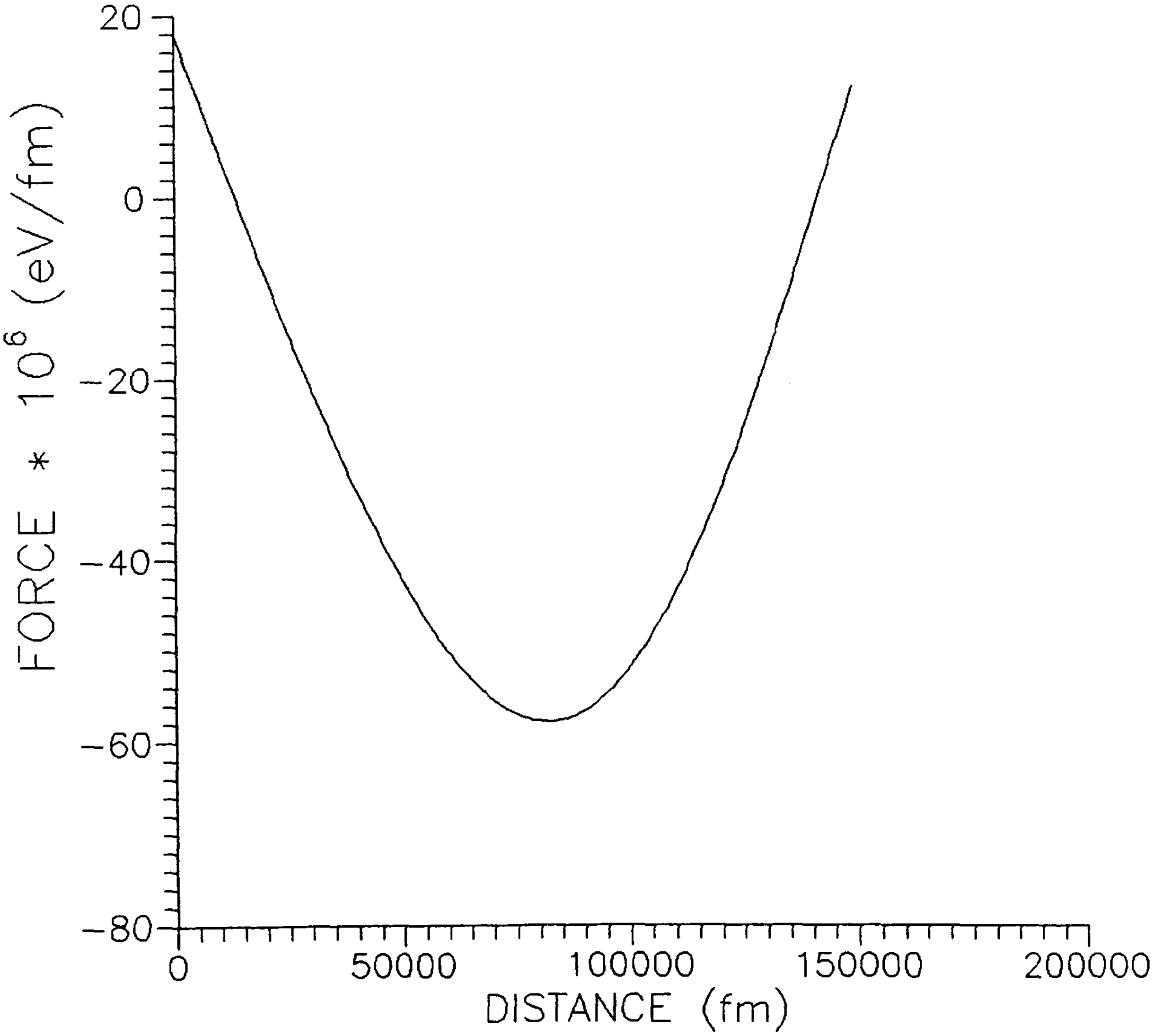

Figure 4.7: Net force versus displacement

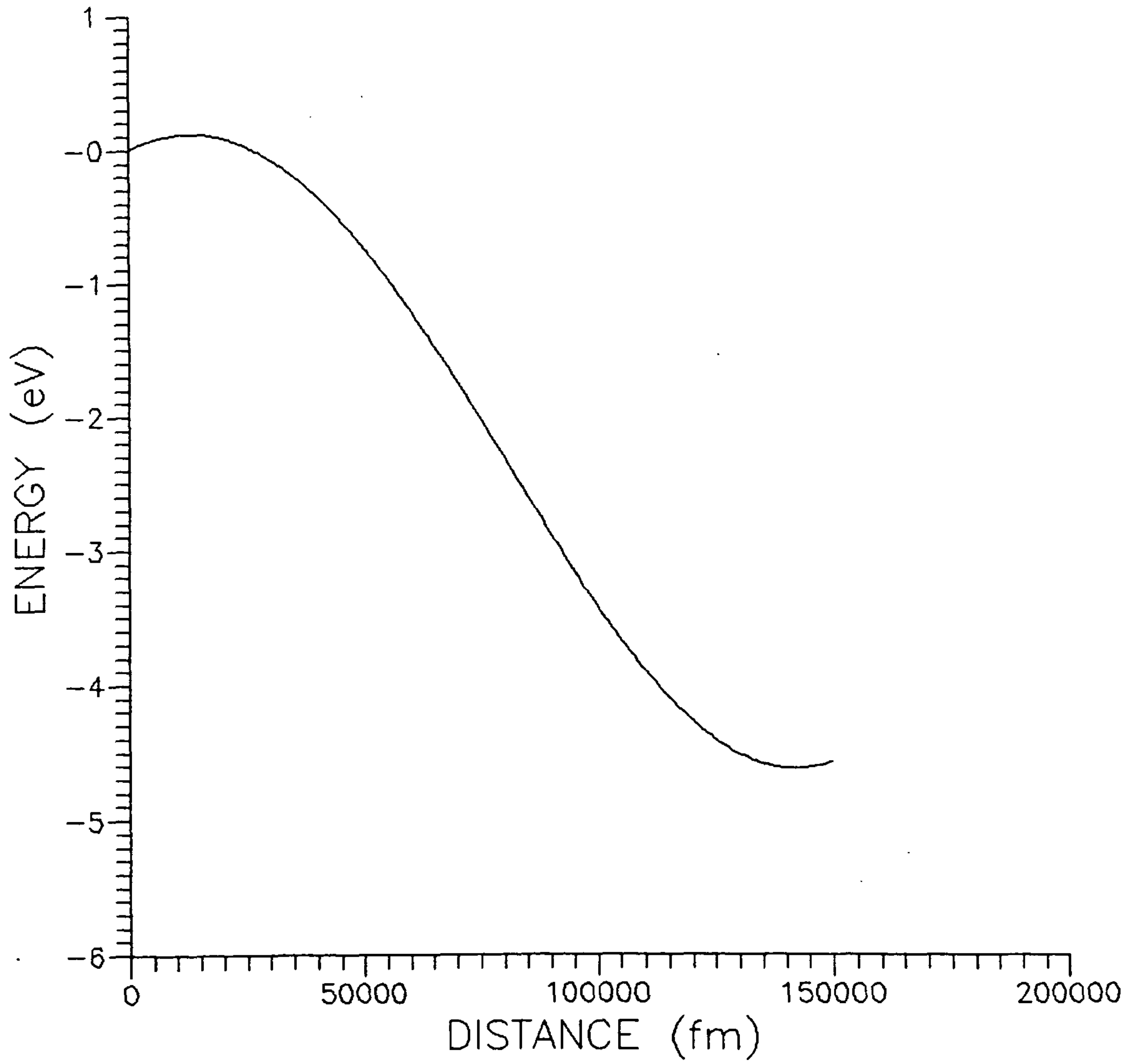

Figure 4.8: Net energy versus displacement

CHAPTER 5. EXPERIMENTS TO INVESTIGATE COLD FUSION PHENOMENON

Behavior of Hydrogen in Palladium

Based on the behavior of hydrogen in palladium, two main questions can be raised.

(1) Exactly how tightly bound is D in the Pd-D lattice? Connected with this question is an auxiliary one as to whether the D atoms behave as impurities in the Pd lattice, in which case they would have appreciable negative charge associated with them.

(2) Are the alpha & beta phase really separate or does the Pd lattice simply expand (as it does when the temperature is raised) as deuterium is added?

There are two possibilities for investigating the first question. The first is measuring electrical resistivity of palladium hydride (PdH) as more hydrogen (H) is added. Qualitatively, the metallic nature of the system will be retained up to very high H content, whereas the crystal with fixed H should exhibit behavior more like an ionic crystal. However, this interpretation is inconclusive. The second possibility is performing neutron diffraction studies on the hydride as the amount of H varies. Neutron diffraction should emphasize the properties of the H over that of Pd. If the H is relatively free, the diffraction pattern should resemble that of a liquid. It is unfortunate that the patterns exhibited in reference [15] do not include the results of high-concentration experiments.

Effects of Electric Fields

As discussed in chapter five, the deuterons in the outer layer of the Pd will be in cells that are full of electrons. The electrons could shield the deuterons from their mutual repulsion until they were close enough that fusion by quantum mechanical tunneling could happen easily. This can be tested by deuterating two samples of equal mass, one a very thin ribbon and the other a more compact bar, and contacting each of them in turn with the negative terminal of a highly charged capacitor. If the surface hypothesis is correct, any fusion that might occur would be more likely in the ribbon, where a high electron density could counteract much of the electrostatic field. This would be thought as analogous to meson-catalyzed fusion, with a large number of electrons replacing the pi meson.

A mystery remains in the hydrogen-in-palladium system, nevertheless. Adding energy to the deuterons in solid Pd-D systems through electrostatic fields is only possible if the H motion is decoupled from the Pd lattice. Even if the accelerating force on the hydrogen's can be made stong enough, they should then behave like energetic, charged particles in a solid and lose energy by ionizing the Pd atoms. We have used a simple model of this process and have found that the kinetic energy is very rapidly dissipated in a very short interval of time [Appendix C]. For a sufficient number of accelerated hydrogen's the sample of Pd-H would even melt.

Although this melting seems improbable, experiments on these concepts might be worth doing. Even if nothing happens, as we expect, such a result will not rule out our idea. The lack of interaction might be electrostatic in origi n: namely, the positive palladium atoms repel deuterons, and could thus focus deuteron mobility into the deuteron channel directions.

CHAPTER 6. CONCLUSIONS AND RECOMMENDATION FOR FURTHER WORK

