Model of low energy nuclear reactions in a solid matrix with defects

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This theoretical development consists of several aspects of low energy nuclear reactions, involving both established effects (such as the interaction of hydrogen, or deuterium, with defects in a lattice, e.g. palladium) and proposed solid-state effects. A known effect is the lattice concentration of electrons into local charge pairs, turning Coulomb barriers into attractive configurations. In one configuration, the proposed effect is linear defects that, when filled with hydrogen atoms, form internal lattices with no fixed lattice constant. The resulting multi-atom, linear, hydrogen molecule has a unique property shown quantum mechanically to allow di-atomic approach to within fusion dimensions.

Keywords: Defects, LENR, lochon, screening, tunnelling.

THIS article contains highlights from a number of referenced papers (starting in 1999)¹ that deal with low energy nuclear reactions in great detail. It is hoped that it will provide a useful sample of the numerous terms, conditions and concepts that have been explored and incorporated into models of the complicated system being addressed.

Low energy nuclear reaction (LENR) occurs in PdD_x (or PdH_x) after a high degree of loading by D or H. This results in degradation of crystallinity or amorphization of the system^{2,3}. It produces defect structures such as line defects near the surface in which D or H form their own linear lattice that may be somewhat independent of the lattice or, dependent, as a sub-lattice^{1,4}. The corresponding one-dimensional optical vibrational mode of the defect lattice will contain anharmonic terms also. It may be noted that, in a low-dimension structure, the potential energy between two D (or H) atoms and the resulting electron energy levels is much deeper⁵. After a suitable unitary transformation, one gets the modified single (onsite) electron energy $E_m^* = E_m - E_d$ with $E_d = g^2 \hbar w_D$, where $\hbar w_D$ is the phonon energy, and the hopping integral

$$t_{\rm mn}^* = t_{\rm mn} \exp(-g^2),$$

where g is the dimensionless electron-phonon coupling constant. As a result, the effective electron mass, $m^* =$

 $m_{\rm e} \exp[E_{\rm d}/\hbar w_{\rm D}] = m_{\rm e} \exp[g^2]$. We find that, even for $g^2 = 1.6$, this will give $m^* = 5m_{\rm e}$. The various parameters of the system become $E_{\rm m}^* = E_{\rm m} - E_{\rm d}$ and $U_{\rm e}^* = U_{\rm e} - 2E_{\rm d}$, where $U_{\rm e}$ is the Coulomb repulsion of two electrons on the same atom (D or H). We see that for $U_{\rm e} < 2E_{\rm d}$, $U_{\rm e}^*$ becomes negative. This will make the two-electron ($\uparrow\downarrow$) onsite localized pair (D⁻). Thus, to maintain local charge neutrality, we will have D⁺D⁻ neighbours. The anharmonic term strengthens the electron pair localized on one atom⁶.

The presence of D^+D^- leads to the resonance of the configuration $D^+D^- \ll D^-D^+$ as the two interacting entities come closer together. It is important to consider the screening effect of tightly bound electron pairs (these local charged bosons are the lochons)⁷. This screening can be denoted by an effective charge of the pair^{5,8}.

$$e^2 \rightarrow (e_{\rm s})^2 = e^2 \exp(-a_{\rm s}),$$

where a_s is the dimensionless screening parameter for the D⁻ and H⁻ cases; we estimate the value $a_s(r) = -1.4$. This gives

$$e_{\rm s}^2 = e^2 \exp(-a_{\rm s}) = \sim 0.25 e^2 = \sim 6 \times 10^{-20}$$
 esu.

