



Research Article

Quantum-correlated Fluctuations, Phonon-induced Bond Polarization, Enhanced Tunneling, and Low-energy Nuclear Reactions in Condensed Matter

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Abstract

In heavily (deuterated or hydrogenated) palladium, some of the crystallinity is lost. As a consequence, the localized phonon modes of the crystal/damaged-region interface have a much higher frequency than the host. These high-frequency modes create electrostatic fields that interact strongly with electrons of the local atoms. A resulting instantaneous potential inversion, from polarization, leads to the formation of lochons (local charged bosons—electron pairs in the singlet state, perhaps isolated from the Pd d-orbital energy levels) and of an associated H^+ or D^+ ion (with its two shared electrons instantaneously isolated into the adjacent Pd d-levels). The Coulomb repulsion between the nuclei of these pairs is greatly reduced by strong screening from the lochons that can even generate an attractive polarization potential. Furthermore, the mutual tunneling penetration probability of the Coulomb barrier is enhanced by correlated fluctuations. This arises from the generalized uncertainty relations, $\Delta x \Delta p_x, \Delta E \Delta t \geq (n + 1/2)\hbar/(1 - \rho^2)^{0.5}$, where n may be on the order of 10–100 and where results from two models are combined. The integer n values represent excitations in the phonon modes of the H or D sub-lattice and ρ is the correlation coefficient with $0 < \rho < 1$. Higher values of n and ρ , for a particle in a potential well, imply less localization and greater uncertainties in location (i.e., extending its probability distribution further into the barrier). These periodic fluctuations into the barrier are an interference effect similar to that of beat frequencies.

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1. Introduction

As noted earlier, low-energy nuclear reaction (LENR) occurs in PdD_x (or PdH_x) after considerable loading by D or H [1]. This loading produces degradation of crystallinity or amorphization of the alloy [2]. When extreme, this degradation is known to suppress LENR by allowing H_2 or D_2 to escape from the interior of the crystal along fractures. On the

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other hand, disorder at a lower level may provide some of the necessary conditions for LENR. With this in mind, one has to consider not just the bulk material, but, also its external surfaces, its defects, and its internal crystallite and grain boundaries [3]. Of particular interest at these boundaries are the defects and the interface phonon modes. Associated with the boundary, interface, and defect states is the effect of nanoparticle (NP) surfaces relative to those of bulk or even thin-film material. The large surface to volume ratio of the NPs, relative to Pd thin films and bulk, alters the Pd-lattice size and its response to hydrogen loading [2]. At least in this recent study, the PdH_x beta phase in NPs appears to be dominant at exposure to 2% H gas, but not until 10% H gas for thin films. Thus, both surface and subsurface effects depend on the nature of the interfaces. Linear defects have been addressed earlier [4]. The present paper examines another aspect of these interfaces.

2. Generalized Uncertainty Relation

The wave amplitude of interface phonon modes (in particular, longitudinal-optical modes) decays away from the interface junction. Thus, solutions of the wave equation correspond to localized modes near the interface. Further, these phonons produce electrostatic fields that strongly couple with the electrons and ions confined to the layer in a manner that may differ from that in the bulk. The effect of these fields in introducing paired-electron states (lochons – local charged bosons) has been discussed in detail in earlier papers [5,6]. Here we also explore the local-interface-state phonons as distinct from the bulk phonons.

The frequencies (ω_1) of these localized modes are much higher than those of the phonon modes of the pure (host) lattice [7]. In addition to the higher frequency (energy) of the local-state phonons, we will explore the effects of the phonon populations and of their correlations. Since we are concerned only with these localized-longitudinal-lattice modes, we will just use $\omega_1 = \omega$ in the equations below.