Conclusion

We have postulated that the D is free to move within a lattice cell. This would make it behave like an interstitial atom rather than one tightly bound in the crystal, thus increasing its mobility and therefore the probability of fusion. Some solid state investigations have been proposed to verify these possibilities.

The deuteron at the (0,0,0) lattice site with a hole at its adjacent lattice site, is subjected to a net electrostatic force of $0.18E - 4eV/fm$. This force is mainly due to attraction of the hole, which contributes $0.18E - 4eV/fm$. The contribution from the neighboring deuterium atoms is $-0.74E - 12eV/fm$ and from palladium atoms it is $2.66E - 13eV/fm$, which shows that they have a negligible effect on the net force at this point. The deuteron at this position has a kinetic energy of $0.0089eV$.

The maximum amplitude of the moving deuteron is 26550 fm (0.266Å) [Table 4.1], with the kinetic energy being approximately zero [Table 4.2].

At the saddle point, i.e. 142000 fm, the net force acting on the deuteron is $0.2E - 6eV/fm$. This small value of the net force means that the components of the net force are balancing each other. The net energy of the deuteron at the saddle point is 4.62 eV, which is its activation energy.

If static electric fields can enhance fusion, as discussed in Chapter five, then enhanced fusion in the surface layers of Pd-D where lattice cells are full of electrons seems likely.

As discussed in Chapter five, we still have a mystery regarding the hydrogen-in-palladium bonding. We have concluded that there must be some kind of focusing of deuteron motion such that deuterium will not collide with Pd lattice atoms. Then deuterium can be quite energetic and remain so far a longer time. Some of this focusing could be due to the electrostatic repulsion between deuterium and palladium ions.

Recommendation for Further Work

The theoretical concept of cold fusion is based on many assumptions. These assumptions are explored and investigations are proposed to determine whether they are justified. Further work into some of these investigations are needed. These investigations can be categorized into two main types.

Solid state investigations

With neutron diffraction experiments, we can answer several questions:

(1) In alpha Pd at moderately low H concentrations (slightly more than 1 H atom per 4 Pd atoms), are the hydrogen atoms in a reasonable organized lattice of their own?

(2) At higher concentrations, do the H exhibit the sharp peaks interpretable as fixed lattice positions or the broad peaks that characterize liquid structure?

System investigations

(1) A thin ribbon of Pd-D should be compared to a more compact bar of the same weight to determine whether there is any preference for skin fusion or for volume fusion.

These investigations would help to clarify the assumptions made in our model for cold fusion and thus strengthen the theoretical concept behind that model.

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APPENDIX A. RATE OF ENERGY LOSS OF DEUTERIUM TO THE PALLADIUM LATTICE

If we consider that D atom while passing through the Pd lattice undergoes collision with the PD atoms and this results in transferring large amount of energy to the atomic electrons of the Pd lattice, such that some of the electrons are knocked out to join to join the electron sea, thus ionizing the Pd crystal.

