2	Determination of Cross Section for Different Fusion Reactions in Terms of Lattice Effects in Solid State Internal Conversion for Different metallic
3 1	Lattice Effects in Sond State Internal Conversion for Different metanic Crystalline Environments
4	Crystanne Environments
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9	Abstract
10	In present paper, the cross section for $D(d,p)T$, $D(d,\gamma)^4He$, $T(d,n)^4He$ and $D(p,\gamma)^3He$ fusion reactions in
11	terms of the lattice effect in solid state internal conversion for different structures and different metallic
12	crystalline environments in comparison with palladium environment has been determined. Elements that
13	we used in this article are Ni, Ru, Rh, Pt, Ta, Ti, Zr,which arecontained FCC, BCC and HCP lattice
14	structures. Fusionable particles are solved as a sublattice in mentioned crystalline
15	metals.Fusionreactionsare generated by flux of incoming fusionableparticles.We took lattice effect part
16	into our calculations with regarding the Bloch function for the initial and final state of three body system.
17	Three-body system involved the host lattice, sublattice and incident particles. The cross section to
18	perform each fusion reaction inside different metal is computed using the state of initial and final system.
19	Then our resultsfor cross section of different metal are compared with palladium metal. Finally, the solid
20	state internal conversion coefficient is obtainedby considering the lattice effect.

21 *Key words*: internal conversion, fusion cross section, lattice effect in solid state internal conversion

22 **1. Introduction**

1

Nowadays using nuclear energy is very important as a clean source of energy. There are two kinds of nuclear reactions, fusion and fission. Since fusion reaction has less radioactive radiation and the fusion fuels required for these reactions are more sufficiently available in the nature, therefore fusion reactions are important to study.

In 1995, many experimental works is done on gaseous metals for determining screening effect 27 [1]. From 1998 to 2001, these experiments continued on metallic environments [2-4]. In 2000, 28 the electron screening effect on cold fusion reaction was studied for D + D in the metallic 29 environment [5]. In 2002, they released a two-volume report, "Thermal and nuclear aspects of 30 the Pd/D₂O system," with a plea for funding [6]. In 2002, the enhancement of cold fusion and 31 solid state effect were studied in deuterated metal for D+D [7]. From 2002 to 2004, the screening 32 effect on 50 metals and insulator is checked by series of experiments [8-10]. In 2003, the 33 enhancement of deuteron-fusion reactions in metals and experimental implications were studied 34 for electron screening effect [11]. In 2004, the subject of solid state internal conversion came up 35 [12].In 2005, many efforts were done to make an apparatus according to the Fleischmann and 36 pons' works; finally, Cold fusion apparatus was made at San Diego Space and Naval Warfare 37 Systems Center. They used other names instead of cold fusion to reduce the effect of previous 38

39 failures.Often they prefer to name their field Low Energy Nuclear Reactions (LENR) or

40 Chemically Assisted Nuclear Reactions (CANR), also Lattice Assisted Nuclear Reactions

41 (LANR), Condensed Matter Nuclear Science (CMNS) and Lattice Enabled Nuclear

42 **Reactions** [13-16].

In 2002, Peter Kalman and Thomas Keszthelyi studied this problem (enhancing cross section) 43 on different metals. They studied many different factors to explain the enhancement of cross 44 section. For example, the electron screening was checked for 29 deuterated metals and 5 45 deuterated insulators/semiconductors from periodic tables. Among them, metals were most 46 47 convenient. Some of the other factors that they considered were: stopping power, thermal motion, channeling, diffusion, conductivity, and crystal structure and electron configuration. 48 None of them could explain the observed enhanced cross section [7, 9, 11, 17-19]. In 2004, they 49 found a reason to explain the enhancement of cross section that was called solid state internal 50 conversion [12]. In 2008, screening effect is studied for the first time on metals by considering 51 52 solid state; actually solid state of metals is expressed in experiments [20]. Finally, in 2009, they considered a metal with its lattice structure and entered the lattice shape of the solid in their 53 54 internal conversion calculations [21]. Their calculations were just for $D(p,\gamma)^{3}$ He reaction.

In this paper, different metals are considered. We choose such metals that are shown the best results in term of screening effect and the density of deuterium [22]. In this article, in order to compare internal conversion(IC)with lattice effect in solid state internal conversion(LEISSIC), we calculate cross section for different seven particles plus palladium for $D(p,\gamma)^{3}He$, D(d,p)T, $D(d,\gamma)^{4}He$, $T(d,n)^{4}He$.