The expectation values of the number of these phonons at a particular frequency $\langle n_{r,\omega} \rangle$ about an interface D* or H* sub-lattice atom (or ion) and the expectation values of their amplitudes $\langle A_{r,\omega} \rangle$ are related [7].

$$\langle n_{r,\omega} \rangle = 2M\omega \langle A_{r,\omega} \rangle^2 / \hbar, \quad (1)$$

where M is the mass of the atom. For $M_D \approx 3.3 \times 10^{-24}$ g, $\omega \approx 5 \times 10^{14}$ to 10^{15} s⁻¹ and $\langle A_{r,\omega} \rangle \approx 3 \times 10^{-9}$ cm, $\langle n_{r,\omega} \rangle$ is of the order of tens of phonons. Why do we choose this value for A ? If the spacing between the interstitial D site and the lattice barrier containing the deuterium is on the order of 10^{-8} cm, then a quadratic potential well, with a broad minimum would allow motion within its walls that would be dependent on the square root of the energy, e.g., on the number of phonons in a given direction and frequency (defining a mode). With many variables determining the actual average motions (temperature, direction, etc.), a ball-park value is the best that can be suggested. While the room-temperature mean-squared displacement [8] is ~ 0.09 au $\approx 5 \times 10^{-10}$ cm, the transitory displacement into preferred directions (e.g., between Pd atoms and with another polarized deuterium atom approaching from the adjacent cell) will be significantly greater. The lattice-assisted nuclear reaction, LANR, depends on this increased displacement and the ‘additional effects’ mentioned below.

In the context of the present problem, we have to consider the time (t) energy (E) uncertainty relation as generalized by Schrodinger [9] and Robertson [10] and extended by Roy and Singh and others [11–13]. Since the maximum energy in phonons of a given mode is equal to the sum of the n phonons plus the zero-point energy ($\hbar\omega/2$) of the mode (ω), and each phonon has $E = \hbar\omega$, and the cycle time is inversely proportional to (ω), then:

$$\Delta x \Delta p_x \text{ and } \Delta E \Delta t \geq (n_{r,\omega} + 1/2)\hbar. \quad (2)$$

Accordingly, the fluctuation-enhanced uncertainty in energy (the dynamic portion of the phonon that goes through zero twice a cycle) turns out to be:

$$\Delta E > (n_{r,\omega} + 1/2)\hbar/\Delta t \approx 2M_D\omega \langle A_{r,\omega} \rangle^2 / \Delta t. \quad (3)$$

It now becomes important to determine the appropriate value of Δt . Since E varies between 0 and $E_{\max}$ in $1/4$ of a cycle, the time of that maximum uncertainty should also be $1/4$ of a cycle. With $\omega = 2\pi\nu > 0.5 - 1 \times 10^{15}$ rad/s, we can assume a period of $T \sim 10^{-14}$ s and $\Delta t \sim 2 \times 10^{-15}$ s. With values of the other parameters given above, we have $\Delta E = 1.5 - 3 \times 10^{-11}$ ergs $\sim 10 - 20$ eV. This energy is very high for phonons and even for plasmons. However, when we take into account the polarization-induced dynamic, short-range, attractive forces (Eq. (A.4) in the Appendix) of the deuterium and the Pd atoms near the collision point of the lattice barrier, the value is more realistic. Furthermore, this is close to the ~ 40 eV associated with the plasma frequency of the Pd electron cloud [14].

If the preferred directions are along a linear harmonic chain (spacing = a), then with only nearest-neighbor interaction, oscillations $\omega(k) = \omega_0 |\sin(ka/2)|$ result, where ω_0 is the resonance frequency. The phonon density of this level (density of normal modes) [15] is given by $g(\omega) = 2/\pi a (\omega_0^2 - \omega^2)^{1/2}$. The number of phonons in this ‘van Hove singularity’ is limited by many things; but, populations in resonant states can still be high. By increasing the local fields and displacement amplitudes, such resonance may greatly enhance the polarization potential $V_{pp}(r)$ [16].

Tunneling probabilities in the classically forbidden region will have the form

$$P(E) = \exp\left[(-2/\hbar) \int (2M(V(r) - E))^{1/2} dr_i\right]. \quad (4)$$

Taking the above polarization and fluctuation into account, the factor $(V(r) - E)$ changes to

$$V(r) + V_{pp}(r) - \Delta E(\rho) - E, \quad (5)$$

where $V_{pp}(r) = -|\alpha|^2/2r^4$ is an attractive short-range potential (Appendix). Even for low-energy situations, where E is almost negligible compared to $V(r)$, the phonon-induced $\Delta E(\rho)$ can rise to the tens-of-eV range. The difference between this and the ~ 26 meV of room temperature energy, generally considered in such problems, may increase the tunneling probability of D–D fusion by many tens of orders of magnitude.