From the Bethe's formula for the rate of loss of energy or stopping power is given by:

$$\frac{dE}{dX} = \frac{4\pi Z^2 e^4 NZ}{m_o v^2}[ln\frac{2m_o v^2}{I} - ln(1-\beta^2) - \beta^2] \tag{A.1}$$

where Ze=charge on the particle, esu

N= number of absorbing atoms cm^{-3}

Z= atomic number of the absorber

I= average excitation potential, erg

m_o= rest mass of the electron

v= velocity of the particle

β= v/c for the particle

The values of these terms are as follows:

Ze= $4.8E-10esu$

N= $\frac{4}{(4.02E-8)^3} = 6.157E22atoms/cm^3$

I= 500

$m_o = 9.1E - 28gm$

mass of the deuteron= $1875.628MeV/c^2 \sim 2E9eV - s^2/cm^2$

If the initial energy given to the deuterium is 10000 ev then,

$$mv^2/2 = 10000eV$$

$$2E9\frac{v^2 ev}{2c^2} = 10000eV$$

$$v^2 = E - 5c^2$$

$$v = 9.3E7cm/sec$$

$$\beta = v/c = 3.1E - 3$$

$$\frac{dE}{dX} = \frac{4\pi(4.8E-10)^4(6.157E22)46}{(9.1E-28)(9E15)}[ln(\frac{2*9.1E-28*E15*9}{500}) - ln(1-10^-5) - 10^-5] \quad (A.2)$$

$$\frac{dE}{dX} = 7.9erg/cm$$

$$\frac{dE}{dX} = 4.94E12ev/cm \quad (A.3)$$

The time in which D will lose its energy to the Pd lattice is given by:

$$\tau = \frac{T}{v*\frac{dE}{dX}} \quad (A.4)$$

$$\tau = \frac{5E4}{9.3E7*4.94E12}$$

$$\tau = 1.088E - 16sec \quad (A.5)$$

From this we could conclude that only a few fusions would occur before the deuterium will lose all its energy to the palladium lattice.

APPENDIX B. SIMPLIFICATION OF FORCE EQUATIONS USED IN PROGRAMMING

Force Due to Palladium

The force due to Pd is given by:

$$F_{Pd} = 3e^2 \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \left(\frac{(s-\sqrt{2}it)\vec{s}}{[(s-\sqrt{2}it)^2 + (2j^2 + 4[q+\frac{1}{2}]^2)t^2]^{\frac{3}{2}}} + \frac{(s-\sqrt{2}[i+\frac{1}{2}]t)\vec{s}}{[(s-\sqrt{2}[i+\frac{1}{2}]t)^2 + (2[j+\frac{1}{2}]^2 + 4q^2)t^2]^{\frac{2}{3}}} \right) \tag{B.1}$$

We do some revisions on the sums involving $(i + \frac{1}{2})$, $(j + \frac{1}{2})$ and $(q + \frac{1}{2})$ terms to get, finally

$$F_{Pd} = 6e^2\vec{s} \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \sum_{q=0}^{\infty} \frac{s-\sqrt{2}it}{[(\sqrt{2}it-s)^2 + 2j^2t^2 + (2q+1)^2t^2]^{\frac{3}{2}}} + 6e^2\vec{s} \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \sum_{q=-\infty}^{\infty} \left(\frac{s+\sqrt{2}[i+\frac{1}{2}]t}{[(\sqrt{2}[i+\frac{1}{2}]t+s)^2 + (2[j+\frac{1}{2}]^2t^2 + 4q^2t^2]^{\frac{3}{2}}} - \frac{\sqrt{2}[i+\frac{1}{2}]t - s}{[(\sqrt{2}[i+\frac{1}{2}]t-s)^2 + 2(j+\frac{1}{2})^2t^2 + 4q^2t^2]^{\frac{3}{2}}} \right) \tag{B.2}$$

Or, for easier computation;

$$F_{Pd} = \frac{6e^2\vec{s}}{t^2}\{\sum_{i=-\infty}^{\infty}\sum_{j=-\infty}^{\infty}\sum_{q=0}^{\infty}\frac{(\sqrt{2}i+\frac{s}{t})}{[(\sqrt{2}i+\frac{s}{t})^2+2j^2+(2q+1)^2]^{\frac{3}{2}}}$$
$$-\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}\sum_{q=-\infty}^{\infty}(\frac{\sqrt{2}(i+\frac{1}{2})-\frac{s}{t}}{[(\sqrt{2}[i+\frac{1}{2}]-\frac{s}{t})^2+(2[j+\frac{1}{2}]^2+4q^2]^{\frac{3}{2}}}$$
$$-\frac{\sqrt{2}(i+\frac{1}{2})+\frac{s}{t}}{[(\sqrt{2}[i+\frac{1}{2}]+\frac{s}{t})^2+2(j+\frac{1}{2})^2+4q^2]^{\frac{3}{2}}})\} \quad (B.3)$$

This can be broken into two parts and we call the first triple sum F_1 and second triple sum F_2, so we get:

$$F_{Pd} = \frac{6e^2\vec{s}}{t^2}(F_1 - F_2) \quad (B.4)$$

$$F_{Pd} = F_{1Pd} - F_{2Pd} \quad (B.5)$$

To evaluate the triple sums, we rely on neighborhood of the origin. The numbers $(2i^2+2j^2+(2q+1)^2)^{1/2}$ for F_1 and $(2(i+\frac{1}{2})^2+2(j+\frac{1}{2})^2+4q^2)^{1/2}$ for F_2 represents the radial distance (in units of t) of force points from the origin. We note that the terms in j and q in the denominators represent tubes of spaced charge surrounding the channel along which the deuterium moves. At a certain distance, these tubes will start behaving like uniformly charged tubes whose force on a charge moving along the channel will be zero.

We take this distance to be any number greater than 5t. Thus, we retain, in the first sum, only those terms in the (j,q) sum for which $2j^2+4(q+\frac{1}{2})^2 \leq 25$, and in the second sum, those for which $2(j+\frac{1}{2})^2+4q^2 \leq 25$.

For the first sum, these terms are: $j=0, |q+\frac{1}{2}| = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}$; $j=\pm 1, |q+\frac{1}{2}| = \frac{1}{2}, \frac{3}{2}$; $j=\pm 2, |q+\frac{1}{2}| = \frac{1}{2}, \frac{3}{2}$; $j=\pm 3, |q+\frac{1}{2}| = \frac{1}{2}$.

