Evaluation of d/d Reaction Rates in Metallic Lattices as a Function of the Deuteron Energy. A Phenomenological Model of Nuclear Fusion in Solids

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Abstract. Recently, unexplained enhancements of d/d reaction rates in solids were observed. This enhancement is lower than a factor of 10 at low energies of the deuteron (a few keV) and as high as a factor of 10^{18} for extremely low energies (0,025 eV). Based on the calculation of d/d reaction rates in a lattice, a phenomenological model is proposed to infer the enhancement that can be expected for deuterons of energies in between these two extremes. A potentially interesting zone (between 500 and 2000 eV) has been identified.

1. Introduction

Recently, experiments on d/d reactions were run, in 2 zones of the reacting deuteron energy: the zone of low energy (3 to 20 keV) [1] and the zone of extremely low deuteron energy (eV level, SPAWAR heavy water electrolysis experiments [2]). In [1], the cross sections of the d/d reactions were measured using a high energy proton (deuteron) generator. In [2], track-etching detectors (CR 39 chips) were used to record tracks of high energy charged particles. The number of tracks recorded gives an estimation of the reaction rates (assuming these tracks come from d/d fusion products). In [1] and [2] an enhancement is observed compared to the calculated reaction probabilities. The enhancement factor is 2 to 10 in [1] and many orders of magnitude (10^{18}) in [2]. This was in both cases attributed to the screening effect of the electrons of the metallic lattice where the reactions take place.

In [3], the contribution to the d/d reaction rate enhancement, of an attractive Yukawa type of potential, acting between nucleons, was evaluated. Its effect was shown to be of the same order of magnitude as the screening of the lattice electrons for deuteron energies of a few keV [1]. Nevertheless, the combined effect of this potential and of the screening of the lattice electrons (150 to 300 V) was shown not to be sufficient to explain the whole enhancement [1,3]. Under SPAWAR electrolysis experimental conditions, the effect of the Yukawa potential was found to be negligible compared to the screening effect of the lattice electrons, which in turn fails by a many orders of magnitude to explain the enhancement observed [3].

A coupling between the deuterons in the target with the incident deuteron beam was thus suggested [3] to explain the enhancement observed, by fusion reactions taking place between the deuterons already trapped in the target. The consequences of this hypothesis on d/d reaction rates are examined, for energies of the incident deuteron beam varying from 2 to some 100 000 eV.

2. Evaluation of d/d reaction rates as a function of the reacting deuteron energy

Using the model developed in [3], the reaction rates and the power production resulting from the interaction of a 1 W beam of deuterons with a metallic target (palladium) loaded with deuterium (1 mmole, loading ratio 0.7), was evaluated as a function of the incident deuteron energy. For a thick target, the reaction rate r is: $r(cm^{-3}s^{-1}) = \sigma(cm^2)\varphi(cm^{-2}s^{-1})N_0(cm^{-3})$, with $\sigma\ (cm^2)$ being the reaction cross-section, $\varphi\ (cm^{-2}s^{-1})$ the deuteron flux and $N_0\ (cm^{-3})$ the deuteron concentration in the target. From [3], the reaction cross section is: $\sigma = \sigma_{geom.} P(E_d)$ with $\sigma_{geom.}$ being the geometrical cross section of the target deuteron ($\approx 0.5\, barn$) and $P(E_d)$ the probability for the deuteron of energy E_d, to tunnel through the potential barrier of the target deuterons, calculated from [3]. The probability $P_{S+Y}(E_d)$ of tunneling through the screened Coulomb potential under the influence of the Yukawa potential is $P_{S+Y}(E_d) = F_{S+Y} P_B(E_d)$, the probability of tunneling through the bare Coulomb potential being $P_B(E_d)$ (corresponding to a rate r_B) and F_{S+Y} being the enhancement factor due to the screening of the electrons and the action of the Yukawa potential. Hence, $r_{S+Y} = F_{S+Y} r_B$. The deuterons concentration n_0 (cm^{-3}) outside the target, corresponding to a deuteron flux (mass m and energy E_d (J)), depositing 1W on the target is:

$$n_0 = \frac{1}{100 E_d}\sqrt{\frac{m}{2E_d}}\ ,(cm^{-3}) \text{ corresponding to a flux: } \varphi = \frac{1}{E_d}\ \left(cm^{-2}s^{-1}\right)$$

For 1 mmole of deuterium (d) loaded in a palladium target with loading ratio 0.7:

$N_0 = 4.74*10^{22}$ (cm^{-3}, palladium thickness:127µm)

For an incident deuteron flux of 1 Wcm^{-2} and for 1 mmole of deuterium in the target, the power produced from the fusion reactions is (after correction for the target thickness):

$$W_{S+Y} = r_{S+Y}\, {}^{Q}\!/_{2}\ 1.6\ 10^{-13}*0.0127 = 7.39\ r_{s+y}\ 10^{-15}\quad \left(\text{J.s}^{-1}.\text{cm}^{-2}.\text{mmole}^{-1}\right)$$

Q= 1+ 3+ 0.83+ 2.44= 7.27 MeV is the total energy of the two main d/d fusion channels.

