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Study Of Lattice Potentials On Low Energy Nuclear Processes In Condensed Matter

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1. Introduction

The phenomena of anomalous heating effects in deuterated metals gained worldwide attention through the famous announcement of "cold fusion" in 1989. Recently, a number of experiments have identified nuclear reaction products that are attributed to hydrogen or deuterium interaction with the host metal. Consequently workers have renamed this field as "Low Energy Nuclear Reactions in Condensed Matter". This work has used a variety of configurations and a variety of loading techniques giving reaction products ranging from Helium-4, Tritium, to an array of heavy elements.

The mounting evidence that soft X-rays and energetic particles are revealed during LENR experiments pushed to consider that lattice potentials can have a significant role in the nuclear processes occurring in condensed matter at low energy. Local potentials in the order of some

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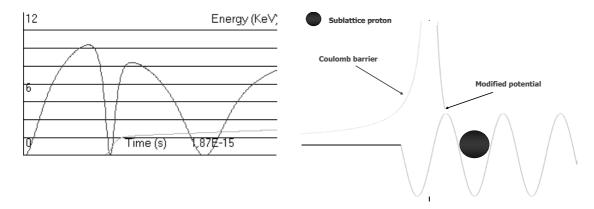


Figure 1. Energy evolution of an **Figure 2.** Modified potential due to an energetic hydrogen isotope confined in oscillating electric field Pd lattice (theoretical result)

tenth of keV and ions having energies within such a range have been predicted (see fig. 1) [1,2] by means of a theoretical picture proposed by some of the authors.

The present study has been carried out within a cooperative frame involving ENEA, University of Illinois and SRI.

In a condensed matter, at high densities, the effects of electron screening become so relevant that rates of nuclear reactions at relatively low temperature take on considerable magnitude independent of the temperature (*pycnonuclear* reactions). In addition to those screening effects by electrons, strong spatial correlation between atomic nuclei in dense matter due to their mutual Coulombic repulsion tends to enhance the rates of reactions through an effective reduction of the overall internuclear repulsion [3-10]. In our model we consider that the basic mechanism is a charge separation effect, due to the coherent oscillations of the Fermi Level (FL) electrons, that creates an intense oscillating electric field in the sublattice (i.e. within the lattice cell).

However, even if the e.m. triggering is produced at the surface of the hydrogenated metal also a region of the bulk is involved in the process, at least some hundreds of angstrom.

Simple calculations taking into account the electron density at the FL show that the local field can reach values of about 1E+13 V/m, at a frequency ranging between 1E14 and 1E15 1/s.

Such a signal can be seen only by particles having an energy enough to do that, i.e. the hydrogen isotopes going into the sublattice. As matter of fact the energy required for hydrogen to jump into the sublattice is around 0.45 eV for Pd and Ni. The corresponding frequency is in the range 1E14 - 1E15 1/s.

Hydrogen isotopes in Pd or Ni lattices may be considered as ions since their electronegativity is much less than the metal atoms one. Ions entering the sublattice, with a proper phase, feel the field created by charge separation and are accelerated achieving energies up to 10 keV or more. The shape, the frequency and the amplitude of the signal control the energy gained by the particle.

We have studied such an effect with the CLAIRE code that performs a calculation of the trajectories of the particles under several conditions within a 3D environment [1,2].

The particle dynamics simulation showed that frequency and amplitude of the oscillating field in the lattice are strongly affected by the electronic status for the system under study.

Distribution of the energy of the particles has been estimated in the computations, so that we have seen, in some conditions, that a significant fraction of the particles can gain an energy, let us say in the order of 10 keV (peak around 6 keV). Particles can be accelerated, by the field, in one direction or in the opposite one and a particle passing from one cell to the other can increase or decrease its energy depending on the phase there. A trapping mechanism occurs due to the local field into the lattice.

Generally speaking we can say that the effect produced by thermalization in our case is produced by the signal phase for particles entering the sub-lattice.