Following is a table generated on these values:

$j\backslash q$	-3	-2	-1	0	1	2
-3	43	27	19	19	27	43
-2	33	17	9	9	17	33
-1	27	11	3	3	11	27
0	25	9	1	1	9	25
1	27	11	3	3	11	27
2	33	17	9	9	17	33
3	43	27	19	19	27	43

Then, the first triple sum can be written as:

$$F_{1Pd} = \frac{6e^2\vec{s}}{t^2}\sum_{l=1}^{7} a_l \sum_{i=-\infty}^{\infty} \frac{\frac{s}{t} - \sqrt{2}i}{([\frac{s}{t} - \sqrt{2}i]^2 + b_l)^{\frac{3}{2}}} \tag{B.6}$$

Where the value of l,a_l and b_l are given as:

l	1	2	3	4	5	6	7
a_l	1	2	3	2	2	2	1
b_l	1	3	9	11	17	19	25

A similar table for the second sum is given below:

$j\backslash q$	-2	-1	0	1	2
-4	$\frac{81}{2}$	$\frac{57}{2}$	$\frac{49}{2}$	$\frac{57}{2}$	$\frac{81}{2}$
-3	$\frac{57}{2}$	$\frac{33}{2}$	$\frac{25}{2}$	$\frac{33}{2}$	$\frac{57}{2}$
-2	$\frac{41}{2}$	$\frac{17}{2}$	$\frac{9}{2}$	$\frac{17}{2}$	$\frac{41}{2}$
-1	$\frac{33}{2}$	$\frac{9}{2}$	$\frac{1}{2}$	$\frac{9}{2}$	$\frac{33}{2}$
0	$\frac{33}{2}$	$\frac{9}{2}$	$\frac{1}{2}$	$\frac{9}{2}$	$\frac{33}{2}$
1	$\frac{41}{2}$	$\frac{17}{2}$	$\frac{9}{2}$	$\frac{17}{2}$	$\frac{41}{2}$
2	$\frac{57}{2}$	$\frac{33}{2}$	$\frac{25}{2}$	$\frac{33}{2}$	$\frac{57}{2}$
3	$\frac{81}{2}$	$\frac{57}{2}$	$\frac{49}{2}$	$\frac{57}{2}$	$\frac{81}{2}$

Then, the second triple sum can be written as:

$$F_{2Pd} = \frac{6e^2\vec{s}}{t^2}\sum_{L=1}^{7} a_L \sum_{i=-\infty}^{\infty} \frac{\frac{s}{t} - (i+\frac{1}{2})\sqrt{2}}{[(\frac{s}{t} - [i+\frac{1}{2}]\sqrt{2})^2 + b_L]^{\frac{3}{2}}} \tag{B.7}$$

with:

L	1	2	3	4	5	6	7
a_L	1	3	2	1	4	2	1
b_L	$\frac{1}{2}$	$\frac{9}{2}$	$\frac{17}{2}$	$\frac{25}{2}$	$\frac{33}{2}$	$\frac{41}{2}$	$\frac{49}{2}$

Next, we approximate the i sums for large values of $|i|$. In the first sum, F_{1Pd}, we note that when $|i| \geq 4$,the points are very far away from the action, which takes place between i=0, $\frac{s}{t}$=0 and i=0 or 1, $\frac{s}{t} = \frac{1}{\sqrt{2}}$. Thus, we approximate the terms in the F_{1Pd} equation with $i \leq -4$ by:

$$= \frac{6e^2\vec{s}}{t^2}\sum_{l=1}^{7} a_l \int_{i=-\infty}^{-3.5} \frac{(\frac{s}{t} - \sqrt{2}i)}{([\frac{s}{t} - \sqrt{2}i]^2 + b_l)^{\frac{3}{2}}} di \tag{B.8}$$

$$= \frac{6e^2\vec{s}}{t^2\sqrt{2}}\sum_{l=1}^{7}a_l\left(\frac{1}{(\frac{s}{t}+\frac{7\sqrt{2}}{2})^2+b_l}\right)^{\frac{1}{2}} \tag{B.9}$$

Those for $i \geq 4$ are similarly approximated to:

$$= -\frac{6e^2\vec{s}}{t^2\sqrt{2}}\sum_{l=1}^{7}a_l\left(\frac{1}{(\frac{7\sqrt{2}}{2}-\frac{s}{t})^2+b_l}\right)^{\frac{1}{2}} \tag{B.10}$$

The denominators of these terms can be written as:

$$(b_l+\frac{49}{2}+\frac{s^2}{t^2}\pm\frac{7\sqrt{2}s}{t})^{\frac{1}{2}} \tag{B.11}$$

This can be written as power series in the following form:

$$\frac{(\frac{s}{t})^n}{(b_l+\frac{49}{2}+\frac{s^2}{t^2})^{n+\frac{1}{2}}} \tag{B.12}$$

When this is done, the first term and the third terms cancel, the fourth terms are always very small, and only the second (n=1) terms are left. The results is:

$$= -\frac{6e^2\vec{s}}{t^2}(\frac{7s}{t})\sum_{l=1}^{7}\frac{a_l}{(\frac{49}{2}+b_l+\frac{s^2}{t^2})^{\frac{3}{2}}} \tag{B.13}$$

This result is clearly quite precise for small values of $\frac{s}{t}$. We also note that for $\frac{s}{t}=\frac{\sqrt{2}}{2}$, the combined sums beyond i=-4 and i=4 cancel out exactly except for the $i = \pm 4$ term, which becomes:

$$= -\frac{6e^2\vec{s}}{t^2}(\frac{7s}{t})\sum_{l=1}^{7}\frac{a_l}{(\frac{49}{2}+b_l)^{\frac{3}{2}}} \tag{B.14}$$

Thus even at this point, the error is less than 3% of a small number. With this term, and unreeling the remaining i sum terms, we get, finally, (after just a little algebra) the final equation used in the program.

$$
\begin{aligned}
F_{1Pd} &= \frac{6e^2\vec{s}}{t^2}\sum_{l=1}^{7} a_l\{\frac{\frac{s}{t}}{([\frac{s}{t}]^2+b_l)^{\frac{3}{2}}} - \frac{\frac{7s}{t}}{(\frac{49}{2}+b_l)^{\frac{3}{2}}} \\
&- \sum_{i=1}^{3}(\frac{\sqrt{2}i-\frac{s}{t}}{([\sqrt{2}i-\frac{s}{t}]^2+b_l)^{\frac{3}{2}}} - \frac{\sqrt{2}i+\frac{s}{t}}{([\sqrt{2}i+\frac{s}{t}]^2+b_l)^{\frac{3}{2}}})\} \qquad \text{(B.15)}
\end{aligned}
$$

