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Research Article

Formation of Hydrogen Miniatoms in the Medium of Free Electrons–the Key to the Mechanism of Low-energy Nuclear Reactions

A. I. Goncharov*

Institute of Digital Technologies, Electronics and Physics, Altai State University, Prospect Lenina, 61, Barnaul, 656099, Russia

V. A. Kirkinskii

Institute of Geology and Mineralogy, Siberian Branch of the Russian Academy of Sciences, Prospect Akad. Koptyuga, 3, Novosibirsk, 630090, Russia E-mail: kirkinsky2011@yandex.ru

Abstract

We have modeled the behavior of hydrogen atoms in the flow of free electrons in metals by the molecular dynamic method. The trajectories of the particles were calculated by numerically solving a system of differential equations of mechanics. Relativistic equations were used, and the interaction of particles was considered Coulombic without taking into account magnetic effects. About 10^4 stories were modeled, each of them containing up to 100 collisions of free electrons with a hydrogen atom. The total number of simulated atoms that experienced collisions was $\sim 10^6$. Dynamic modeling revealed the formation of neutral particles consisting of protons (deuterons) with an electron rotating around them in nonstationary, close to elliptical orbits with an apogee to a distance of less than 10^{-11} cm and to a perigee of $\sim 10^{-12}$ cm. These particles, which are continuously changing in size and shape, are up to 3 to 4 orders of magnitude smaller than ordinary hydrogen atoms, and 1-2 orders of magnitude larger than neutrons. Such nonstationary hydrogen miniatoms can exist for a short time (on our estimate, up to $\sim 10^{-12}$ sec.) in the environment of free electrons of metals, easily move in them and, like neutrons, approach the nuclei of isotopes of hydrogen or other elements at a distance at which nuclear fusion reactions or transmutation of elements are possible due to the tunneling effect. Taking into account the formation of such hydrogen miniatoms the previously calculated rate of low-energy nuclear reactions in metals[1–6] increases more than by 5 – 6 orders of magnitude, that is, to values corresponding to experimental data. Formation of hydrogen miniatoms in the medium of free electrons is of primary importance in the mechanism of low-energy nuclear reactions.
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*Corresponding author: goncharov.ai@mail.ru

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1. Introduction

In computer simulations using molecular dynamics methods, it was previously shown that the electrons of the outer shells of metals have a shielding effect on deuterons and significantly accelerate nuclear fusion reactions. The results of quantitative calculations of the reaction rates of hydrogen isotopes in a number of metals are published in Refs. [1]–[6]. In this paper, we model the behavior of hydrogen atoms in the flow of free electrons in metals.

1.1. Description of the Model

At the first stage, within the frame of classical (non-quantum) mechanics, the behavior of a single deuterium atom is simulated when acted upon by a flow of free electrons[7]. It is assumed that the particles do not radiate electromagnetic waves. The system consists of a deuteron and two electrons. At the initial moment, one of the electrons (orbital) is in the circular orbit of Bohr radius 0.529 Å. The flow of incoming electrons is isotropic; the impact parameter is limited by the value 0.53 Å.

The incoming electrons appear at the 1 Å distance from the deuteron; the kinetic energy of the incoming electrons follows the Fermi distribution with the parameters characteristic of free electrons in a Pd crystal at room temperature[8]:

$$f(\varepsilon) = const\sqrt{\varepsilon}/\{1 + \exp[(\varepsilon - \varepsilon^*)/kT]\},$$

where $\varepsilon^* = h^2(3n_e/\pi)^{3/2}/8m_e$ is the so-called characteristic energy, $n_e$designates the free electrons concentration, h is Planck's constant, k is the Boltzmann constant; and the absolute temperature T is assumed to be equal to 350 K. According to Ref. [3], we assume that for every atom there is a single free electron. Then $n_e \approx N_A \cdot \rho/A$. For palladium, $n_e \approx 6.8 \times 10^{22}\text{cm}^{-3}$, $\varepsilon^*/k \approx 7 \times 10^4$ K. The average kinetic energy of free electrons in palladium is $3\varepsilon^*/5 \approx 3.6$eV, the average electron velocity $v \approx 1.13 \times 10^8$ cm/s.