Then the proposed picture allows us to define two populations of particles 1) "Target particles" at the rest (metal atoms or hydrogen isotopes within sub-lattice sites 2) "Shot particles" at some keV.

Then the effect of the periodic potential can be neglected because of the higher energy level of the "shots" that may be considered as free particles in the sublattice scale.

Plasmons-polaritons are coherent oscillations of FL electrons, so that we can estimate a coherent domain in the order of 100 - 1000 A for the e.m. field.

The density number of shots can be estimated by means of the Boltzmann statistic, by considering that only particles having ~ 0.45 eV may enter the sublattice. Such a condition allows roughly 1E+14 (protons/deuterons)/cc to enter the sublattice and give rise a temperature effect on the excess of power production for D-D in Pd that is in rough accordance with the experimental data [1,2].

This is, in a few words, the proposed picture of a condensed matter plasma as statistical system of charged particles.

I addition it has been observed, by means of the CLAIRE code, that the flight time of the shots are very close to the oscillation period of the FL electrons, so that one may assume that a significant fraction (calculated by a Montecarlo option of CLAIRE code) of the shot particles is tuned with the negative signal of the field, then a screening effect turns out. We used such a picture to estimate an effective screening length.

Oscillating local potentials, created by separation of charges (due to plasmons-polaritons), within the range of the energy of the observed soft X-rays have been considered to produce a modified potential for the Gamow factor calculation, so that an effective short distance screening length has been estimated for protons interacting with metal atoms. Fig. 2 shows the modified potential. One may assume that such potentials are screening a charged particles, e.g. proton impinging an heavier nucleus, if the charged particle travels tuned with the negative phase of the e.m. signal.

The interaction Hamiltonian, for the energy transfer mechanism, is calculated through the minimal coupling by assuming the single particle approximation to calculate the nuclear current. The product A x J results to be significant because of the amplitude of the field that makes the potential vector large enough.

The lattice is considered as an infinite reservoir and is not involved in the calculation of the matrix element on the basis of the approximation that the lattice doesn't change dramatically from the initial to the final state [1,2]

An approach based on statistical physic of dense plasmas is proposed to have an estimate of the reaction rate between the hydrogen isotopes loaded in the lattice and the metal atoms.

In the past it has been emphasized that the features of nuclear reactions in dense matter differ in a fundamental way from those in a low density environment, since the joint probability densities

between reacting nuclei at nuclear reaction distances, the quantities representative of the tunnelling probabilities through the Coulombic barriers, are affected sensitively by the internuclear correlation, as well as by the screening action of dense electrons. Treatments of such joint probability densities and the resultant pycnonuclear rates depend crucially on the quantum-statistic of the reacting nuclei.

The scope of the computations described in the paper is to have indicative values for reactivity under the considered hypothesis.

2 Nuclear Reactions

The system under study, of reacting nuclei in condensed matter, may be traced back to a binary ionic mixture (BIM) with mass density ρ_m , pressure P and temperature T, consisting of nuclear species with charge number Z_i , mass number A_i , and molar fraction x_i (i=1,2). The thermonuclear reaction rate is given by:

$$R_{ij}^{s}(\rho_{m},T) = \frac{2n_{i}n_{j}}{I + \delta_{ij}} S_{ij}(E_{eff}) \sqrt{\frac{2}{\pi\mu_{ij}k_{B}T}} \cdot \left\{ w_{ij}^{T}(\rho_{m},T) R_{ij}^{T}(\rho_{m},T) + w_{ij}^{p}(\rho_{m},T) R_{ij}^{p}(\rho_{m},T) \right\}$$
(1)

where

$$R_{ij}^{T}(\rho_{m},T) = \frac{2\sqrt{\pi\tau_{ij}}}{3} exp\left[-\tau_{ij} + \frac{E_{s}}{k_{B}T} \frac{\tanh(\tau_{ij}^{2}/9s_{ij}^{2})}{\tau_{ij}^{2}/9s_{ij}^{2}} \left[1 - \tanh\left(\frac{3}{2\tau_{ij}} - \frac{\tau_{ij}^{2}}{12s_{ij}^{2}}\right)\right]\right]$$
(2)