Similar manipulation on the second set of sums yields:

$$
\begin{aligned}
F_{2Pd} &= -\frac{6e^2\vec{s}}{t^2}\sum_{L=1}^{7} a_L\{\frac{\frac{8s}{t}}{(32+b_L)^{\frac{3}{2}}} + \sum_{i=0}^{3}[\frac{\sqrt{2}(i+\frac{1}{2})-\frac{s}{t}}{([\sqrt{2}(i+\frac{1}{2})-\frac{s}{t}]^2+b_L)^{\frac{3}{2}}} \\
&- \frac{\sqrt{2}(i+\frac{1}{2})+\frac{s}{t}}{[(\sqrt{2}(i+\frac{1}{2})+\frac{s}{t}]^2+b_L)^{\frac{3}{2}}}]\} \qquad \text{(B.16)}
\end{aligned}
$$

Force from D Atoms in PdD on a D at (0,0,0) Lattice Position

The force due to Deuterium is given by:

$$
\begin{aligned}
F_D &= \frac{e^2\vec{s}}{t^2}\sum_{i=-\infty}^{\infty}\sum_{j=-\infty}^{\infty}\sum_{q=-\infty}^{\infty}\{\frac{\frac{s}{t}-\sqrt{2}i}{[(\frac{s}{t}-\sqrt{2}i)^2+2j^2+4q^2]^{\frac{3}{2}}} \\
&+ \frac{\frac{s}{t}-\sqrt{2}(i+\frac{1}{2})}{[(\frac{s}{t}-\sqrt{2}[i+\frac{1}{2}])^2+2(j+\frac{1}{2})^2+(2q+1)^2]^{\frac{3}{2}}}\} \qquad \text{(B.17)}
\end{aligned}
$$

$$F_D = F_{1D} + F_{2D} \qquad \text{(B.18)}$$

In the above equation, the case of $i = j = q = 0$ is excluded from the first term only. To evaluate the triple sum, we rely on neighborhood of the origin. The numbers $(2j^2+2q^2)$ for the first part and $2(j+\frac{1}{2})^2+(2q+1)^2$ for the second part, representing the radial distance terms in j and q in the denominators,this also represent tubes of spaced charge surrounding the channel along which the deuterium moves. At a distance, these tubes will start behaving like uniformly charged tubes whose force on a charge moving along the channel will be zero.

We take this distance to be any number greater than 5t. Thus, we retain, in the first sum, only those terms in the (j,q) sum for which $(2j^2 + 4q^2) \leq 25$ and in the second sum for which $(2(j + \frac{1}{2})^2 + (2q + 1)^2) \leq 25$

Based on $(2j^2 + 4q^2) \leq 25$ for the first sum, a table of sum is given:

$j\backslash q$	-3	-2	-1	0	1	2	3
-3	54	34	22	18	22	34	54
-2	44	24	12	8	12	24	44
-1	38	18	6	2	6	18	36
0	36	16	4	0	4	16	36
1	38	18	6	2	6	18	36
2	44	24	12	8	12	24	44
3	54	34	22	18	22	34	54

The first sum is then reduced to:

$$F_{1D} = \frac{\vec{s}e^2}{t^2}\left(\sum_{l=1}^{10} a_l \sum_{i=-\infty}^{\infty} \frac{\frac{s}{t} - \sqrt{2}i}{[(\frac{s}{t} - \sqrt{2}i)^2 + b_l]^{\frac{3}{2}}} - \frac{t^2}{s^2}\right) \tag{B.19}$$

Where the value of l, a_l and b_l from the above table are as follows:

l	1	2	3	4	5	6	7	8	9	10
a_l	1	2	2	4	2	4	2	6	4	4
b_l	0	2	4	6	8	12	16	18	22	24

The subtracted term in the above equation represents the exclusion of the l=1, i=0 term from the double sum.

Based on this equation $(2q+1)^2 + 2(j+\frac{1}{2})^2 \leq 25$, a table for the second sum is given below:

$j\backslash q$	-3	-2	-1	0	1	2	3
-3	$\frac{75}{2}$	$\frac{43}{2}$	$\frac{27}{2}$	$\frac{27}{2}$	$\frac{43}{2}$	$\frac{75}{2}$	$\frac{123}{2}$
-2	$\frac{59}{2}$	$\frac{27}{2}$	$\frac{11}{2}$	$\frac{11}{2}$	$\frac{27}{2}$	$\frac{59}{2}$	$\frac{107}{2}$
-1	$\frac{51}{2}$	$\frac{19}{2}$	$\frac{3}{2}$	$\frac{3}{2}$	$\frac{19}{2}$	$\frac{51}{2}$	$\frac{99}{2}$
0	$\frac{51}{2}$	$\frac{19}{2}$	$\frac{3}{2}$	$\frac{3}{2}$	$\frac{19}{2}$	$\frac{51}{2}$	$\frac{99}{2}$
1	$\frac{59}{2}$	$\frac{27}{2}$	$\frac{11}{2}$	$\frac{11}{2}$	$\frac{27}{2}$	$\frac{59}{2}$	$\frac{107}{2}$
2	$\frac{75}{2}$	$\frac{43}{2}$	$\frac{27}{2}$	$\frac{27}{2}$	$\frac{43}{2}$	$\frac{75}{2}$	$\frac{123}{2}$
3	$\frac{99}{2}$	$\frac{67}{2}$	$\frac{51}{2}$	$\frac{51}{2}$	$\frac{67}{2}$	$\frac{99}{2}$	$\frac{147}{2}$

The second term is reduced to:

$$F_{2D} = \frac{\vec{s}e^2}{t^2} \sum_{L=1}^{5} a_L \sum_{i=-\infty}^{\infty} \frac{\frac{s}{t} - \sqrt{2}(i+\frac{1}{2})}{[(\frac{s}{t} - \sqrt{2}[i+\frac{1}{2}])^2 + b_L]^{\frac{3}{2}}} \qquad \text{(B.20)}$$

where the values of L, a_L and b_L from the above table are as follows:

L	1	2	3	4	5
a_L	4	4	4	8	4
b_L	$\frac{3}{2}$	$\frac{11}{2}$	$\frac{19}{2}$	$\frac{27}{2}$	$\frac{43}{2}$