It is interesting that this result, when combined with the low energy, zero angular momentum corrections [4] to the normal Gamow tunneling-cross-section equation, corresponds roughly to those results predicted by the high values of ΔE (~ 400 eV) determined by low-energy deuteron-beam experiments and the uncorrected Gamow equation [17]. The researchers involved in such experiments attribute the result to screening of the D–D interactions by electrons of the embedding material. *However, theoretical calculations for conventional screening effects are only one-quarter to one-half of these experimental values.* Screening effects, addressed in the next section, are not included in these calculations above.

3. Correlated Fluctuation

Phonons, as bosons, are self-correlating when in the same mode. That is why their ability to transfer energy is additive. However, any lattice has many modes. Not being in the same state as in other modes, most phonons do not necessarily add. However, if they are correlated, they can phase lock because of the non-linearities within a lattice and become coherent. A subset of these correlated phonons, the longitudinal-optical mode, is of particular interest to us.

An example of the consequences of this coherence is pictured by considering the probabilities of deuterons penetrating the lattice barrier if their periodic motion is in phase with a periodic motion of the Pd atoms. If the phases are such that the Pd atoms are further apart [18] at the time that the D atoms are approaching the barrier, the penetration will be much greater than if either phase were reversed. If these particular phonon frequencies of the Pd and D lattices are equal, or harmonic, then the number of deep penetrations for in-phase motion is increased relative to that of non-resonant phasing.

To carry this picture into the real world, assume the motion modes are not independent. This is likely, since real potentials are not truly simple harmonic oscillators (as generally assumed in QM). The anharmonicity or non-linearity of

the modes may allow them to couple to other modes (or result from such coupling). Even anharmonic correlation of the modes will create periodic fluctuations large enough to permit fusion under the right circumstances. Such events would just happen less often than they would with harmonic correlations. If the modes are of equal or multiple frequencies, the coupling can grow and reach a folding point (something breaks). Does this apply to the LANR experiments? Two examples described below indicate that this may be so.

Experiments with laser stimulation of deuterium sub-lattice phonon modes (using beat frequencies of laser pairs to get into the correct frequency range [19]) have demonstrated enhanced heat output at specific ranges. This is expected from any model based on lattice barrier penetration by deuterons. However, stimulation of PdD by lower frequencies, e.g., those produced by complex acoustic stimulation [20] (deliberately constituted to create high-frequency overtones) and even high-frequency electrical stimulation [21] have also shown positive results.

These lower frequencies could stimulate the Pd-lattice resonant modes and thereby enhance the motion that could permit the deuterons greater access to adjacent sub-lattice sites. They could also stimulate the much higher deuteron phonon harmonic frequencies that are many multiples of the Pd-phonon and source frequencies. However, the sub-lattice frequencies that are most critical may be harmonics generated by non-linearities of the Pd phonon modes and would then have both the correct frequencies and phase relationship for enhanced deuteron transport into and across the lattice barriers.

What are the quantitative consequences of this coherent-correlation effect? Given a correlation factor ρ , where $0 \leq \rho < 1$, that increases with correlation, we find an effect on the uncertainty relation such that

$$\Delta E \Delta t = \Delta x \Delta p_x \geq \hbar/2(1 - \rho^2)^{0.5}. \quad (6)$$

This means that as correlation increases, the fluctuations in energy, time, position, or momentum increase as well. For highly correlated states in which $\rho \Rightarrow 1$, the fluctuations in position or momentum can be quite high. If the states are also coherent, then these fluctuations can seldom occur or can occur all of the time (every cycle or n^{th} cycle) depending on the phase and harmonic. If we couple the phonon effects with the correlated-coherence effects, then Eq. (2) becomes:

$$\Delta E \Delta t = \Delta x \Delta p_x \geq (n_{r,\omega} + 1/2)\hbar/(1 - \rho^2)^{0.5}. \quad (7)$$

If n is of order 10 and ρ is 0.9, the fluctuations in energy, relative to standard calculations, can increase by $\sim 20\times$. This value can be larger and readily enhanced. Specifically, the effects of proper laser stimulation of phonon modes can greatly increase $n_{r,\omega}$ and the selection, modifications, and chance correlation of material properties can be explained and shown to contribute greatly to the energy of the deuteron fluctuations within a Pd lattice.