This is a reduction in the repulsive potential between like charges. However, with the lochon bound to one deuteron and a bare deuteron in its proximity, we have to include the attraction between D^+ and D^- to the overall interaction

$$V_{\rm c}(R) = \frac{-e_{\rm s}({\rm D}^-)e_{\rm s}({\rm D}^+)}{R_{{\rm D}^-{\rm D}^+}} = -\frac{e_{\rm s}e}{R_{{\rm D}^-{\rm D}^+}}$$

For $R_{D^-D^+} = 10^{-10}$ cm, a small value only possible under special circumstances, the attractive potential is -8.3×10^{-10} erg = $- \sim 500$ eV. This value is close to that observed experimentally in low-kilo-electron volt d–d collisions⁹, where bare energetic deuterons (multi-keV) are injected into a lattice already saturated with deuterium. This value is greater than that predicted by normal screening calculations⁹, which do not involve the chargestate effects of deuterons in a solid matrix. Thus, this analysis provides a possible solution to the dilemma presented by the experimental data for these low-energy

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'hot fusion' nuclear interactions. It also provides a basis for considering much higher-than-ambient-temperature effective energies from phonon-induced deuterium and deuteron motion within the lattice.

The polarization potential, induced by local vibrational modes (e.g. longitudinal-optical phonon) of the hydrogen sub-lattice interacting with those of the phonon fields of the host lattice, can also play a significant role in countering the Coulomb barrier^{4,10}. We have $V_{pp} = 1/2\mathbf{P}\cdot\mathbf{E}$, where \mathbf{P} is the induced dipole moment which can be expressed as $\mathbf{P} = \alpha E$, where α is the polarizability of the interacting entity. This leads to an approximation of the complex, short-range, attractive, near-field relation that greatly reduces the lattice barriers separating interstitial hydrogen atoms and/or the tunnelling distance through the Coulomb potential between protons¹¹.

$$V_{\rm pp} = -\frac{1}{2} \frac{\alpha e_{\rm s}^2}{R^4},$$

R being the distance between the target and the incoming projectile. The R^{-4} dependence of the attractive potential is altered beyond the near-field, since the polarization at larger separations depends more on the lattice fields rather than the point-charge fields.

At this point, we must emphasize the tunnelling of a slow quantum wave packet through a high Coulomb barrier. This has been done long ago (in 1932) by Mac-Coll¹² and in recent papers by Dodonar and collaborators $(2002-2014)^{13}$. It has been found that the transmission probability *D* through the potential barrier is modified to

$$T = \int_{0}^{\alpha} \mathcal{D}(p) |\varphi(p)|^2 d_{\rm p},$$

where $\varphi(P)$ is the wave function of the quantum in the momentum space. It is found that even a small dispersion of the momentum can produce large increase of the transmission probability. To this effect one should consider the enhancement of tunnelling penetration probability of the Coulomb barrier by correlated fluctuations^{10,14}, and as shown by Vysotskii and Vysotskyy in p. 524.

We now briefly discuss the laser stimulation of LENR¹⁵. The penetration probability per $D^- - D^+$ interaction is given by

$$P_{\rm T} = \exp(-G),$$

where *G* is the Gamow factor, $G = e^2/\hbar v_d$, v_d being the velocity of the deuterons prior to their encountering the Coulomb barrier. The interaction cross-section σ (D⁻, D⁺) is given by

$$\sigma(\mathbf{D}^-, \mathbf{D}^+) = \left(\frac{\pi}{k^2}\right) P_{\mathrm{T}} = \left(\frac{\pi}{k^2}\right) \exp\left(-\frac{e^2}{\hbar v_{\mathrm{d}}}\right)$$

CURRENT SCIENCE, VOL. 108, NO. 4, 25 FEBRUARY 2015

This value is modified due to laser stimulation of the local phonon modes. The light-induced enhancement of interaction per $D^- - D^+$ becomes

$$P_{\rm E} = P_{\rm T}(G') \times P_{\rm oe}\left(\frac{N}{P_u}\right) = \exp[-G' + |N|],$$

where G' is the reduced-Gamow factor due to screening of the charge and |N| arises from the laser enhancement.

Summary

These models of the pairing, polarization and localization of electrons, along with laser-enhancement and correlated motion of phonon modes and atoms within a solid lattice and its defects^{4,16}, led naturally to the extended-lochon model^{17,18}. This combination answered even more questions as to how cold fusion occurs in the solid matrix and why the results differ from those predicted from high-energy nuclear-fusion experiments (see also Meulenberg's article in p. 499).

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