is the thermonuclear reaction rate and

$$R_{ij}^{P}(\rho_m, T) = \sqrt{\frac{\pi k_B T}{4E_s + \pi k_B T}} \cdot exp\left(-\pi \sqrt{\frac{D_s}{r_{ij}^* (I + \pi k_b T / E_s)}}\right)$$

$$\tag{3}$$

is the pycnonuclear reaction rate, $w_{ij}^{T,P}(\rho_m,T)$ are the weighting factors for thermonuclear and pycnonuclear reactions:

$$w_{ij}^{T}(\rho_{m},T) = \frac{\exp[-(\tau_{ij}/2s_{ij})^{2}/2]}{I + \exp[-2(\tau_{ij}^{2}-30)]}, \quad w_{ij}^{P}(\rho_{m},T) = I - w_{ij}^{T}(\rho_{m},T)$$
(4)

$$s_{ij} = \frac{\pi}{2} \sqrt{\frac{D_s}{r_{ij}^*}}, \qquad r_{ij}^* = \frac{\hbar^2}{2\mu_{ij} Z_i Z_j e^2}, \qquad \tau_{ij} = 3 \left(\frac{\pi^2 E_G}{4k_B T}\right)^{1/3}, \quad E_s = \frac{Z_i Z_j e^2}{D_s}$$
 (5)

 S_{ij} is the astrophysical factor, n_{ij} the reacting nuclei densities, δ_{ij} the Konecker's delta distinguishing between the cases with $i \neq j$ and i = j, E_G the Gamow energy, μ_{ij} the effective mass of the colliding nuclei and D_s the short length screening distance.

3 Enhancement Factors

In addition to the screening effects of electrons manifested in the reaction rate (1), Coulombic cohesive effects between atomic nuclei in dense matter act to enhance the reaction rates through the effective reduction of internuclear repulsion.

The rates of nuclear reactions are proportional to the statistical averages of the penetration or contact probabilities, $|\Psi_{ij}(0)|^2$, which are the joint probability densities, $g_{ij}(r)$, between nuclei i and j at a nuclear-force distance, $r = r_N$ (zero separation point).

Enhancement factors for thermonuclear rates have been evaluated through quantum statistical calculations of such joint probability densities [8], [11], [12] in the form

$$A_{ij}^{s}(\rho_{m,T}) = exp(Q_{ij}^{s})$$

$$\tag{6}$$

where [7-8]

$$Q_{ij}^{s} = \beta H_{ij}^{s}(0) - \frac{5}{32} \Gamma_{ij}^{s} \left(r_{TP}^{s} / a_{ij} \right)^{2} \left| 1 + \left(C_{1} + C_{2} \ln \Gamma_{ij}^{s} \right) r_{TP}^{s} / a_{ij} + C_{3} \left(r_{TP}^{s} / a_{ij} \right)^{2} \right|$$
(7)

$$C_1$$
=1.1858, C_2 =-0.2472, C_3 =-0.07009 (8)

$$a_{ij} = \frac{1}{2} \left[\left(\frac{3Z_i}{4\pi n_e} \right)^{1/3} + \left(\frac{3Z_j}{4\pi n_e} \right)^{1/3} \right]$$
 (9)

$$\Gamma_{ij}^{s} = \Gamma_{ij} \exp\left(-\frac{a_{ij}}{D_{ij}}\right); \quad \Gamma_{ij} = \frac{Z_i Z_j e^2}{a_{ij} k_B T}; \quad r_{TP}^{s} = D_s \left(1 - \frac{D_s}{2\Gamma_{ij} a_{ij}}\right); \tag{10}$$

$$D_{ij} = 14.83 + 1.31 \ln \Gamma_{ij}, \qquad \beta H_{ij}^{s}(0) = 1.148 \Gamma_{ij}^{s} - 0.00944 \Gamma_{ij}^{s} \ln \Gamma_{ij}^{s} - 0.000168 \Gamma_{ij}^{s} \left(\ln \Gamma_{ij}^{s} \right)^{2}$$
(11)