The aim of this work is to determinate fusion cross section (FCS) for above reactions in different 60 metallic environments regarding LEISSIC in order to find the reason of enhanced FCS in these 61 metallic media then recommend the best metal. Toapproachthis aim, following steps are 62 studied: First, right after introduction, the aspects of IC, SSIC and LEISSIC are explained. 63 Second, different special lattice such as Face Cubic Centered (FCC), Body Cubic Centered 64 (BCC) and Hexagonal close Packed (HCP) are introduced in details. Third, LEISSIC and other 65 required quantities to determinate FCS and LEISSIC coefficient forPd environment are 66 67 computed. Fourth, all calculations in the third step are repeated for Ni, Ru, Rh, Pt, Ta, Ti, Zr. Fifth, microscopic FCS for all elements are determined in different reaction for the case that 68 these metals are considered as host particle in lattice. Finally, we can suggest the best kind of 69 lattice, fusion reaction and metallic environment which have high value LEISSIC when cold 70 71 fusion happening.

72 **2.** Internal Conversion (IC) and Solid State Internal Conversion (SSIC)

Internal conversion is a radioactive decay process where an excited nucleus interacts with an electron in one of the lower atomic orbitals, causing the electron to be emitted from the atom. Thus, in an internal conversion process, a high-energy electron is emitted from the radioactive atom, but without beta decay taking place. Since no beta decay takes place in internal conversion, the element atomic number does not change, and thus (as is the case with gamma).

decay) no transmutation of one element to another is seen. Also, no neutrino is emitted in internal conversion.Most internal conversion electrons come from the K shell (1s state, see electron shell), as these two electrons have the highest probability of being found inside the nucleus. After the electron has been emitted, the atom is left with a vacancy in one of the inner electron shells. This hole will be filled with an electron from one of the higher shells and subsequently a characteristic x-ray or Auger electron will be emitted[23,24]



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HIGHTE	1.	Internal	conversion
Inguie	т.	memu	conversion

The enhancement in the fusion rate, which is observed in solid metallic environments, is attributed to the presence of solid state material but up till now the theoretical explanation of the phenomenon is still missing [25-27]. In what follows we suggest a possible mechanism called solid state internal conversion process that should be considered when trying to understand the extra fusion events. [28].

91

92 A similar process to IC can take place in a solid between fusionable nuclei and any charged particle in the crystal. The solid state internal conversion process, e.g. $D(p,\gamma)^{3}$ He nuclear 93 reaction, can be processes consisting of (a) a bound-free electron transition $p + d + (e) \rightarrow {}^{3}He +$ 94 e and (b) a bound-free deuteron transition $p + d + (d) \rightarrow {}^{3}He + d$. Therefore, as internal 95 conversion happened in solid environment in addition of electron channel, we have deuterium 96 channel too [12].Increasing absorption is shown that in a solid material, nuclear fusion 97 98 reactions(NFR) can happen in solid state internal conversion that creates transit for every charged particle by electromagnetic reaction [12]. 99

3. Describing mentioned latticestructure in this article: FCC, BCC, HCP

101

102 In this paper, these elements are studied: Ni, Ru, Rh, Pt, Ta, Ti, Zr. Which, Ni, Pt, Rh have a

103 FCC lattice such as Pd. Ru, Ti, Zr have a HCP lattice and the lattice of Ta is BCC.

After investigating prior experimental work, finally in 2008 solids are considered without 104 their lattice crystal [20]. Then, in 2009, calculations are continued for Pd and with regarding the 105 crystalline lattice [21]. Before study on solid state internal conversion the scientists examined 106 screening effect on metals to finding the reasons of the enhancement FCS of metals which was 107 observed^[22].In this article chosen element are significant in screening effect or deuterium 108 density. For example, Ti and Zr showed the most screening potential in the experiments [11]. Ta 109 110 and Zr had the most solved deuterium density [22]. Whereas having a maximum deuterium density in Ti depends on having high temperature [12]. 111

112 The most important quantities that change during calculations are unit cell volume and the 113 number of atom that belongs to each kind of lattice. Those quantities are explained for each 114 lattice that is following.

In each unit cell of FCC and BCC lattice, eight atoms stand on the corner of cubic that are collaborative between eight other closed cubic (Fig 2, a_1 and a_2),thus, each unit cell has one atom from corners ($8 \times \frac{1}{8} = 1$). For FCC there is one atom which belongs to two closed cubic but for BCC one atom locates in the center of each unit cell. So, FCC and BCC lattice have respectively 3 atoms from all 6 sites ($6 \times \frac{1}{2} = 3$) and one atom from its center. Therefore, FCC and BCC have four(1 + 3 = 4) and two (1 + 1 = 2) atoms for each unit cell respectively.

HCP lattice: In each unit cell of HCP (see fig.2,a₃), there are two atoms on the top and down sides that are shared between two closed unit cells $\left(2 \times \frac{1}{2} = 1\right)$, on the other sides of the unit cell there are six atoms. Each atom belong two closed unit cells $\left(6 \times \frac{1}{2} = 3\right)$. There are twelve atoms in the corners that are collaborating between three closed unit cells $\left(12 \times \frac{1}{3} = 4\right)$. Consequently, there are eight atoms that are completely belonging to one unit cell. In this lattice there are two lattice constants: c height of unit cell and a, the face of hexagonal.



127

128

Figure 2: Shape of unit cell; a1: FCC unit cell, a2: BCC unit cell, a3: HCP unit cell.