3. Effect of electron screening and Yukawa potential on reaction rates and energy production

The reaction rates *r* and the power produced *W*, were evaluated, for the incident deuteron energy varying from 2 to 100 000 eV. Calculations were run in two situations: bare Coulomb potential (r_B and W_B) and screened (screening energy 150 V) Coulomb and Yukawa potential (r_{S+Y} and W_{S+Y}). Results are summarized in *Fig. 1* and *Fig. 2*

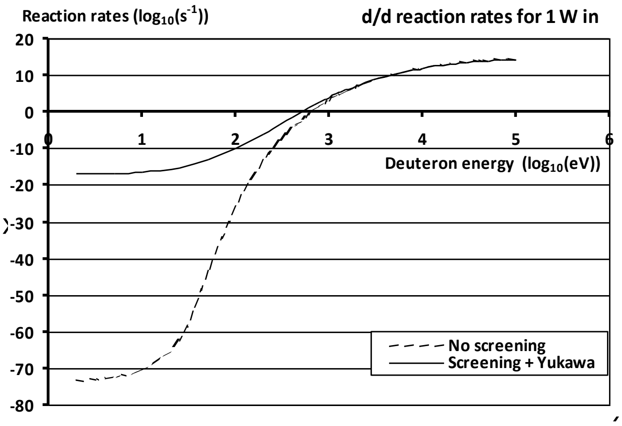

Fig. 1 – d/d reaction rates for 1W in.

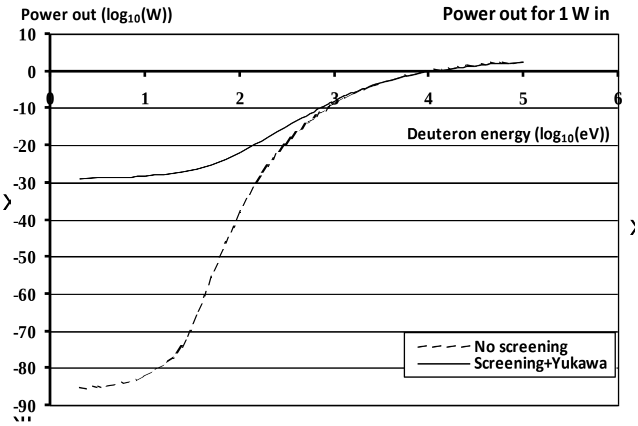

Fig. 2 – Power out for 1W in.

It can be seen from *Fig. 1*, that for deuteron of energy 0,025 eV, the reaction rates *r* without screening, are extremely low (1.32*10^{-74} reactions per second), corresponding to a very small amount of produced power *W* (1.9*10^{-88} W). Taking into account the screening effect of the electrons acting on the combined repulsive Coulomb potential and the attractive Yukawa one, considerably increases the reaction rates r_{S+Y} (7*10^{-18} reactions per second) and the power production W_{S+Y} (some 1.1*10^{-31} W). At these extremely low energies, the contribution of the Yukawa potential and of the energy of the deuteron (up to 2 to 3 eV), are negligible compared to the screening of the electrons. Anyhow, the reaction rates are still very much lower than what is observed in SPAWAR experiments (which can be estimated to be round 10^{-1} reactions per second (≈ 7*10^{4} in 1 week), assuming that the charged particles observed in SPAWAR experiments are the signature of d/d reactions. At energies of the deuteron round 2 to 3 keV, the effects of the screening of the electrons and of the Yukawa potential are of the same order of magnitude, but their combined effects do not account for the totality of the enhancement factor observed at these energies. In [3] it was thus proposed that the incoming deuteron could couple with the deuterons already present in the lattice, inducing additional fusion reactions between them. A phenomenological model based on these ideas is proposed.