The condition to have a strong screening is:

$$T \ll T_{cs} \,, \tag{12}$$

where

$$T_{cs} = \frac{2}{\pi} \left(\frac{r_{ij}^*}{D_s} \right)^{1/2} \frac{Z_i Z_j}{k_B D_s} . \tag{13}$$

If the condition (12) is not satisfied we are dealing with a weak electron screening process so that

$$A_{ij}^{e} = exp\left(Q_{ij}^{e}\right) \tag{14}$$

$$Q_{ij}^{e} = \langle Z \rangle^{1/3} \frac{a_{e}}{D_{s}} \left\{ I - I.057 \frac{D_{s}}{a_{ij}} \left[I - exp \left(-\frac{a_{ij}}{D_{s}} \right) \right] \right\} \Gamma_{ij} + \left[0.342 - 0.354 exp \left(-\frac{3\Gamma_{ij}}{\tau_{ij}} \right) \right] \Gamma_{ij} \frac{3\Gamma_{ij}}{\tau_{ij}}$$

$$- \frac{3}{8} \left(\langle Z \rangle^{1/3} \frac{a_{e}}{D_{s}} \right)^{2} \Gamma_{ij} \frac{3\Gamma_{ij}}{\tau_{ij}} + 0.09I \left(\langle Z \rangle^{1/3} \frac{a_{e}}{D_{s}} \right)^{2.923} \Gamma_{ij} \left(\frac{3\Gamma_{ij}}{\tau_{ij}} \right)^{1.897}$$

$$(15)$$

being

$$\langle Z \rangle = \sum_{i} x_i Z_i , \quad a_e = \left(\frac{3}{4\pi n_e}\right)^{1/3}$$
 (16)

 x_i and n_e denoting the molar fraction of the i nuclei and the electron density respectively.

In order to calculate the reaction rate for LENR in condensed matter an estimate of an effective value for the screening distance is required. If a dynamic condition in the lattice is considered, where charge density oscillation produces a screening potential, due to the oscillating electric field, the effective value of the screening distance may be calculated.

The effective electron density, in general, may be calculated by the D_s value by resolving the following equation:

$$\frac{a_e}{D_s} = 1.23r_s^{\nu} \left(\tanh\frac{1.061}{\theta}\right)^{\frac{1}{2}}$$

if $r_s < 1$ and $\theta < 0.01$, where

$$v = \frac{0.435 + 0.024\theta^{2.65}}{1 + 0.048\theta^{2.65}}; \quad \theta = \frac{2m_e k_{BT}}{\hbar^2 (3\pi^2 n_e)^{2/3}}; \quad r_s = \frac{m_e e^2 a_e}{\hbar^2}$$

Notice that for relativistic electrons

$$\frac{a_e}{D_s} = 0.1718 + 0.09283 \cdot r_u + 1.591 \cdot r_u^2 - 3.8 \cdot r_u^3 + 3.706 \cdot r_u^4 - 1.311 r_u^5$$
where $r_u = 10r_s$.

Screening Distance

In dense systems D_s is a function of the electron density, in the case under study one may estimate an effective screening distance on the basis of the effect of local potentials created by electron density oscillations within a lattice (e.g. plasmons-polaritons).

A simple way to estimate D_s is given by the following relationship:

$$E_{s} = \frac{Z_{i}Z_{j}e^{2}}{D_{s}} \tag{17}$$

We may consider a screening potential in the order of the experimentally observed e.m. emitted signals (some tenths of KeV, close to the calculated values [1,2]), by assuming a proton colliding with an ion having a charge $Z \sim 30$: a screening distance in the order of 10^{-10} cm turns out. The alternative is to consider the screening effect on the Gamow factor.