129 The volume of unit cell for each lattice is defined by equation 1,

$$v_{cell} = \begin{cases} \frac{a^3}{4} & FCC\\ \frac{a^3}{2} & BCC\\ \frac{3\sqrt{3}}{16}a^2c & HCP \end{cases} , (a, c: lattice \ constant) (1)$$

132 4. Lattice Effect in Solid State Internal Conversion

4.1. Cross section theory of LEISSIC

Since particles in the crystal are placed in specific sites, we can estimate fusion cross section (FCS) reactions using Block theorem for describing initial and final states of this system (palladium environment). In all formulas subscripts 1, 2 and 3 are respectively pointed at incoming, sublattice and host particles. Also, the state of particles in the lattice is determined by Block function [28]

139
$$\varphi_{k_{3,i}}(r_3) = \frac{1}{\sqrt{N}} \sum_{l_s} e^{ik_{3,i} \cdot l_s} a_3 (r_3 - l_s - u_3(l_s)) (2)$$

140 where, r_3 , $k_{3,I}$ and a_3 are respectively introduced host-particle coordinate, a wave vector of the first 141 Brillouan zone of the reciprocal lattice, and Wannier function. Here, Pd (palladium), d (duetron) 142 and e (electron) are considered as host particles. Lattice site and the displacement of the atom 143 located at lattice site are symbols to represent l_s and $u_3(l_s)$. Here N is the number of lattice 144 point. The sublattice particle also is described by Block function (Eq3). Lattice contains N_2 145 fusionable particles, for palladium system it is assumed that $N_2 = N$.

146
$$\varphi_{k_{2,i}}(r_2) = \frac{1}{\sqrt{N_2}} \sum_{l_s} e^{ik_{2,i} \cdot l_s} a_2 (r_2 - l_s - u_2(l_s)) (3)$$

147 Here, a_2 and a_3 are Wannier functions for sublattice and host particles respectively that are determined 148 by equation 4[20],

$$a_j(x) = \left(\frac{\beta_j^2}{\pi}\right)^{3/4} e^{-\frac{\beta_j^2}{2}x^2} (x = r_2 - l_s), j = 2,3$$
(4)

149 In the above formula, $\beta_j = \sqrt{m_j \omega_j / \hbar}$ [6]. The initial state Ψ_i for the three particles that participate 150 in solid state assisted fusion reaction is described by,

151
$$\Psi_i = \varphi_{k_{2,i}}(r_2)\varphi_{k_{3,i}}(r_3)\varphi_1(r_1 - r_2)(5)$$

where, $\varphi_1(r_1 - r_2)$ is the Coulomb wave function corresponding to the state of a sublattice and incoming particle. The Coulomb wave function is[20],

$$\varphi_1(r_1 - r_2) = e^{ik_1 \cdot (r_1 - r_2)} \frac{f(k_1, r_1 - r_2)}{\sqrt{V}}$$
(6)

154 V is the volume of normalization, k_1 is the wave vector, r_1 is the coordinate of incoming particle,

- and f function is defined as the following:
- 156 $f(k_1, x) = e^{-\pi \eta/2} \Gamma(1 + i\eta) {}_1F_1(-i\eta, 1; i[k_1x k_1 \cdot x])$ (7)
- ¹⁵⁷ ${}_{1}F_{1}$ is the confluent hyper geometric function [4]. η is determined by using the eq. 8 and 9 [29].

$$\eta = 0.1575 \, z_1 z_2 \left(\frac{A}{E}\right)^{1/2} (8)$$
$$A = \frac{A_1 A_2}{A_1 + A_2} (amu) (9)$$

- where z_1 and z_2 are the charge number of particles 1 and 2 and E is the energy of incoming
- particle. A_1 and A_2 are the mass of incident and sublattice particles that are measured in amu unit. The final state of this three- body system is defined by,
- 161 $\Psi_f = \psi_f(r_1, r_2)\varphi_f(r_3)F_{Cb}(z_3, z_{12}, v_{3,12})$ (10)
- 162 Where φ_f is a plane wave of wave vector k_3 that is corresponded to an outgoing particle 3.

$$\varphi_f(r_3) = \frac{1}{\sqrt{V}} e^{ik_3 \cdot r_3} \tag{11}$$

- 163 ψ_f stands for the outgoing fusion product leaving a deuteron lattice point vacant that is given in
- 164 the relative coordinate $(r = r_1 r_2)$ and the center of mass coordinate $(R = m_1r_1 + m_2r_2/m)$ of the
- 165 particles of the rest masses m_1 and m_2 then we have,

166
$$\psi_f(r,R) = \frac{1}{\sqrt{V}} e^{iK.R} \chi(r)$$
 (12)

167 where K and $\chi(r)$ are the wave vector of fusion product and a nuclear wave function, 168 respectively.

$$\chi(r) = \left(\frac{\lambda^2}{\pi}\right)^{3/4} e^{-\lambda^2 r^2/2}$$
(13)