Next, we approximate the i sums for the large $|i|$. In the first sum, F_{1D}, we note that when $|i| \geq 5$ the points are very far away from the action. Thus we approximate the i terms in the first sum in the following way:

$$= \sum_{l=1}^{10} a_l \{ \sum_{i=-\infty}^{-5} + \sum_{i=5}^{\infty} \} [\frac{\frac{s}{t} - \sqrt{2}i}{((\frac{s}{t} - \sqrt{2}i)^2 + b_l)^{\frac{3}{2}}}] \qquad \text{(B.21)}$$

$$= \sum_{l=1}^{10} a_l \{ \int_{i=-\infty}^{-4.5} di + \int_{i=4.5}^{\infty} di \} [\frac{\frac{s}{t} - \sqrt{2}i}{((\frac{s}{t} - \sqrt{2}i)^2 + b_l)^{\frac{3}{2}}}] \qquad \text{(B.22)}$$

$$= \sum_{l=1}^{10} \frac{a_l}{\sqrt{2}} \{ \frac{1}{([\frac{s}{t} + \frac{9\sqrt{2}}{2}]^2 + b_l)^{\frac{1}{2}}} - \frac{1}{([\frac{s}{t} - \frac{9\sqrt{2}}{2}]^2 + b_l)^{\frac{1}{2}}} \} \quad (B.23)$$

Let us write $D = \frac{s^2}{t^2} + \frac{81}{2} + b_l$. Then the above equation can be written in the following form:

$$= \sum_{l=1}^{10} \frac{a_l}{\sqrt{2}D} \{ \frac{1}{(1 + \frac{9\sqrt{2}s}{D^2 t})^{\frac{1}{2}}} - \frac{1}{((1 - \frac{9\sqrt{2}s}{D^2 t})^{\frac{1}{2}}} \} \quad (B.24)$$

On expanding the denominators in the braces by the rule of $(1-\epsilon)^{-\frac{1}{2}} = 1 + \frac{\epsilon}{2} + \frac{1}{2}.\frac{3}{4}.(\epsilon)^2 + \frac{1}{2}.\frac{3}{4}.\frac{5}{6}.(\epsilon)^3$....., we get:

$$= \sum_{l=1}^{10} \frac{a_l}{D\sqrt{2}} (1 - \frac{\frac{9}{2}.\sqrt{2}.\frac{s}{t}}{D^2} + \frac{\frac{3}{8}.\frac{81}{2}.\frac{s^2}{t^2}}{D^4} - \frac{\frac{5}{16}.\frac{81}{2}.\frac{9}{2}.\sqrt{2}.\frac{s^3}{t^3}}{D^6} \ldots$$

$$- 1 - \frac{\frac{9}{2}.\sqrt{2}.\frac{s}{t}}{D^2} - \frac{\frac{3}{8}.\frac{81}{2}.\frac{s^2}{t^2}}{D^4} - \frac{\frac{5}{16}.\frac{81}{2}.\frac{9}{2}.\sqrt{2}.\frac{s^3}{t^3}}{D^6} \ldots) \quad (B.25)$$

The last term is very small ($D^4 > \frac{(81)^2}{4}$) and may dropped, giving

$$= -\sum_{l=1}^{10} \frac{9\frac{s}{t}}{(\frac{81}{2} + b_l + \frac{s^2}{t^2})^{\frac{3}{2}}} \quad (B.26)$$

Note that when $\frac{s}{t} = \frac{1}{\sqrt{2}}$, then the above term reduces to:

$$= -\sum_{l=1}^{10} \frac{\frac{9}{\sqrt{2}}}{(\frac{81}{2} + b_l + \frac{1}{2})^{\frac{3}{2}}} \quad (B.27)$$

Thus from this we can see that an exact summation is possible, which is:

$$= -\sum_{l=1}^{10} \frac{\frac{9}{\sqrt{2}}}{(\frac{81}{2} + b_l)^{\frac{3}{2}}} \quad (B.28)$$

This suggests that dropping $\frac{s^2}{t^2}$ from the denominator will improve accuracy for the largest $\frac{s}{t}$ of our problem, and will hardly effect the answer for smaller $\frac{s}{t}$. Thus, force due to D can be written as:

$$F_{1D} = \frac{\vec{s}e^2}{t^2}\{\sum_{l=1}^{10} a_l[\sum_{i=-4}^{4} \frac{\frac{s}{t} - \sqrt{2}i}{([\frac{s}{t} - \sqrt{2}i]^2 + b_l)^{\frac{3}{2}}} - \frac{9\frac{s}{t}}{(\frac{81}{2} + b_l)^{\frac{3}{2}}}] - \frac{t^2}{s^2}\} \qquad \text{(B.29)}$$

Rearranging for convenience in computing we get:

$$\begin{aligned} F_{1D} &= \frac{\vec{s}e^2}{t^2}\{\sum_{l=2}^{10} a_l \frac{\frac{s}{t}}{(\frac{s^2}{t^2} + b_l)^{\frac{3}{2}}} - \sum_{l=1}^{10} a_l \sum_{i=1}^{4}[\frac{i\sqrt{2} - \frac{s}{t}}{([i\sqrt{2} - \frac{s}{t}]^2 + b_l)^{\frac{3}{2}}} \\ &- \frac{i\sqrt{2} + \frac{s}{t}}{([i\sqrt{2} + \frac{s}{t}]^2 + b_l)^{\frac{3}{2}}}] - \sum_{l=1}^{10} \frac{9\frac{s}{t}a_l}{(\frac{81}{2} + b_l)^{\frac{3}{2}}}\} \end{aligned} \qquad \text{(B.30)}$$

Now same procedure is applied in solving the second term of the D force.

$$F_{2D} = \frac{\vec{s}e^2}{t^2}\sum_{L=1}^{5} a_L\{\sum_{i=0}^{\infty}\frac{\frac{s}{t} - \sqrt{2}[i+\frac{1}{2}]}{[(\frac{s}{t} - \sqrt{2}[i+\frac{1}{2}])^2 + b_L]^{\frac{3}{2}}} + \sum_{i=0}^{\infty}\frac{\frac{s}{t} + \sqrt{2}[i+\frac{1}{2}]}{[(\frac{s}{t} - \sqrt{2}[i+\frac{1}{2}])^2 + b_L]^{\frac{3}{2}}}\} \qquad \text{(B.31)}$$

This can be also be written as:

$$\begin{aligned} F_{2D} &= -\frac{\vec{s}e^2}{t^2}\sum_{L=1}^{5} a_L \sum_{i=0}^{4}\{\frac{\sqrt{2}(i+\frac{1}{2}) - \frac{s}{t}}{[(\sqrt{2}[i+\frac{1}{2}] - \frac{s}{t})^2 + b_L]^{\frac{3}{2}}} - \frac{\sqrt{2}(i+\frac{1}{2}) + \frac{s}{t}}{[(\sqrt{2}[i+\frac{1}{2}] + \frac{s}{t})^2 + b_L]^{\frac{3}{2}}}\} \\ &+ \sum_{l=1}^{10} a_l\{\int_{i=-\infty}^{-4.5} di + \int_{i=4.5}^{\infty} di\}[\frac{\frac{s}{t} - \sqrt{2}(i+\frac{1}{2})}{(\frac{s}{t} - \sqrt{2}[i+\frac{1}{2}]^2 + b_l)^{\frac{3}{2}}}] \end{aligned} \qquad \text{(B.32)}$$