The expansion in partial waves leads the cross section expression for the reaction between the particles 1 and 2 for the l^{th} partial wave [13]

$$\sigma = \pi \lambda^2 (2l+1)T_l(E) \tag{18}$$

where

$$\lambda = \frac{\hbar}{(2\mu_{ii}E)^{1/2}} \tag{19}$$

is the reduced De Broglie wave length and T_l is transmission coefficient inside the nucleus.

At low energy (typically E << 100 KeV) the energy dependence of σ is dominated by the transmission coefficient T_l , which is basically proportional to the tunneling factor across the interaction potential U,

$$U = V + \frac{\hbar^2}{2\mu_{II}} \frac{l(l+I)}{r^2}$$
 (20)

where l is the relative orbital momentum; for l=0 (s-wave scattering) T_l is only determined by the potential V, while for l > 0 T_l depends on the centrifugal potential too.

The transmission factor T_l can be written in the form

$$T_l \approx C_l e^{-2G_l} \tag{21}$$

 C_l is a factor approximately independent on the energy and

$$G_{l} = \frac{(2\mu_{ij})^{1/2}}{\hbar} \int_{R_{i}}^{R_{o}} (U - E)^{1/2} dr$$
 (22)

is the so called Gamow factor; here R_i and R_o are the inner and the outer classical turning points, respectively, associated with the potential U (i.e. the points such that $U(R_o)=U(R_i)=E$); R_i is in the order of the nuclear radius 3-6 10^{-13} cm.

For $l\neq 0$ but not too large

$$G_{l} = G_{o} + \sqrt{l(l+1)} \left[ln \left(\frac{4l(l+1)a_{N}}{R_{i}} \right) - 2 \right]$$
(23)

$$a_N \equiv \frac{\hbar^2}{2\mu_{ii}Z_1Z_2e^2}$$

It is evident from Eq. (21) and Eq. (23) that at low energies the cross section for $l\neq 0$ is depressed for several order of magnitude with respect to the s-wave, l=0, cross section.

A modified potential can be assumed for the case under study where we consider an effective screening length in the order of 10^{-10} cm. Considering that the region closed to the nucleus is traceable to the vacuum we can assume the vacuum dielectric constant so that the resulting expression for the potential with screening is

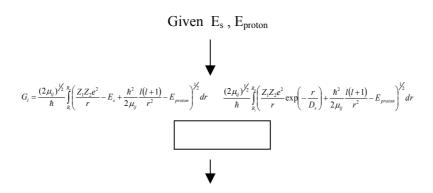
$$U = V' + \frac{\hbar^2}{2\mu_{ij}} \frac{l(l+1)}{r^2}$$
 (26)

where

$$V'(r) = \frac{Z_1 Z_2 e^2}{r} - E_s \tag{27a}$$

$$V'(r) = \frac{Z_1 Z_2 e^2}{r} exp\left(-\frac{r}{D_s}\right)$$
 (27b)

Assuming a value for E_s as above and an energy value for the shot particle in the order of the considered lattice potentials (~10 KeV) one may calculate the Gamow factor by using eq. (26) and (27a) with eq. (22) and then evaluate D_s by iterative calculation of eq.(22) by using eq. (26) and eq. (27b). Values of D_s in the order of 10^{-10} cm are calculated again. Similar values can be also obtained by using the tunnelling probability relationships for screened and not screened systems [10]. Figure 3 shows the calculation scheme; Fig. 4 shows the behaviour of the screening length as function of the screening potential in the lattice. Figure 5 shows the effect of the screening distance on the Gamow factor by considering 10, 20 and 30 KeV as values of the energy of a proton impinging a target Ni nucleus. It turns out that the barrier is reduced of 30-40 orders of magnitude.