We determine the Coulomb interaction between host particle and the product of the incident andsublattice reaction using the Fermi correction;

171
$$F_{Cb} = \sqrt{2\pi\xi} \frac{e^{-\pi\xi}}{\sqrt{1 - e^{-2\pi\xi}}}$$
 (14)

172 Where, $\xi = z_3 z_{12} \alpha_f \sqrt{\mu c^2/2Q}$ and α_f is the fine structure constant. μ is the reduced mass

$$\mu = \frac{(m_1 + m_2)m_3}{m_1 + m_2 + m_3}$$
(15)

(16)

173 The element of s-matrix that is used for determining of the cross section of the different fusion

174 reaction is known as,

175
$$S_{fi} = \frac{2\pi}{i\hbar} \iiint \Psi_f^* \frac{z_1 z_3 e^2}{|r_1 - r_3|} \Psi_i d^3 r_1 d^3 r_2 d^3 r_3 \delta(E/\hbar)$$

- 176 With a little simplification on this integral and using the HatreeFok approximation for Coulomb
- 177 interaction part of integral, we have

178
$$\frac{z_1 z_3 e^2}{|r_1 - r_3|} = \frac{z_1 z_3 e^2}{2\pi^2} \int d^3 q \, \frac{1}{q^2} e^{iq.(r_1 - r_2)} \tag{17}$$

Putting the Fourier transform of Eq.12 in Eq.15, and applying the approximation 16 and 179

comparing it with $\langle \sigma v \rangle$ formula, the cross section of fusion reaction between host and target 180 181

$$\sigma_2 = C_0 \frac{\exp\left(-2\pi\eta\right)}{E} \tag{18}$$

E is the energy of incoming particle and C_0 is determined by, 182

183
$$C_0 = |F_{Cb}|^2 A_0 k_\mu \left(\frac{\beta_2}{K_Q}\right)^3 \langle |\tilde{\chi}|_{K=K_Q}^2 \rangle_{\Omega_K}$$
(19)

With Ω_K denoting the solid angle in the K space, $\beta_2 = \sqrt{m_d \omega/\hbar}$, $A_0 = 128\alpha_f^3 z_1^3 z_2^2 z_2 m_1 c^2 \sqrt{\pi}$, 184 $K_Q = \sqrt{2\mu c^2 Q}/(\hbar c)$, Q is the energy of the reaction, $k_\mu = \mu c/\hbar$. The average of nuclear wave 185

function is defined by, 186

$$\langle |\tilde{\chi}|_{K=K_Q}^2 \rangle_{\Omega_K} = \left| \tilde{\chi} \left(\frac{m_2}{m} K \right) \right|^2 = \frac{8\pi^{3/2}}{\lambda^3} e^{-\frac{4K^2}{9\lambda^2}}$$
(20)

m_n, nucleons mass, ω_n angular frequent of binding energy are calculated for each reaction 187 separately (table 4). 188

$$\lambda = \frac{\sqrt{m_n \omega_n}}{\hbar}$$

$$m_n = m_i + m_{He}, i = d \text{ or } t$$

$$binding energy of He(MeV)$$
(21)
(22)

$$\omega_n = \frac{binaing \, energy \, of \, He(MeV)}{\hbar} (23)$$

- Here, C_0 is calculated for one d or one Pd. In order to compare C_0 with astrophysical factor (S(0)) in 189
- ordinary state, it must be calculated considering the density of these particles. So, we use the 190
- Eq.23, 191

$$NC_0 = A\Delta R_h C_1 \tag{24}$$

In this case, N is defined by, 192

$$N(Pd) = V_{eff} / v_{cell}$$
(25)
193 Where $v_{cell} = d^3/4$, $V_{eff} = A\Delta R_h$ and $d = 3.89 \times 10^{-8} cm$ is the lattice constant

$$N(d) = u V_{eff} / v_{cell}$$
(26)

In Eq.26, u is the ratio of deuteron to palladium number density. For electron u = 10 which is the 194 number of electron valence in palladium. Co contains all the properties of the lattice. For 195 comparison the fusion cross section with and without LEISSIC we have to determine the 196 macroscopic cross section. 197

(27)

198
$$\Sigma = N\sigma_2$$

4.2. Results of numerical calculations for each reaction 199

There are two tables for all reactions that can aid in plotting the cross section and comparing 200 201 with the ordinary state. The suppositions of host, sublattice and incoming particles are expressed for all reactions in this way: the host particles are Pd,d,e for Palladium. The sublattice is 202 deuterium for all reactions. The incoming particles are proton (p) in $D(p,\gamma)^{3}$ He, deuterium (d) in 203 D(d,p)T and $D(d,\gamma)^4He$ and tritium (t) in $T(d,n)^4He$. Our calculation for obtaining the cross 204

section for all three kind of host particles are accomplished by using equations: 12,13,17,19 and

206 our obtained results are given in tables 1 and 2.