4. The resonant coupling phenomenological model

4.1 The concepts that back the phenomenological model

A plasma is a globally neutral collection of free charged particles, with the same concentrations: 10^{20} m^{-3} (T≈ 10 keV) in nuclear fusion and 10^{29} m^{-3} (T≈ 3 keV) in dense astrophysical plasmas. In both cases, nuclear fusion reactions occur at a high rate, only because the high thermal energy of the hydrogen isotopes ions allows significant tunneling through their Coulomb potential barrier.

In order to measure the d/d nuclear fusion reactions rates, use is made of a deuteron gun that projects deuterons on a target loaded with deuterium, under vacuum and with a controlled energy. Recently it has been experimentally observed [1], that at low energy (3 to 20 keV) of the impinging deuteron, the reaction cross sections are increased by a factor that can reach 2 to 10 compared to what is expected from the Gamow factor at these low energies. This was attributed [1], to the screening effect of the electrons of the target. The corresponding potential was experimentally found to be as high as 500 V. It is only 150 V when evaluated from the Thomas Fermi approximation (low temperature of the deuterons) and some 300 V when considering the Debye-Hückel one (high temperature > tens of keV of the deuterons). Similar screening effect is invoked when considering the calculation of alpha disintegration constants from the tunneling of the alpha particle through the Coulomb barrier of the daughter nucleus of the decaying atom [1,4].

A screened potential naturally arises for the conduction electrons in a metal. The screening acts on the pseudo potential that the electrons of the conduction band experience from the cations in the lattice. In first approximation, this unscreened pseudo-potential is taken equal to zero for distances lower than a distance in the order of the Bohr radius and equal to the Coulomb one for distances higher. This is a semi-empirical way to simplify, in a representative way, the wave functions of the electrons in the conduction band of the metal, which mostly ignore the cations of the metal, (hence the empty lattice name of the method) [5].

The interactions of charged particles with a metallic lattice, are understood in two extreme situations:

- Extremely low energy charged particle: metallic hydrides can be viewed as the typical interaction. They have a metallic character (electrical conduction). The protons (deuterons) in the lattice are very mobile: their diffusion coefficients are very high and they move under the influence of an electrical field. In that respect, metallic hydrides can be viewed as a plasma of protons (deuterons) and electrons embedded in the lattice of the host metal. But contrary to electrons, protons (deuterons) in a lattice experience the screened full Coulomb potential of the lattice ions and not the screened pseudo-potential, resulting in potential wells at tetrahedral or octahedral sites, where the hydrogen isotopes find a stable equilibrium position. So they are not completely free to move, but the potential wells have a depth E_A (activation energy of the diffusion process) in the order of a few tenths of eV. They are thus easy to activate (acquiring an energy higher than E_A) and can thus move more or less freely.

- High energy charged particle. This is typically the interactions of an alpha particle (a few MeV energy) impinging a metallic lattice (in that case the interaction would be similar with a non metallic lattice) the alpha looses most of its energy through inelastic collisions with the electrons of the lattice (ionization, resulting in the range of the alpha measured by nuclear physicists) and rarely with the nuclei of the lattice.

- A situation much less explored, is that of a metallic lattice loaded with deuterium, submitted to a flux of deuterons of energy between say a few eV to 15 000 eV. In that case, the impinging deuteron will mainly exchange energy with the loaded deuterons, through very efficient elastic collisions (same mass). A non equilibrium situation is created where the hotter part of the deuterons partition could activate the main deuteron population, inducing movements of the deuterons in the lattice beyond the diffusion rates observed at thermodynamic equilibrium and yielding an increase of the fusion reaction rates (note that hot spots, even macroscopic, have been observed in certain experiments). Moreover, the possible focusing action of the periodic potential of the embedding metallic lattice ("conduction band" of the activated deuterons) could result in increasing the apparent geometric cross sections determining the fusion reactions rates.

4.2 Proposed phenomenological model

So far, no model exists describing this hypothetical mechanism. It is reasonable to think that it is more and more efficient as the de Broglie wavelength of the impinging deuteron increases with the decrease of its energy E_d (2 eV = 15 000 fm, 10 000 eV = 200 fm). It is thus proposed to describe this interaction by a phenomenological model: a resonant coupling enhancement factor F_C, which adds its effects to the already observed enhancements due to the electron screening (and to the Yukawa potential for low energies used in [1]). The reaction rates are given by $r_{S+Y+C} = F_C F_{S+Y} r_B = F_C r_{S+Y}$. In this concept, F_C is a function of the energy of the impinging activating deuteron. The Fermi energy E_f of the metal is likely to play a role in this mechanism. The maximum of F_C is thus hypothesized to occur at this energy. The deuteron plasma activation mechanism is rather clear in the case of deuteron gun experiments. It requires some additional hypothesis in the case of electrolysis and more generally of extremely low energy experiments. Modifications of surface and bulk conditions (cracks) of the cathode during electrolysis, conditions of preparation of the cathode (metallurgy and pretreatment, size and morphology of the small metal particles when supported on a porous dielectric material etc…) forced diffusion of deuterons through the embedding metal, could provide explanations for the formation of a hot population of deuterons of energy E_d of a few eV.