4. Additional Effects

There are combined effects that might go beyond the non-linearities that can couple orthogonal modes. For example, if the optical modes of the Pd lattice allow the lattice barrier to be lowered at a time when the deuteron pair is approaching it, the amplitude of oscillation in that particular deuteron lattice mode may be significantly increased. The increased amplitude does not necessarily mean that the number of phonons increases in this case (Eq. (8)). The effective mass of the deuterons could be altered by the motion of the Pd lattice. Barrier penetration attributed to stochastic extremes [22] could, in fact, be a result of these coherent-correlated effects. There are so many variables in this problem that it is unlikely that theory alone will be able to determine which is most important (until experimental results point the way).

Beside the mechanical resonances that are obviously important, there are electric field effects of the phonons that may be even more important for the heat versus fragmentation balance in any resulting D–D fusion. Palladium, as a metal, clearly has many or most of its lattice atoms ionized. Hydrogen, with its much deeper ground-state energy levels, would not be ionized much, if any, of the time. However, it shares its electron with the adjacent ionized-Pd atoms. The Pd ion(s) also shares d-orbital electrons with the H atom. This results in a covalent bond sharing the H ground-state

orbital and yet leaving it with a net positive charge in the lattice [23,4]. The polarized covalent bond between the H and Pd atoms raises the average H energy level (Appendix) and population of the Pd valence electrons and therefore increases the conductivity of the material as H is added (nearly up to saturation, at $x = 1$ in PdD_x). Pd-ion and PdD-dipole phonon modes will generate oscillating electric fields. These fields interact with the H or D electrons, thereby polarizing the deuteron pairs colliding (at a Pd lattice barrier) in the longitudinal optical-phonon modes. The phonon-induced colliding motion of the H (or D) atomic pairs in the sub-lattice, means that the bound electrons, attracted to the opposing D nucleus will do more work ($W = \text{Force} \times \text{distance}$, T. Barnard, <http://www.ichaphysics.com/the-science-of-cold-fusion>) than they could without the phonon assist.^a

An aspect of this E -field interaction that ties in with the correlated-coherent phonon modes and the deep orbit is the Extended Lochon Model [24]. This model makes use of these fields to create stable hydrogen–electron pairs in an s-orbital that is momentarily, but cyclically, much below the Pd d-orbitals. This periodically decouples the D–Pd covalent bonds and creates a D^- ion within the lattice. Similarly, the fields can momentarily polarize valence electrons away from an adjacent lattice and sub-lattice location. This means that the shared Pd and D electrons shift more toward the Pd atoms leaving these D atoms/ions with a greater net positive charge. The result is a D^+D^- pair that is attractive and aids in the collision process by reducing the Coulomb barrier in size and magnitude. Thus, coupled-phonon modes, which might not appear to have any mechanical connection with the deuterons' motion toward the lattice barrier, may have a major role simply by altering the electron concentration/polarization in the right place at the right time.

The above examples provide physical intuition for the theoretical papers on coherent-correlated-enhancement [12] and anharmonic-fluctuation effects. These dynamic resonance and non-linear effects are seldom treated well in QM because they are so dependent on material properties. Therefore, it is an open question as to which is more likely to succeed in determining the best materials and conditions for LENR and LANR, theory or experiment. Here-to-fore, experiment has provided the only basis for moving forward. Only now, is there a glimmer that theory can help guide in the selections.

5. Strong-screening Contribution

In our earlier papers [3–6], we have invoked the concept of strong-screening and attraction as a result of the doubly negative lochon being present in a tight orbit about a deuteron. The advantage of this concept is that the electron effective size and orbits shrink as the colliding deuterons approach on another. They shrink for two reasons. First, the long-range Coulomb fields of the electrons and protons cancel each other more completely as they approach one another. The screened long-range monopole charge field becomes a short-range dipole field. Second, if the electrons do work on bringing the deuterons together, they move deeper into the potential well converting potential energy into kinetic energy and work. This lowers the orbit radius. At the sub-atomic level, shrinking the average electron distance from the nuclei, which determines the 'effective size' of the electron, has the greatest effect on tunneling probability by reducing the length of the nuclear-Coulomb barrier.

There is a point to our considering that electrons reduce their average distance from a nucleus just by doing work. It allows them to reach the postulated deep-electron location (at least a metastable or resonance state), which is not accessible by normal means, i.e., photon emission [25]. It is also expedient to consider that a strong-screening effect of these tightly bound electron pairs is created assuming a lochon in this deep orbit.