207

Type of Reactions	host parti cles	A ₀ (Me V)	μ(gr)	$K_Q(\mathrm{cm}^{-1})$	$ \widetilde{\chi} _{K=K_Q}^2$ (cm ³)	າງແ
	Pd	175	5.013×10^{-24}	8.91×10^{12}	3.95×10^{-38}	10.755
D(p,y)3He	d	0.0827	2.005×10^{-24}	5.64×10^{12}	5.13×10^{-38}	0.1477
	e	0.0103		2.78×10^{11}	6.11×10^{-38}	-560382
	Pd	349	6.686×10^{-24}	8.82×10^{12}	3.15×10^{-38}	14.462
D(d,p)T	d	0.165	2.229×10^{-24}	5.09×10^{12}	3.97×10^{-38}	0.181
	e	0.021		2.05×10^{11}	4.45×10^{-38}	-0.0011
	Pd	349	6.686×10^{-24}	7.93×10^{12}	3.69×10^{-38}	16.075
D(d,y)4He	d	0.165	2.229×10^{-24}	4.58×10^{12}	4.51×10^{-38}	0.202
	е	0.021		1.65×10^{11}	4.98×10^{-38}	-0.0022
	Pd	524	8.35×10^{-24}	2.05×10^{13}	2.89×10^{-39}	5.863
T(d,n)4He	d	0.248	2.387×10^{-24}	1.10×10^{13}	4.24×10^{-39}	0.09
	e	0.031		8.90×10^{11}	4.30×10^{-38}	-4.228

Table 1: our numerical calculation of necessary quantities for obtaining C_0 for all chosen reactions

208

From the results of table 1 and Eqs. 17 and 27 for different reactions and host particle, we can calculate the required parameters such as C_0 and C_1 which are important for estimating cross

211 section of the fusion reactions.

212

Table 2: our numerical calculation C_0 and C_1 for different host particle and different reactions

Type of Reactions	host parti cles	k_{μ} (cm ⁻¹)	$ F_{Cb} ^2$	C ₀ (MeV b)	С ₁ (MeV b)
	Pd	1.42×10^{14}	3.14×10^{-28}	4.92×10^{-38}	3.36×10^{-24}
D(p,y)3He	d	0.57×10^{14}	0.61	2.30×10^{-13}	u × 15.6
	e		1	9.10×10^{-13}	6.18×10^{2}
	Pd	1.90×10^{14}	3.27×10^{-38}	1.11×10^{-47}	7.53×10^{-34}
D(d,p)T	d	0.63×10^{14}	0.5371	1.88×10^{-13}	u × 12.78
	e		1	2.48×10^{-12}	1.687×10^{3}
	Pd	1.90×10^{14}	7.02×10^{-41}	3.83×10^{-50}	0.26×10^{-35}
D(d, y)4He	d	0.63×10^{14}	0.4964	2.70×10^{-13}	u × 18.35
	e		1	4.31×10^{-36}	2.93×10^{-21}
	Pd	2.37×10^{14}	4.44×10^{-15}	2.05×10^{-25}	1.39×10^{-12}
T(d,n)4He	d	0.68×10^{14}	0.7438	4.45×10^{-15}	u × 0.3024
	e		1	1.87×10^{-13}	127.1

213

Since each palladium unit cell has 4 Pd atoms purely and since we suppose that the number ofhost and sublattice particles are equal, then we have

$$N_{Pd} = \frac{1}{4} \times 4.22 \times 10^{22} \tag{(}$$

- 216 The other quantities such as, m_n , β_2 and Q which is mentioned before are calculated and
- 217 numerical results are summarized in table 3.

Type of Reactions	λ (cm ⁻¹)	$\beta_2(\mathrm{cm}^{-1})$	Q (MeV)	Binding Energy (MeV)
$D(p,\gamma)^{3}He$	9×10^{12}	4.81×10^{14}	5.49	7.718
D(d,p)T	10×10^{12}	4.81×10^{14}	4.04	8.482
$D(d,\gamma)^4$ He	9.63×10^{12}	4.81×10^{14}	3.27	28.3
T(d,n) ⁴ He	21.8×10^{12}	4.81×10^{14}	17.59	28.3

218 Table 3: our obtaining required quantities which are calculated for determination of different fusion

219

4.3. Calculations the solid state internal conversion coefficient for different fusion reactions in Palladium crystal environment

With regarding to definition that exists in Ref.11, we can write $v_{eff} = A\Delta R_h$, where A is the cross section of the beam, ΔR_h is the "differential" range, that is, the distance within which the energy of the incoming particle can be considered unchanged. The $\Delta R_h \ll R_h$ condition helps in an order of magnitude estimate of ΔR_h , where R_h is the stopping range of a proton which is about $8 \times 10^{-2} \mu m$ at $E = 0.01 \, MeV$ in Pd [22]. The quantities A and R_h were measured in $mm^2 and 10^{-3} \mu m$ units. The solid state internal conversion coefficient is introduced as,

$$\alpha_{SSIC} = A \Delta R_h C_1 / S(0) (29)$$

D(d,p)T

0.056

 $D(d,\gamma)^4$ He

0.054

 $T(d,n)^4$ He

10

S(0) is the astrophysical factor and the amounts of S(0) were calculated completely in the ref 27. Here since the issue is studied on the low energy (5-30 eV), the amounts of S(0) for each reaction is a constant that are shown in table 4.