The integeral term reduces to:

$$\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{50 + b_L + \frac{s^2}{t^2} - \frac{10\sqrt{2}s}{t}}} - \frac{1}{\sqrt{50 + b_L + \frac{s^2}{t^2} + \frac{10\sqrt{2}s}{t}}}\right) \qquad \text{(B.33)}$$

This can be approximately be written as:

$$10\left(\frac{\frac{s}{t}}{(50+b_L+\frac{s^2}{t^2})^{\frac{3}{2}}}\right) \tag{B.34}$$

Again we can see that the result is quite precise for $\frac{s}{t}$ small. Thus we can neglect the $\frac{s^2}{t^2}$ term to get get a more precise value.

The final result for the second term becomes as follows:

$$\begin{aligned} F_{2D} &= -\frac{\vec{s}e^2}{t^2}\{\sum_{L=1}^{5} a_L \frac{10\frac{s}{t}}{(50+b_L)^{\frac{3}{2}}} + \sum_{L=1}^{5} a_L \sum_{i=0}^{4}[\frac{\sqrt{2}(i+\frac{1}{2})-\frac{s}{t}}{([\sqrt{2}(i+\frac{1}{2})-\frac{s}{t}]^2+b_L)^{\frac{3}{2}}} \\ &- \frac{\sqrt{2}(i+\frac{1}{2})+\frac{s}{t}}{([\sqrt{2}(i+\frac{1}{2})+\frac{s}{t}]^2+b_L)^{\frac{3}{2}}}]\} \end{aligned} \tag{B.35}$$

Thus the final form of the D force used reduces to:

$$\begin{aligned} F_{1D} &= \frac{\vec{s}e^2}{t^2}\{\sum_{l=2}^{10} a_l \frac{\frac{s}{t}}{(\frac{s^2}{t^2}+b_l)^{\frac{3}{2}}} - \sum_{l=1}^{10} a_l \sum_{i=1}^{4}[\frac{i\sqrt{2}-\frac{s}{t}}{([i\sqrt{2}-\frac{s}{t}]^2+b_l)^{\frac{3}{2}}} - \frac{i\sqrt{2}+\frac{s}{t}}{([i\sqrt{2}+\frac{s}{t}]^2+b_l)^{\frac{3}{2}}}] \\ &- \sum_{l=1}^{10} \frac{9\frac{s}{t}a_l}{(\frac{81}{2}+b_l)^{\frac{3}{2}}}\} \end{aligned} \tag{B.36}$$

$$\begin{aligned} F_{2D} &= -\frac{\vec{s}e^2}{t^2}\{\sum_{L=1}^{5} a_L \frac{10\frac{s}{t}}{(50+b_L)^{\frac{3}{2}}} + \sum_{L=1}^{5} a_L \sum_{i=0}^{4}[\frac{\sqrt{2}(i+\frac{1}{2})-\frac{s}{t}}{[(\sqrt{2}[i+\frac{1}{2}]-\frac{s}{t})^2+b_L]^{\frac{3}{2}}} \\ &- \frac{\sqrt{2}(i+\frac{1}{2})+\frac{s}{t}}{[(\sqrt{2}[i+\frac{1}{2}]+\frac{s}{t})^2+b_L]^{\frac{3}{2}}}]\} \end{aligned} \tag{B.37}$$