After random initial conditions have been specified, particle trajectories are calculated by numerically solving a system of differential equations of mechanics. Relativistic equations are used but without allowance for magnetic effects, i.e. the particle interaction is considered purely Coulomb interaction. The system of equations is solved by Runge-Kutta method of the fourth order with the relative error less than 10^{-5}.

As has already been mentioned, at any instant three particles can be tracked, i.e., two electrons and one deuteron. When one of the electrons travels at a distance exceeding 10 Å, the remaining system (unsteady state of deuterium D* atom) is bombarded by a new free electron, etc. $N_{\max} = 10^4$ model experiments have been conducted. Number l of free electrons collisions with the D* "atom" could reach up to $l_{\max} = 100$.

When one of the electrons approached the deuteron at a distance less than 10^{-13} cm, trajectories were no longer calculated. This implementation of incoming electron parameters was excluded from consideration and a transition to a new implementation of a system took place with an initial Bohr orbit of the deuterium atom. Therefore, the number of simulated D* "atoms", which underwent l collisions with electrons, $N(l) < N_{\max}$. For instance, $N(10) = 9101$, $N(50) = 3331, N(80) = 1489, N(100) = 847$. The total number N* of simulated D* "atoms"

$$N* = \sum_{l=1}^{l_{\max}} N(l) = 420748 \quad < N_{\max} \times l_{\max} = 10^6.$$

A high proportion of electrons collisions with D* results in the decreased energy of D* and its size. For the D* size the distance r from the electron to the deuteron is taken at the apogee of the orbit. The size distribution density of D*, which underwent l collisions with electrons, will be designated as $f(r|l)$.

We had to exclude from our consideration trajectories in the region of small distances in order to prevent the degradation of the trajectories calculation accuracy and to enhance the program response. Special calculations showed that for a significant proportion of neglected trajectories there was a pronounced trend for the electron impingement on

the deuteron, which could have resulted in the formation of a bineutron. The program, however, was not yet sufficient to calculate this process accurately enough. Part of the neglected trajectories could have also lead to the formation of D* of even smaller sizes. Those two possibilities potentially can significantly increase the theoretically estimated value of the fusion reaction rate and require supplementary research. For the time being, we assume that under more accurate trajectories calculation all the excluded implementations result in the formation of D* whose size obey the same distributions $f(r|l)$. In this connection, distributions are normalized similarly for any *l*:

$$\int_0^\infty f(r|l)dr = 1.$$

The number *l* of the D* "atom" collisions with free electrons obeys Poisson distribution $P_a(l)$ with the parameter *a*; the average number of collisions *a* is proportional to the electron flow density and time.

The main contribution to the reaction rate make small D* ($r\sim10^{-11}$ cm), that have a high mobility. So, the crystal lattice does not strongly interfere with D*-D* collisions. Let *n* and *N* be the concentration and full quantity of D* atoms in the working volume of crystal. The proportion of deuterons λ, which reacted in a unite time (fractional reaction rate λ) is equal to:

$$\lambda(a) = -\frac{1}{N}\frac{dN}{dt} = \sum_{l=0}^{l_{\max}}\sum_{m=0}^{l_{\max}} P_a(l)P_a(m)\lambda(l,m),$$
$$\lambda(l,m) = \frac{n}{2}\int_0^\infty dr_1 \int_0^\infty dr_2 f(r_1|l)f(r_2|m)\int_0^\infty dE v\sigma(v)F_M(E),$$

where *v* is the relative speed of deuterons, $E = \mu v^2/2$; μ – reduced mass of deuterons pair; F_M(E) – Maxwell distribution at room temperature normalized as:

$$\int_0^\infty F_M(E)dE = 1.$$

The cross-section of D*−D*-collisions resulting in a fusion reaction in the quasiclassical approximation is $\sigma(v) = S_0P(E)/E$, where $S_0 = 0.55\times10^{-19}$ cm^2 eV;

$$P(E) = \exp\left(-\frac{4\pi}{h}\int_0^R \sqrt{2\mu[V(r)-E]}dr\right),$$

where $R = V^{-1}(E)$ is the turning point of a classical trajectory.