231Table 4: the amounts of astrophysical S-factor for different reactions in ordinary state in low energy

 $D(p,\gamma)^{3}He$

 $0.2\times~10^{-6}$

Reactions

Astrophysical

S(0)

MeV barn

factor

232

233

--

234

235

236

237	By using the amounts exist in tables 2, 4 and replacing them into Eq.28 the solid state internal
238	conversion coefficient for different reactions can be found. This coefficient indicates the internal
239	conversion rate in different reactions. The result of the calculations summarize in table 5.

240

Table 5: solid state internal conversion coefficient in different reactions for e, 4d and d channels

$D(p,\gamma)^{3}He$	$u \times 7.8 \times 10^{5}$	3.1×10^{9}
D(d,p)T	$u \times 3.03 \times 10^4$	3.2×10^{6}
$D(d,\gamma)^4$ He	$u \times 3.398 \times 10^{2}$	5.42×10^{-20}
$T(d,n)^4$ He	u × 0.03	12.7

We find out the solid state internal conversion happens in $D(p,\gamma)^{3}$ HeandD(d,p)T reactions with 242 more rates. All calculations in this part are shown for palladium. In the next part we show the 243

results for other elements in detailed. 244

5. Calculations of LEISSIC forother elements 245

5.1. Tables of Calculation for Different Elements and Reactions 246

247 By using all formulas in section 3, such as what we have done for palladium, all required

quantities can be computed for mentioned elements. Because other host particles (deuterium and 248

249 electron) don't change in these calculations and the only thing that changes is the first row of the

- Table.1. Meanwhile, C₁ and C₀which changes only for the elements are respectively showed in 250
- Table 6 and 7. 251

	1		1	
Quantity	С _{0,D(р,ү)3He} (MeV barn)	C _{0,D(d,p)T} (MeV barn)	C _{0,D(d,γ)4He} (MeV barn)	C _{0,T(d,n)4He} (MeV barn)
Pd (FCC)	4.92×10^{-38}	1.11×10^{-47}	3.83×10^{-50}	2.05×10^{-21}
Ni (FCC)	3.44×10^{-27}	6.79×10^{-33}	2.56×10^{-35}	6.98×10^{-23}
Pt (FCC)	1.34×10^{-57}	1.95×10^{-74}	1.21×10^{-81}	1.63×10^{-4}
Rh (FCC)	1.08×10^{-36}	7.43×10^{-47}	6.61×10^{-51}	1.38×10^{-2}
Ru (HCP)	8.49×10^{-37}	5.07×10^{-46}	5.56×10^{-50}	1.21×10^{-3}
Ti (HCP)	1.10×10^{-23}	4.63×10^{-28}	6.49×10^{-30}	1.93×10^{-2}
Zr (HCP)	2.25×10^{-34}	1.01×10^{-42}	2.69×10^{-46}	6.27×10^{-2}
Ta (BCC)	1.30×10^{-54}	3.10×10^{-70}	5.79×10^{-77}	2.64×10^{-43}

252 e

253

254

255

257 Table 7: Our numerical calculations of C₁ for different elements and reactions with FCC, BCC and HCP lattice

elements				
	D1			
Pd	Pa			
(FCC)	d			
. ,	e			
Ni	Ni		(
(FCC)	d			
(100)	e			
D.	Pt	ť		
Pt (FCC)	d			1
(FCC)	e			
~	Rh	5	1	
Rh (ECC)	d			
(FCC)	e			
Du	Ru	Ľ		
(HCP)	d			
(1101)	e			
т	Ti	5		
(HCP)	d			
(IICI)	e			
7r	Zr	8		
(HCP)	d			
(IICI)	e			
Та	Та	7	-	
(BCC)	d			
(BCC)	e			

For comparing C_0 , the microscopic FCS of these metallic environments for all elements,

numerical values from Table.6 can be useful. For studying the comparison of the C_1 quantity see table 7.

According to table 7, we find out that: wherever elements themselves are considered as host particles, the results of C₁ from large too small values for all reactions are: Ti, Ni, Zr, Ru, Rh, Pd, Ta and Pt. For cases that deuterium and electron are host particles, our comparing values lead to Ru, Ni, Ti, Rh, Pd, Pt, Zr, Ta and Ni, Ru, Pd, Pt, Rh, Ti, Ta,Zr respectively. In case that electron is host the number of electrons in capacity layer is too important indeed whatever the numbers of electrons increases the screening effect is enhanced. Between all reactions, $D(p,\gamma)^{3}$ He , D(d,p)T and $D(d,\gamma)^{4}$ He have larger values of C₁ than T(d,n)⁴He.