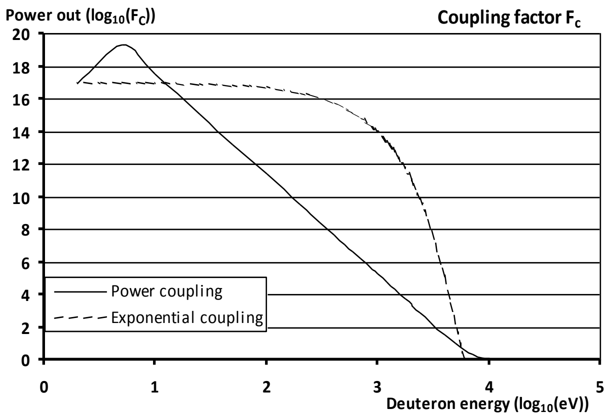

Fig. 3 – Coupling factor F_C.

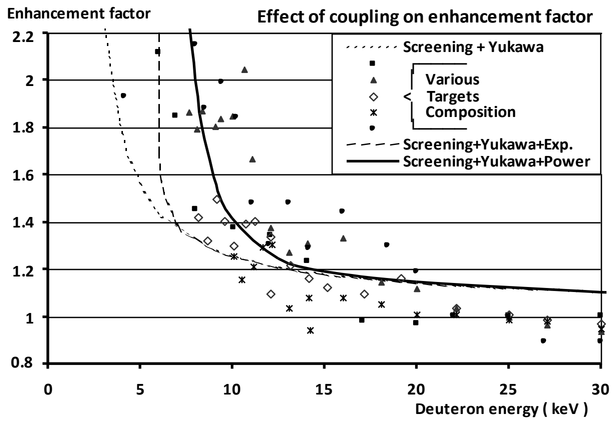

Fig. 4 – Effect of coupling on enhancement factor.

The coupling invoked in [3] could thus be a general phenomenon, extending form extremely low energies (a few eV) to low energies (a few keV) of the deuteron. To define the coefficients of the resonance coupling curve, use is made of the experimental results given by [1] and [2]. In the case of [1], an additional enhancement factor (F_C) of 6 is required for E_d = 5500 eV (see *Fig. 4*). From the experimental results of [2], a reaction rate of 10^{-1} s^{-1} can be inferred. In that case, the energy of the activating deuterons is supposed to be 2 eV. The corresponding calculated (screened) reaction rate $r_{S+Y} = F_{S+Y} r_B$ is $1.3*10^{-17}$ [2], requiring for F_C a value F_C *(2)* = $8.14*10^{16}$, giving $r_{S+Y+C} = F_{S+Y+C} r_B = 0.1\ s^{-1}$. Two coupling laws have been examined: a power law and an exponential one.

4.3 Determination of the coupling factor F_C as a function of E_d

4.3.1 Power coupling: in that case, $F_C = 1 + \lambda \left(E_d / E_f \right)^{\pm n}$, + for $E_d \le E_f$ and - for $E_d > E_f$

λ ($2.24*10^{19}$) is determined by the condition F_c*(2)*= $8,14*10^{16}$ and n (6.13) by the condition F_c (5500)= 6.

4.3.2 Exponential coupling: in that case: $F_C = 1 + \lambda' \exp\left(-n' \left(\left| E_d - E_f \right| / E_f \right) \right)$

λ' ($8.31*10^{16}$) is determined by the condition F_C *(2)= $8.14*10^{16}$* and n' (0.034) by the condition F_C (5500)= 6. The two laws are shown on *Fig. 3*

5. Effect of the coupling on reaction rates r_{S+Y+C} and power production W_{S+Y+C}

Fig. 5 and *6* give the result of the calculation of r_{S+Y+C} and W_{S+Y+C} , for both coupling laws.