Effective screening Length

Figure 3. Screening distance calculations scheme

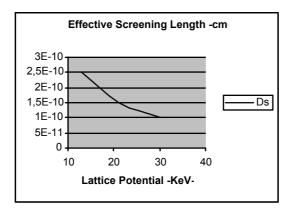


Figure 4. Screening length Vs lattice potential

5. Energy transfer mechanism to lattice

Mechanism for direct energy transfer to the lattice by coupling with the lattice e.m. field created by the electron oscillations has been proposed for nuclear process in condensed matter by some of the authors [1,2]. Transition from an excited status of the composite nuclei can be approached in similar way leading to the conclusion that proton capture reaction, in principle, may decay also without any emission of radiation in condensed matter since the energy is transferred to the system as lattice thermal vibration. For a *d wave* process the following relationship has been found for decay probability [1]

$$\left|a_{fi}\right|^2 \simeq \gamma^2 \left[3 - 2(\cos(\omega_{10}T) + \sin(\omega_{10}T))\right] \tag{28}$$

where

$$T \cong \frac{1}{(\omega_{\theta} - \omega_{I})}, \qquad \omega_{\theta I} = \omega_{\theta} - \omega_{I}, \qquad \gamma = -\frac{1}{\hbar^{2}} \frac{a^{2}}{(\omega_{\theta} - \omega_{I})^{2}} \quad \text{and} \quad a = \langle I | H_{I} | \theta \rangle$$
 (29)

$$\langle I|H_I|0\rangle = \frac{eA_0}{m} \langle I|\hat{p}|0\rangle \tag{30}$$

$$\langle I|\hat{p}|0\rangle = \frac{1}{i\hbar} m\langle I|\hat{r}H - H\hat{r}|0\rangle = im(\omega_I - \omega_0)\langle I|\hat{r}|0\rangle \tag{31}$$

(the considered characteristic length of the system is the nuclear radius) so that the transition probability results to be a function of the amplitude/frequency ratio of the e.m. signal in the lattice A similar calculation leads the following relationship for a *p wave* decay process.

$$\left|a_{fi}\right|^{2} = \frac{2}{\hbar^{2}} e^{2} A_{0} \omega_{fi}^{2} R_{0}^{2} \frac{\sin^{2}(\omega_{fi}/2)}{\omega_{fi}^{2}}$$
(32)

In this case also the probability is a function of the amplitude/frequency ratio of the e.m. signal in the lattice.

6 Results

Experiments [16] showed a strong shift in the isotopic composition of Cu giving a decreasing of the 63 Cu/ 65 Cu ratio, from the natural value (2.25) up to 0.165 on thin Ni films undergone to electrochemical loading of protons. An estimate can be done, on the basis of the experimental data, about the apparently observed reactivity for p+ 64 Zn \rightarrow 65 Cu reaction. The knowledge of the cross section factor Sij is required in order to apply eq.(1) for the reaction rate calculation. An estimate of Sij for a certain energy can be done on the basis of known values of the reaction cross section by means of the following relationship

$$\sigma_{ij}(E) = \frac{S_{ij}(E)}{E\left\{exp(\pi\sqrt{E_G/E}) - 1\right\}}$$
(33)

Since the cross-section factors are the quantities intrinsic to the nuclear reactions and thus should not be affected by the features of electronic and atomic configurations, in our conditions, we may write the eq.(33) as [8]

$$\sigma_{ij}^{s}(E) = \frac{S_{ij}(E)}{\sqrt{E(E+E_s)} \{exp(\pi\sqrt{E_G/E+E_s}) - 1\}}$$
(34)

Cross section DataBase are available for proton capture reaction up to energies of 200 KeV (i.e NOT-SMOKER DataBase http://quasar.physik.unibas.ch/~tommy/reaclib). Eq. (34) allows to calculate the factor for the known cross section values, then, since S_{ij} doesn't change too much with energy, the astrophysical factor S_{ij} may be extrapolated at lower energies (10-30 keV) in order to have a rough calculation of the reactivity for the system under study.

The hydrogen sublattice population density is estimated by means of the Boltzman distribution for an activation energy of 0.45 eV, that is the typical activation energy for hydrogen jumping in Ni lattice.