269 (According Table.7 the result of comparing C₁ for different host particles in different metallic 270 environments are: element host particle, $C_{1,Ti} > C_{1,Ni} > C_{1,Zr} > C_{1,Ru} > C_{1,Rh} > C_{1,Pd} > C_{1,Ta} >$ 271 $C_{1,Pt}$; deuterium host particle, $C_{1,Ru} > C_{1,Ni} > C_{1,Ti} > C_{1,Rh} > C_{1,Pd} > C_{1,Pt} > C_{1,Zr} > C_{1,Ta};$ 272 electron host particle, $C_{1,Ni} > C_{1,Pd} > C_{1,Pt} > C_{1,Rh} > C_{1,Ti} > C_{1,Ta} > C_{1,Ta}$

273

Table 8: Our numerical calculations of LEISSIC for all elements in different reactions

quantity					
elements					
Pd (ECC)	d	U	ι		
Tu (FCC)	e				
Ni (ECC)	d	Ů	ι		
n (rec)	e				
Dt (ECC)	d	U	ι		
	e				
Ph (FCC)	d	U	ι		
	e				
D ₁₁ (HCD)	d	U	ι		
	e				
T; (HCD)	d	U	ι		
II (HCF)	e				
7r (HCP)	d	U	ι	ι	
	e				
	d	U	l		
Ia (DCC)	e				

In the each environment, IC coefficient shows internal conversion rate and determined the cross

section enhancement in each environment. By studying table 8, we find out that the internal

277 conversion coefficient of deuterium for $D(p,\gamma)^{3}$ He is the largest one. IC coefficient for $D(p,\gamma)^{3}$ He

for different reactions from larger to smaller value is: Ru, Ni, Rh, Pt, Zr, Ta, Ti and Pd. As you

see in this reaction Pd has the last rank. In D (d,p)T, the arrangement of the elements is: Pd, Ru,

280 Ni, Ti, Rh, Pt, Zr and Ta.

281 Electronic internal conversion coefficientarrangement for different elements is: Ni, Ru, Pd, Rh, Ti,

282 Ta, Zr, Pt. $(\propto_{e,Ni} > \propto_{e,Ru} > \propto_{e,Pd} > \propto_{e,Rh} > \propto_{e,Ti} > \propto_{e,Ta} > \propto_{e,Zr} > \propto_{e,Pt})$

283 (According to Table.8, comparing ICC values of deuterium host particle for the two largest

reactions D(p, γ)3He and D(d,p)T are respectively: $\propto_{d,Ru} > \propto_{d,Ni} > \propto_{d,Pt} > \propto_{d,Zr} > \propto_{d,Ta} > \infty_{d,Ta} > \infty$

285 $\alpha_{d,Ti} > \alpha_{d,Pd}$ and $\alpha_{d,Pd} > \alpha_{d,Ru} > \alpha_{d,Ni} > \alpha_{d,Ti} > \alpha_{d,Rh} > \alpha_{d,Pt} > \alpha_{d,Zr} > \alpha_{d,Ta})$

6. Microscopic cross section for all elements in different reactions

287 Microscopic FCS for all metallic environments when metal considers as a host particle are plotted 288 by replacing numerical values in Table 6 and Eq.16. All FCS are divided into two groups in 289 order to show changes clearly: 16 maximum and 16 minimum which are respectively shown in 290 Fig 3 and Fig 4. Numbers 1 to 4 besides the name of the elements shows $D(p,\gamma)^{3}$ He , D(d,p)T , 291 $D(d,\gamma)^{4}$ He and $T(d,n)^{4}$ He .





Figure3:16 maximum of microscopicFCS in terms of incoming energy for all reactions

In the above graph, different colors shows kinds of elements and the styles of shape introduce kinds of reactions. $D(p,\gamma)^{3}$ He by "dash", D(d,p)T by "dashdot", $D(d,\gamma)^{4}$ He by "longdash" and T(d,n)^{4}He by "dot" are shown. The color of Pd, Ni, Pt, Rh, Ru, Ti, Zr, and Ta are respectively: Green, red, navy, cyan, dark pink, coral, aquamarine and brown. As you see Ti and Ni have the lager cross section. After them palladium shows up just in the T(d,n)^{4}He reaction.



Figure 4: 16 minimum of micFCS in terms of incoming energy for all reactions

299

301 To realize the best kinds of lattice structure, microscopic FCS related to element host particles are

302 plotted for each fusion reactions separately.Here in these graphs colors shows kinds of elements

and the styles of the graph indicate the kind of the lattice. BCCshows by "dot", FCC by "long"

304 dash" and HCP by "dashpot".

305



307

Figure 5: Microscopic FCS of all elements for $D(p,\gamma)^{3}$ He.