The local screening effect may be represented by an equation normally used to describe an 'effective charge' of a unit charge in a plasma or free electron environment:

$$e^2 \rightarrow (e_{\text{eff}})^2 = e^2 \exp(-\alpha_s), \quad (8)$$

^aWithout phonon assist, the electrons move in the atomic Coulomb potential, not the nuclei; thus, the work they do is generally negligible. If the phonons move the nuclei, then the work done by the electrons can be significant.

where α_s is the dimensionless screening parameter [26]. This α_s is not the same as the polarizability α in the appendix; however, it is very similar in both nature and effect. Values of $\alpha_s = 1, 2$, which give $e_{\text{eff}} \sim e/2$, provide screening sufficient to raise the energy level of a bound hydrogen electron pair beyond their binding energy. In the presence of the electron pair's bound double-negative charge, what is the effective charge of the deuterium nucleus as seen by another charge. Since H^- in the lattice is instantaneously stable, the paired electrons must be in a much deeper orbit or at least not provide the same value of e_{eff} as would a free-electron density giving $\alpha_s = 1.2$. However, since the lochon model requires close proximity of the second deuteron to bring the lochon to a deep orbit, the paired deuterons must already be very close together. For even instantaneous stability at this point, the new screening parameter, α'_s , is once again on the order of 1 and the effective charge of one of the deuterons (as seen by the other) is $e_{\text{eff}} \sim 0.6e$.

For the H^- and D^- lochon cases, our estimated value of $\alpha'_s (\sim 1)$, gives $e^2 \exp(-\alpha_s) = 23 \times 10^{-20} \times 0.37 \sim 8 \times 10^{-20}$ esu. Thus, to reach a micro-molecule orbit (e.g., $\sim 2 \times 10^{-11}$ cm) at which point fusion occurs rapidly, the nuclei have to climb a Coulomb barrier of energy:

$$V(R) = e^2 \exp(-\alpha_s)/R \sim 8 \times 10^{-20} \text{ esu} / 2 \times 10^{-11} \text{ cm} = 4 \times 10^{-9} \text{ erg} = \sim 3 \text{ keV}. \quad (9)$$

This is compared to the ~ 10 keV at which D–D colliding beam experiments start seeing measurable deviations from the Gamow tunneling model. The actual attraction and repulsion of the electron charges with the protons and each other must be examined in this context, since the protons will screen the electrons as well.

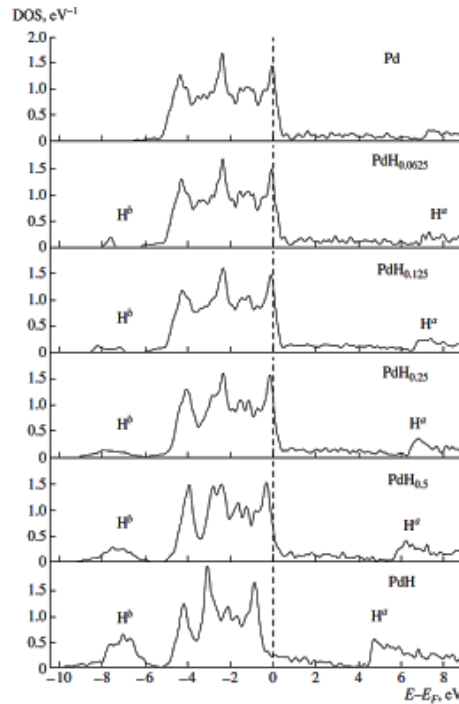


Figure 1. Density-of-states, DOS, in pure Pd and in PdH_x solid solutions for different H concentrations x . H^b and H^a are peaks corresponding to bonding and antibonding states of Pd–H ([28] with permission).

6. Conclusions

It is seen that no single mechanism can account for the D–D fusion observed in cold-fusion experiments. However, a combination of effects can explain some of the results. Individual phonons are below the 100 meV range; however, as bosons, they seek the same states and can increase the effective energy of their combined action by more than an order of magnitude. Random fluctuations of the lattice-barrier height can permit deuterons to penetrate the barrier, if they are at the right place at the right time. This is unlikely for truly random fluctuations. Therefore, it is important to seek correlated and coherent motions of the deuterons and Pd atoms within the lattice.