It will be assumed that D* "atoms" with the shell sizes r_1, r_2 move freely if the "shells" do not overlap, i.e., if the distance between the D* "atoms" is $r > r_1 + r_2$. If the "shells" overlap, a purely Coulomb repulsion of the D* "atoms" is observed. The potential deuterons interaction energy in this approximation is equal to

$$V(r) = \begin{cases} e^2/r - E_s & \text{if } r < r_1 + r_2, \\ 0 & \text{if } r > r_1 + r_2, \end{cases}$$

where $E_s = e^2/(r_1+r_2) = m_ec^2r_e/(r_1+r_2)$ is the screening energy, $r_e = 2.82\times10^{-13}$ cm is the classical radius of an electron. By integration, we obtain

$$P(E) = \exp\left(-993.09\ \text{eV}^{1/2}/\sqrt{E+E_s}\right).$$

Since at any energy E contributing to λ there holds a condition $E << E_s$, the approximation $P(E) \approx P(0)$, $F_M(E) = \delta(E - \overline{E})$ can be used where $\overline{E} = 3kT/2$. Then

$$\lambda(l,m) = C\int_0^\infty dr_1 \int_0^\infty dr_2 f(r_1|l) f(r_2|m) W(r_1 + r_2),$$

where $C = (nS_0/2)(2/\mu\overline{E})^{1/2}$, $W(r_1 + r_2) = \exp\left(-1.39\sqrt{(r_1 + r_2)/r_e}\right)$.

Taking into account the probabilistic sense of $f(r|l)$, the reaction rates $\lambda(l, m)$, $\lambda(a)$ could be approximately calculated by the formulas

$$\lambda(l,m) = \frac{C}{N(l)N(m)} \sum_{i=1}^{N(l)} \sum_{j=1}^{N(m)} W(r_i^{(l)} + r_j^{(m)}), \quad \lambda(a) = C \sum_{i=1}^{N*} \sum_{j=1}^{N*} \frac{P_a(l(i))P_a(m(j))}{N(l(i))N(m(j))} W(r_i + r_j),$$

where $r_i{}^{(l)}$, $i = 1, 2, 3, \ldots, N(l)$ are random implementations of the D* "atom" size with l collisions of electrons; r_i, $i = 1, 2, 3 \ldots, N*$ denotes the complete set of implementations. Let every octahedral site contain a deuterium atom. Then the deuterium concentration $n = 6.8 \times 10^{22}$ cm^{-3}; at T = 350 K, $C = 1.2 \times 10^{10}$ s^{-1}.

2. Calculation Results

Recall that *f(r/l)* is the size distribution of the atom that has experienced l collisions with electrons. The simulation showed that the distributions of *f(r/l)*, starting from about $l = 50$, are almost the same with a further increase in l (see Figure 1). The equilibrium distribution can be close to that found if the characteristic time of the quantum relaxation of the "miniatom" exceeds 10^{-13} s.

Table 1 presents the number of events with the size r and the number of collisions l from the different ranges; $\Delta N*$ is the total number of events with l from these ranges.

Table 2 shows the dimensions of the 10 smallest "miniatoms" of deuterium D*, which have $r \leq 2 \times 10^{-11}$cm. The "orbits" are usually very elongated: $r_{\min} << r$, so using the value r as the size of the "atom" should lead to a lower estimate of λ.