308

306

Figure 6: Microscopic FCS of all elements for D(d,p)T







Figure 7: Microscopic FCS of all elements for $D(d,\gamma)$ 4He



Figure 8: Microscopic FCS of all elements for T(d,n)4He

312

From Fig.8 we can understand that Ni with FCC lattice is in the first place of microscopic FCS

and Pd is the fifth. Now the data that are correspond to figures 3 and 4 are summarized in table 9.

318

For $D(p,\gamma)^{3}$ He, D(d,p)T, $D(d,\gamma)^{4}$ He (Figs. 5,6,7 and 8), Ti with HCP lattice has the largest

³¹⁵ microscopic FCS and Pd with FCC lattice is respectively in the sixth, second and fifth place.

320 Table 9: numerical microscopic cross sectioned values in special energy (0.025MeV) for different elements in 321 different reactions 322 323 quantity 324 $D(p,\gamma)^{3}He$ $D(d,\gamma)^4$ He $T(d,n)^4$ He D(d,p)T(MeV) (MeV) (MeV) 325 elements Pd 326 (FCC) Ni 327 (FCC) Pt (FCC) 328 Rh (FCC) 329

7. Discussion and Conclusion

Ru (HCP)

Ti (HCP)

Zr (HCP) Ta

(BCC)

334

333

330

331

332

According to table.7, the result of comparing C₁ for different host particles in different metallic environments are: when the metals are considered as host particle, $C_{1,Ti} > C_{1,Ni} > C_{1,Zr} >$ $C_{1,Ru} > C_{1,Rh} > C_{1,Pd} > C_{1,Ta} > C_{1,Pt}$; whenever deuterium considered a host particle, $C_{1,Ru} >$ $C_{1,Ni} > C_{1,Ti} > C_{1,Rh} > C_{1,Pd} > C_{1,Pt} > C_{1,Zr} > C_{1,Ta}$; electron host particle, $C_{1,Ni} > C_{1,Ni} > C_{1,Ru} >$

339 $C_{1,Pd} > C_{1,Pt} > C_{1,Rh} > C_{1,Ti} > C_{1,Ta} > C_{1,Zr}$.

346 arrangement of the elements is: Pd, Ru, Ni, Ti, Rh, Pt, Zr and Ta.

348 Ti, Ta, Zr, Pt. $(\propto_{e,Ni} > \propto_{e,Ru} > \propto_{e,Pd} > \propto_{e,Rh} > \propto_{e,Ti} > \propto_{e,Ta} > \propto_{e,Zr} > \propto_{e,Pt})$

As you see in table.9 the best cross sections belong to $D(p,\gamma)^{3}$ He and D(d,p)T reactions. In order

to achieve our goals we need to look back to our data about internal conversion coefficient by
 considering lattice effect.

In table 8, we find out that the internal conversion coefficient of deuterium for D $(p,\gamma)^3$ He is the

³⁴⁴ largest one. IC coefficient for $D(p,\gamma)^{3}$ He for different reactions from larger to smaller value is:

Ru, Ni, Rh, Pt, Zr, Ta, Ti and Pd. As you see in this reaction Pd has the last ICC. In D (d,p)T, the

³⁴⁷ Electronic internal conversion coefficient arrangement for different elements is: Ni, Ru, Pd, Rh,

- 349 According to Table.8, comparing ICC values of deuterium host particle for the two largest
- 350 reactions $D(p,\gamma)^{3}$ He and D(d,p)T are respectively: $\propto_{d,Ru} > \propto_{d,Ni} > \propto_{d,Rh} > \propto_{d,Pt} > \propto_{d,Zr} > \propto_{d,Ta} >$
- 351 $\propto_{d,Ti} > \propto_{d,Pd}$ and $\propto_{d,Pd} > \propto_{d,Ru} > \propto_{d,Ni} > \propto_{d,Ti} > \propto_{d,Rh} > \propto_{d,Pt} > \propto_{d,Zr} > \propto_{d,Ta}$)
- As you see Ti and Ni have the lager cross section. After them palladium shows up just in the
- 353 $T(d,n)^4$ He reaction.
- Looking at figs 5, 6, 7 and 8, can show that what the best lattice, kinds of environment and kinds
- of reactions are. Ti with HCP lattice has the largest micFCS and Pd with FCC lattice is
- respectively in the sixth, second and fifth place. From Fig.8 we can understand that Ni with FCC
- 357 lattice is in the first place of micFCS and Pd is the fifth. FCC and HCP are the best lattice
- 358 structures and Ti and Ni are best elements, Ru has a largest ICC In the case that deuterium is the
- 359 host particle.

By comparing FCS in term of LEISSIC, Ti and Ni show maximum data. By comparing in@60al conversion coefficient in term of LEISSIC, the best results belong to Ni and Ru. So Ni canb6e the best option for the next experimental works. We can neglect Ta and the BCC lattice becau362 of its worse results. 363

- 364 The other investigations show that: FCC and HCP lattice have a much closed results. Palladium
- shows good results just in the $D(p,\gamma)^{3}$ He and $D(d,\gamma)^{4}$ He.

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