The parameters of both laws have been computed to fit the experimental data at extremely low (2 eV) and low (5500 *eV*) energy of the deuteron. As can be seen in *Fig. 4* the fitting is not very good, for the exponential law at low energy of the deuteron (5500 eV). The power fitting is better (*Fig. 4*). This could be a consequence of the non thermodynamic equilibrium of the populations of deuterons in the lattice. The objective of the phenomenological model is to infer the behavior of the deuterons in the lattice for all energies E_d, from the 2 extreme and experimentally known situations (E_d = 2 eV and 5500 eV). *Fig. 5* shows that the reaction rates

r_{S+Y+C} are significantly increased by the power coupling when compared to the “Screened + Yukawa” reaction rates r_{S+Y} . Values as high as 10^5 to 10^{10} s^{-1} are predicted, for E_d between 500 and 1000 eV, whereas in this zone, r_{S+Y} vary from 1 to 10^5 s^{-1}. It is thought that this energy window could be used in a research program, to optimize the target characteristics. From results presented in [1] it can be seen that the enhancement factor varies very much with the target used. These variations are of much bigger amplitudes than the standard deviations presented in [1]. They can be attributed to the exact characteristics of the target used, hence opening the possibility for optimization. This optimization could be done, by using as an optimizing criterion the neutron emission of the studied targets. This emission is predicted to be significantly higher than the background against which the optimization would done, the calculated r_{S+Y} emission rate. This optimization could result in a very significant increase of the enhancement factor.

Fig. 6 shows that the reaction rates r_{S+Y+C} are considerably increased by the exponential coupling. From *Fig. 3*, it can be seen that this type of coupling is not representative for energies E_d of the deuteron higher than some 3 keV. It cannot be excluded that with the decrease of the energy, the exponential coupling becomes more and more representative (less departure from thermodynamic equilibrium) and that the true coupling is in between power and exponential for lower values of E_d.

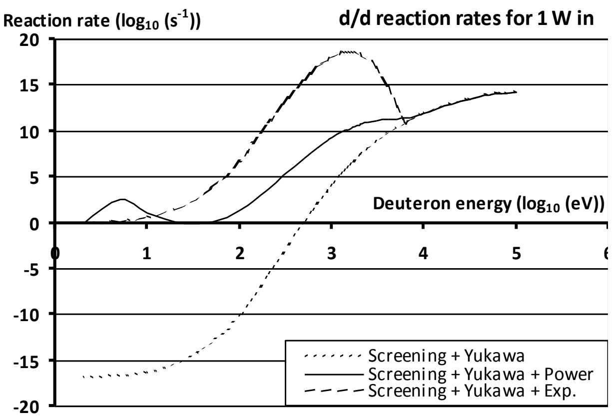

Fig. 5 – d/d reaction rates for 1 W in.

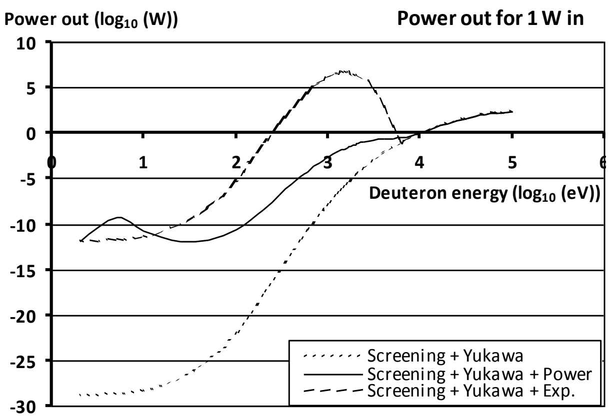

Fig. 6 – Power out for 1 W in.

6. Conclusion

Because of the development of surface treatment and electronic industries, ion generators of several kW power are now available on the market. They can produce ion (proton, deuteron) beams of high intensity (several A), with ion energies in the range 100 to 4000 eV and are thus able to work in the 500 to 1000 eV energy window. Technological devices can be imagined, to generate energy by bombarding appropriate targets with such ion beams.

It is thought that much of the work done in the field (on the cathodes physico-chemical characteristics), could be used to test the possibility of this hypothetical coupling. Such materials could be good candidates as targets for this last approach. A prototype has been built in the lab, using a two steps glow discharge to generate the ions and able to produce currents up to some tens of µA [6]. The energy of the ions is in the order of hundreds eV and the hydrogen (deuterium) pressure at the level of the target is 3 to 4 Pa. A neutron detector (helium 3) monitors the fusion reactions that are expected. Experiments will be run to define precisely the requirements for a lab scale ion generator based on a µwave discharge. Finally, more insight could also be gained on what happens in the extremely low energy region (<2 eV).

7. References

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