If the motions (phonon-induced) are both coherent and correlated, then resonance effects can greatly amplify the deuteron motions within the sub-lattice. If Pd lattice phonons are also coherent and correlated (at least harmonically) with the sub-lattice phonons, then the lattice barriers can be greatly lowered at the correct times for barrier penetration by the deuterons.

Even if the motions of the deuterons and the Pd lattice are correct for barrier penetration, the deuterons cannot overcome their nuclear Coulomb barrier without other mechanisms. The phonon electric fields can provide one of these by cyclically polarizing the deuteron electrons relative to the colliding deuterons. As a result, if the different phonon modes of both the lattice and sub-lattice allow coherent-correlated action, the bound electrons can move deeper into the nuclear-Coulomb-potential well for hundreds of orbits and shrink their orbital radius during a portion of the phonon cycle. This action leads to a strong-screening effect, or actual attraction between the deuterons, that reduces the effective charge of the nuclei and allows them to penetrate through their mutual Coulomb barrier to the attractive nuclear potential well within.

The LENR results, both from the unconventional ‘Cold Fusion’ community and the ‘conventional’ keV D–D collision work, cannot be explained by standard mechanisms. The cumulative effects on the energy barrier proposed in this paper are still small compared to those effects from standard calculations, 10s of eV vs ~ 100 eV for screening, that can enhance fusion results. And these, in turn, are small compared to the experimental values attributed to screening to explain fusion rates for low-energy ($> \text{keV}$) D–D collision experiments [17]. Therefore, there must be a difference between the random nature of screening and the actual cause of the high fusion rates observed. Reducing the randomness and ‘focusing’ the effects of the low energies available in the system appear to be key to the observed LENR results. Even these contributing factors are not likely to be sufficient unless some other mechanism is, or can be, triggered by the additional energies and mechanisms. The ability of the electron pairing (formation of the lochon), to not just overcome

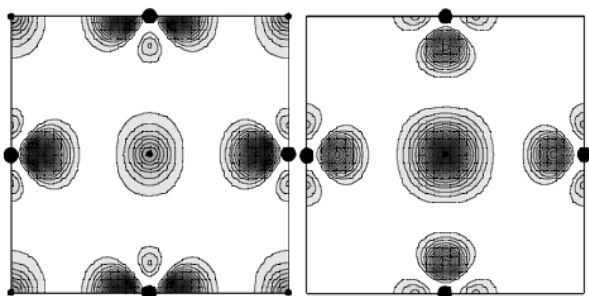


Figure 2. Maps of electron probability-density distributions for H–Pd bonding and anti-bonding states in PdH (*left panel*) and PdH 0.25 (*right panel*). The four large dots in each frame represent Pd atoms and the 5, or 1, small dots represent H atoms. ([28] with permission)

the Coulomb barrier problem but to create an attraction between deuterons under the proper conditions, would appear to be the mechanism that can explain the observed fusion rates. This mechanism also leads to answers [24] of the arguments against LENR based on known high-energy nuclear physics.

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Appendix A. Polarization and Electron-sharing Effects

In the situation of Pd loading by D (or H), one must take into account the polarizability of atoms, covalently bonded molecules, and clusters of atoms. Polarization leads to an attractive (induced-dipole) [27] potential:

$$V_{pp}(r) = -\alpha e^2 / 2r^4, \quad (\text{A.1})$$

where α is the polarizability having the dimension of volume. This will act: against the linear, hard-core, repulsive potential $V(r) = e^2/r$, between the nuclei of two interacting atoms (ions); and against the lattice barrier(s).