Since the signal of the considered isotopes (63 Cu, 65 Cu) is in the order of a factor 10 above the detection limit of the used SIMS instrument, a 65 Cu concentration of about 10^{15} - 10^{16} atoms/cm³ may be estimated after the experiment. So that it turns out that in the whole film the number of Cu atoms are roughly 10^{10} .

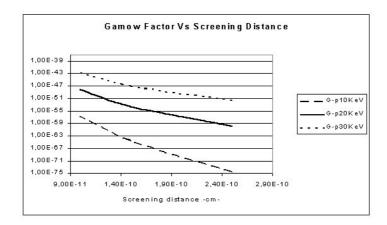


Figure 5. Gamow factor Vs screening distance

Since the experiment elapsed time is about 10⁴ s a conservative reaction rate of 10⁶ atoms/s can be estimated.

In order to estimate the reaction rate the particles dynamics has been studied within a Montecarlo loop leading a distribution of the proton energy in the reaction zone. Since a Maxwellian distribution has been assumed for reaction rate (eq. (1)) a chi-square test has been performed obtaining a satisfactory agreement between the calculated and expected distribution. Fig. 6 shows both the distributions. A binning has been performed with the calculated energy distribution to estimate the reaction rate.

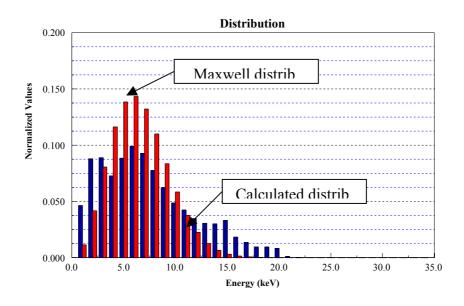


Fig. 6 Comparison between the calculated and Maxwell distribution

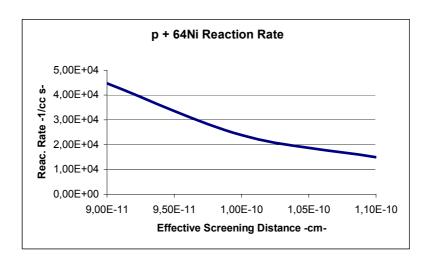


Figure 7. Reaction rate for ⁶⁴Ni proton capture reaction

The reaction rate values shown in Fig.7, calculated for an effective screening distances around $1.0 ext{ } 10^{-10}$ cm that are corresponding to potentials in the lattice in the order of 10^{1} KeV, do not differ dramatically from the experimental ones.

The approximated model may indicate a region of parameters that gives a non zero probability to have reactions in the considered scenario.

Calculations show that the Gamow peak is around 33 keV, not far from the considered energy range. An important effect of the screening at low energies (order 10 keV) turns out, but such an effect disappears at higher energies. The reason is that the effective screening length is estimated on the basis of a screening potential, so that if the particle energy exceeds over the screening potential value the enhancement effect vanishes.

Such a behaviour coupled with the distribution function values, for energies exceeding 30 keV, makes the reaction rate not affected by particles belonging to the tail.

An estimate of the energy released by the energetic particles to the lattice (taking into account the phonon exchange probability) shows that the exchanged power is in the order of some hundreds of mW, as upper limit.

Conclusions

The proposed model describes the system as traceable to a dense solid state plasma leading picnonuclear reactions of proton captures in presence of lattice potentials in the order of 10^1 keV , theoretically predicted to be in the order of 10 keV [14-15] and experimentally observed towards X-Ray measurements (the proposed picture could be also applied to different approaches for estimating the effective screening distance). The calculation results show that the reaction rate estimated on the basis of the experiments [16], in the proposed picture, may be achieved with potentials (and energies) in the lattice in the order of 10^1 keV instead of MeV as in vacuum. The calculated reactivity is in reasonable agreement with the value estimated on the basis of the SIMS analysis performed on hydrogenated Ni thin films [16].

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