Figure 2 shows the functions $\lambda(l, l)$ and $\lambda(a)$. Averaging $\lambda(a)$ over $a \leq l_{\max}$, which is equivalent to averaging over time, leads to the result $\lambda \approx 2 \times 10^{-4}$ s^{-1}, which is 10^6 times greater than the value obtained in Refs. [2] and [4]

Table 1. Number of events with r and l from the indicated ranges

Ranges of l	$\Delta N*$	Ranges of size r of the D* "atom" in units of 10^{-11} cm								
		0.5 – 1.	1. – 1.5	1.5– 2.	2. – 2.5	2.5 – 3.	3. – 3.5	3.5 – 4.	4. – 4.5	4.5 – 5.
1 – 20	177731	0	0	0	0	2	4	7	2	0
21 – 40	114983	0	0	1	5	4	14	19	25	43
41 – 60	66531	0	0	2	10	9	16	23	25	36
61 – 80	39042	0	0	1	3	7	13	17	10	22
81 – 100	22461	1	3	2	2	2	3	8	11	18

Table 2. Sizes of D* "atoms" at the apogee of r and at the perigee r_{min} in units of 10^{-11} cm. l is the number of electron collisions with D*

l	88	83	84	82	25	89	79	56	98	51
r	0.87	1.17	1.27	1.38	1.64	1.69	1.78	1.81	1.82	1.99
r_{min}	0.22	0.41	0.19	0.88	0.12	0.11	0.08	0.19	0.88	0.38

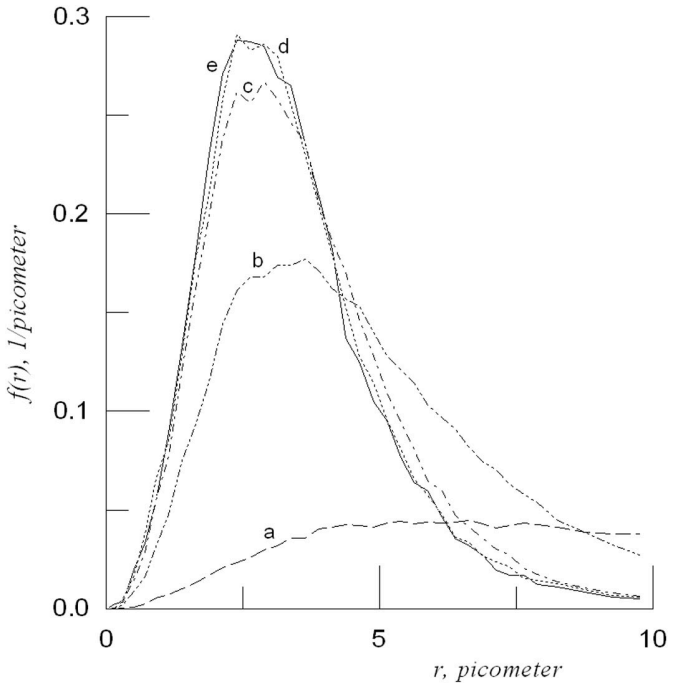

Figure 1. The size distributions of "atoms" D*, averaged over the number l of collisions with electrons: a $- l = 1 \div 20$; b $- l = 21 \div 40$; c $- l = 41 \div 60$; d $- l = 61 \div 80$; e $- l = 81 \div 100$.

on the basis of the dynamic model of electron orbital deformation (EODD). Taking into account that $\lambda(a)$ somewhat increases with the increase in a, the obtained average λ should be treated as a lower-bound estimate. The contribution of 370 events presented in Table 2 to the obtained value of λ is 99%, including the contribution of 10 events from Table 1 amounting to about 80%.