The tunneling probability in the classically forbidden region has the form

$$P(E) = \exp \left[-2/\hbar \int_r^R \sqrt{2M(V(r) - E)} dr \right], \quad (\text{A.2})$$

where E is the energy of the deuteron and r_o and R denote the beginning and the end of nuclear-Coulomb potential barrier. For low-energy situations, E is almost negligible. However, when we consider the lattice, the situation is much more complicated. E now includes the minimum lattice barriers $V_l(r)$ and maximum energies. The average lattice energy may be at room temperature; but, with correlated motion and fluctuations (phonons and plasmons, etc.) arising from the generalized uncertainty, instantaneous energies $\Delta E(\rho)$ can be many eV. These energies can reduce the Coulomb barrier of the nuclei and lattice (assumed to be quadratic) and contribute to bringing adjacent deuterium atoms in the lattice closer together. Localized charge distributions increase the polarization potential $V_{pp}(r)$; and the factor $(2M(V(r) - E))^{0.5}$ for free-space is now modified to:

$$2M(V(r) - E)^{0.5} \Rightarrow (2M(V_l(r) + V_{pp}(r) - \Delta E(\rho)))^{0.5}. \quad (\text{A.3})$$

The values of $V(r)$, $V_l(r)$, and $V_{pp}(r)$ are compared (Table 1) for r values (distance between the H atoms approaching a common point of the lattice barrier) from $\sim 1.4 \times 10^{-8}$ to 7×10^{-9} cm. However, even with detailed modeling [8], predictions of potentials at $< 1.6 \times 10^{-8}$ cm are not considered to be reliable. Assuming unit charges and a value of deuterium polarizability to be $\alpha = 0.68 \times (10^{-8})^3$ – not generally valid in the solid state – an approximation gives Table 1.

Table 1. Comparison of potentials in Eq. (A.3)

	$V(r)$ (eV)	$V_l(r)$ (eV)	$V_{pp}(r)$ (eV)
$r = 1.4 \times 10^{-8} \Rightarrow$	~ 7	~ 4	-1.2
$r = 10^{-8}$	~ 14	~ 4	-5
$r = 7 \times 10^{-9}$	~ 28	~ 4	-20

All of the potentials $V(r)$, $V_l(r)$, and $V_{pp}(r)$ and ΔE are cyclic, but generally at different frequencies. In this region, they are similar in amplitude as demonstrated by the ability of hydrogen to diffuse in a Pd lattice and for plasmon-induced ionization to move throughout the lattice [29].

The attractive polarization potential gives rise to forces with which the interacting atoms (ions) move towards each other.

$$F_{pp} = 2\alpha e^2/r^3. \quad (\text{A.4})$$

With heavy loading, there is breakdown of crystallinity resulting from the amorphization of the alloy along with cluster formation. This can further increase the polarization and decrease the minimum distance of approach between deuterons.

Loading the Pd lattice with hydrogen, introduces an electron s-band below the Pd d-band (Fig. 1) [28]. Hybridization of these levels satisfies the atoms by ‘filling’ both the H s-orbitals and the Pd d-orbitals. However, the electrons are more tightly bound to the H atoms, and the result is a net negative charge on the H atoms relative to the Pd atoms. But, because of the loss of electrons to the conduction band, there is positive charge on both the Pd and H atoms. This relative charge difference produces a polarizable charge dipole that responds to both plasmon and photon fields. Because of the additional covalently-bonded electron in the hydrogen orbits, its induced polarizability is also greater.

As the H content increases with loading and the Pd d-orbitals fill, the Fermi level rises. Conduction eventually (at PdH) takes place only in the Pd 5s-orbital. While H does not ‘lose’ electrons in PdH, it shares electrons in a covalent bond with Pd atoms in a manner that makes it more positive than neutral atoms. Figure 2 displays the electron configurations about the Pd atoms (large dots) and H atoms (small dots) for PdH and for PdH_{0.25}. The electron density about the H atoms in PdH_{0.25} (no H in corners) is greater than that in the PdH because, in the PdH lattice, there are fewer Pd electrons for each H to share.

Another explanation for the change in electron density about the hydrogen atoms is based on lattice strain. Until the Pd lattice is stressed by being filled, the hydrogen 1s- and the Pd 4d-orbitals do not spread sufficiently for them to overlap and share their electrons. Thus, the electrons are more confined than they are when the lattice is full.

A phonon-induced electric field can shift the shared electron(s) from one Pd or H atom (or pair of atoms) to another. Thus, H can change from bonding, H^b , to anti-bonding, H^a , states (Fig. 2). Since the charge densities differ about the H^b and adjacent H^a atoms, they will become polarizable as pairs and respond to the local fields. The H^a sites are dominant plasmon centers [29] and, if resonant with longitudinal optical-phonon modes, can have correlated-coherent effects that would greatly enhance the H–H or D–D fusion probability.

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