APPENDIX C. PROGRAM USED TO CALCULATE THE ELECTROSTATIC FORCES ON THE DEUTERONS

The following four programs are used in calculating separately the net force due to Pd atoms, D atoms, attractive force from an adjacent hole respectively and total effect due to these three combinations.

```
********************************************************
*  PALLADIUM.FOR
*  This program computes the net force due to Pd atoms.
*  By Suneeta Singh
*********************************************************
        PROGRAM Pd
        DIMENSION TERM(4)
*       VARIABLES
        REAL A(7),B(7),C(7),D(7),T,Y,Y1,Y2,YA,YA1,YA2
        INTEGER I,J,K
*       DATA VALUES
        DATA A/1.0,2.0,3.0,2.0,2.0,2.0,1.0/
        DATA B/1.0,3.0,9.0,11.0,17.0,19.0,25.0/
        DATA C/1.0,3.0,2.0,1.0,4.0,2.0,1.0 /
        DATA D/0.5,4.5,8..5,12.5,16.5,20.5,24.5 /
*       OPENING A FILE TO STORE THE OUTPUT
        OPEN(2,'OUTPUT1.DAT')
*       DEFINING CONSTANTS AND VARIABLES
*   T= half of the lattice constant of Pd
*   E= square of charge of electron
*   J= distance travelled by the deuterium till the saddle
*      point
```

```
*    FP= force due to Pd
*    ENP= energy due to Pd
       T=2.01E5
       E=1.44e6
       Z=1.4142136
*        Initialization
         FP=0.0
         ENP=0.0
                DO 10  J=0,150000,500
*        We will now calculate the value of FPd(1) and
*        FPd(2) by breaking the equations into small terms.
*        These terms are then calculated and the results are
*        combined to get the net force result.
         S=REAL(J)
         X2=0.0
                        DO 20 L=1,7
         X1=0.0
                  DO 30 I=1,3
         Y=S/T
         Y1=Z*I-Y
         Y2=Z*I+Y
         TERM(1)=A(L)*(Y1*(Y1**2+B(L))**(-1.5)-Y2*(Y2**2+B(L)
     +    )**(-1.5))
          X1=TERM(1)+X1
 30                    CONTINUE
         TERM(1)=X1
*
         TERM(2)=A(L)*Y*((Y**2+B(L))**(-1.5)-7.*(24.5+B(L))
     +   **(-1.5))-TERM(1)
         X2=X2+TERM(2)
 20                              CONTINUE
         TERM(2)=X2
*
*
         X4=0.
                                  DO 40 K=1,7
         X3=0.0
                 DO 50 I=0,3
         YA=S/T
         YA1=(Z*(I+.5)-YA)
```

```
      YA2=(Z*(I+.5)+YA)
     TERM(3)=C(K)*(YA1*(YA1**2+D(K))**(-1.5)-
   + YA2*(YA2**2+D(K))**(-1.5))
      X3=TERM(3)+X3
50             CONTINUE
      TERM(3)=X3
      TERM(4)=TERM(3)+C(K)*8.0*YA*(32+D(K))**(-1.5)
      X4=TERM(4)+X4
40                     CONTINUE
      TERM(4)=X4
      PRINT*,'FPd(1)= ',TERM(2),'  FPd(2)=  ',TERM(4)
               F=TERM(2)-TERM(4)
*     Calculating The Net Force Due to the Pd Atoms
      FP=F*6*E/(T**2)
*     Calculating The Net Energy Due To the Pd Atoms
      ENP=FP*500+ENP
      PRINT*,'FP=  ',FP,'  J= ',J,'  ENP= ',ENP
*     Writing the output in the file
      WRITE(2,*)FP,ENP,J,TERM(2),TERM(4)
10    CONTINUE
      END

*************************************************************
*   DEUTERON.FOR
*   This program is used to calculate the effect on the net
*   force due to the neighboring deuteriums.
*   By Suneeta Singh
*************************************************************
*
      PROGRAM DEUTERON
*
      DIMENSION TERM(6)
*     VARIABLES
      REAL A(10),B(10),C(5),D(5),T,Y,Y1,Y2,YA,YA1,YA2
      INTEGER I,J,K
*     DATA VALUES
      DATA A/1,2,2,4,2,4,2,6,4,4/
      DATA B/0,2,4,6,8,12,16,18,22,24/
      DATA C/4,4,4,8,4/
      DATA D/1.5,5.5,9.5,13.5,21.5/
```

```
*       DEFINING CONSTANTS AND VARIABLES
*       T= half of the lattice constant of Pd
*       E= square of charge of electron
*       J= distance travelled by the deuterium
*          till the saddle point.
*       Fd= force due to deuterium
*       ENd= energy due to deuterium
*       OPENING A FILE TO WRITE OUTPUT
        OPEN(2,'OUTPUT2.DAT')
*       VALUES OF THE CONSTANTS
        T=2.01E5
        E=1.44E6
        Z=1.4142136
*
*       INITIALIZATION
        Fd=0.
        ENd=0.
        DO 10  J=0 ,150000,500
*       The value FD1 and FD2 are calulated by dividing
*       the equations into small terms. The values of these
*       are calculated and the net force is obtained by
*       joining these results.
        S=REAL(J)
        X1=0.
        DO 20 L=2,10
        Y=S/T
        TERM(1)=A(L)*Y*(Y**2+B(L))**(-1.5)
        X1=TERM(1)+X1
   20   CONTINUE
        TERM(1)=X1
        X3=0.
        DO 30 L=1,10
        X2=0.
        DO 40 I=1,4
        Y=S/T
        Y1=I*Z-Y
        Y2=I*Z+Y
        TERM(2)=A(L)*(Y1*(Y1**2+B(L))**(-1.5)-Y2*(Y2**2+
     +  B(L))**(-1.5))
        X2=TERM(2)+X2
```

```
   40   CONTINUE
        TERM(2)=X2
        TERM(3)=A(L)*9*Y*(40.5+B(L))**(-1.5)+TERM(2)
        X3=X3+TERM(3)
   30   CONTINUE
        TERM(3)=X3
        TERM(4)= TERM(1)-TERM(3)
        X4=0.
        DO 50 K=1,5
        X5=0.
        DO 60 I=0,4
        YA=S/T
        YA1=(I+.5)*Z-YA
        YA2=(I+.5)*Z+YA
        TERM(5)=C(K)*(YA1*(YA1**2+D(K))**(-1.5)
     +  -YA2*(YA2**2+D(K))**(-1.5))
        X5=X5+TERM(5)
   60   CONTINUE
        TERM(5)=X5
        TERM(6)=C(K)*10*YA*(50+D(K))**(-1.5)+TERM(5)
        X4=X4+TERM(6)
   50   CONTINUE
        TERM(6)=X4
        F=TERM(4)-TERM(6)
*       Calculating net force due to neighboring deuteriums.
        Fd=E*F/(T**2)
*       Calculating energy due to neighboring deuteriums.
        ENd=Fd*500+ENd
*     Printing the net force and energy at various distances.
       PRINT*,'Fd= ',Fd,'  F1= ',TERM(4),'  F2= ',TERM(6),'
     +      ENd= ',ENd,'  J=  ',J
*       Writing the values in an Output file
        WRITE(2,*)Fd,END,J,TERM(4),TERM(6)
   10    CONTINUE
        END

************************************************************
*  HOLE.FOR
*  This program is used to calculate the net force on the
*  deuterium when a negative charge is placed at any one
```

```
*  deuterium atom position, such that it behaves as a hole.
*       By Suneeta Singh
************************************************************
        PROGRAM HOLE
*       DEFINING VARIABLES
        REAL T,E
        INTEGER J
*       OPENING A FILE TO WRITE OUTPUT
        OPEN(2,'OUTPUT3.DAT')
*       DEFINING CONSTANTS
*       T= half of the lattice constant of Pd
*       E= square of eletron charge
        T=2.01E5
        E=1.44E6
        Z=1.4142136
*
*       INITIALIZATION
        EX=0.0
        DO 10 J=0.0,150000,500
        S=REAL(J)
*       Calculating the force values
        FX=E/(T*Z-S)**2
*       Calculating the energy values
        X=FX*500.
        EX=EX+X
*       Printing the force and energy at various distances
        PRINT*,'FX= ',FX,'  EX= ',EX,'  J= ',J
*       Writing the output in a file
        WRITE(2,*)FX,EX,J
   10   CONTINUE
        END
*********************************************************
*  CONNECT.FOR
*  This program is used to join the results of all the three
*   above given programs.
*       By Suneeta Singh
************************************************************
        PROGRAM CONNECT
*       DEFINING VARIABLES
        INTEGER J
```

```
*       J= half of the lattice constant of Pd
*   Opening files of the above three programs containing
*   output and opening another file to add results.
        OPEN(2,'FINAL.DAT')
        OPEN(3,'OUTPUT1.DAT',STATUS='UNKNOWN')
        OPEN(4,'OUTPUT2.DAT',STATUS='UNKNOWN')
        OPEN(5,'OUTPUT3.DAT',STATUS='UNKNOWN')
*       INITIALIZATION
        ET=0.
        DO 10 J=0,150000,500
*       Reading  outputs from the  opened files
        READ(3,*)FP,ENP
        READ(4,*)FD,END
        READ(5,*)FX,EX
*       Adding all the three forces
        F=FP+FD+FX
*       Adding all the three energies
        E=ENP+ENd+EX
*       Printing the results
        PRINT*,'F(TOTAL)=  ',F,'  E(T)=',E,'  J= ',J,'
*       Writing the results in a output file
        WRITE(2,*)F,E,J
   10   CONTINUE
        END
************************************************************
```