3. Discussion

The application of classical mechanics usually provokes objections because classical mechanics enables one to put a shielding charge at any point and impart it any initial velocity (e.g., zero velocity). We deem it therefore important to emphasize that the equiprobable initial conditions we employed correspond to the *real-life* situation. In addition, the applied approach, which could be called the Bohr approach, is not a purely classical one, since the radiation has been "turned off". Quantum-mechanical models allowing for elastic processes only give a sufficiently accurate description of real physical processes for a very wide range of phenomena.

It should be noted that from the quantum-mechanical viewpoint, D^* is not a kind of a hypothetical atomic state with energies lower than that of the ground state. D^* should be treated as an unsteady structure within many-particle nonradiating system.

We indicate a possible mechanism for the occurrence of such configurations under the action of a flow of free electrons, having previously made an estimate of the collision frequency of the "atom" D* with electrons. It was said above that the maximum value of the impact parameter of the incoming electrons in our calculations was equal to r_B, and any outcome was counted as a collision. The average number of such collisions of an "atom" with electrons

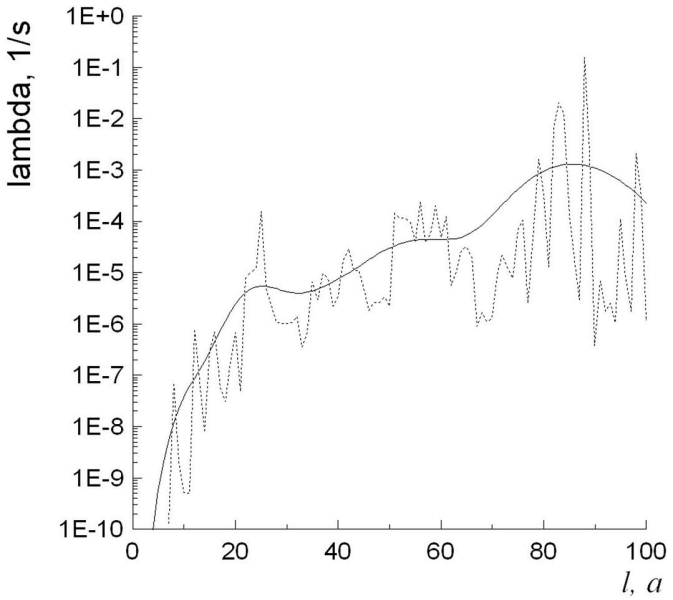

Figure 2. Reaction rate. Dashed line denotes $\lambda(l, l)$; solid line designates $\lambda(a)$.

during time t is equal to $a = \Phi\pi\ r_B^2 t$, where $\Phi = n_e v \approx 7.7 \cdot 10^{30}\ \mathrm{cm}^{-2} s^{-1}$ is the density of the flow of free electrons in a palladium crystal. The average time between two successive collisions of an "atom" with free electrons is equal to $\Delta\tau = 1/\Phi\pi\ r_B^2 \approx 1.5 \cdot 10^{-15}$s. In some cases, as a result of the interaction of electrons, one of them (flying or orbiting, let's call it "electron 1") can fly a sufficiently large distance (several Å) from the deuteron; for a while (Δt) it seems to be out of the game, since it is far away and does not determine the size of the "atom". But it takes away some of the energy, which leads to the fact that the remaining electron ("electron 2") will make revolutions around the center along an open trajectory, which we will call a "non-stationary orbit"; its average dimensions are smaller than the original dimensions of the atom and during Δt these determine the actual dimensions of the "atom". The returned electron 1 returns part of the energy to electron 2, which as a result flies away to infinity. If the final energy of the atom is not less than the initial energy, then such a classical movement of electrons does not contradict the fact of the existence of a lower energy stationary state of the atom. Since electron 1 can fly far enough away, a non-stationary orbit may well exist for a time of order $\Delta t = 10^{-15} s$; then it is very likely that it will be exposed to the next free electron, and this may lead to the formation of a non-stationary orbit of an even smaller size, etc.

4. Conclusions

Dynamic modeling without taking into account quantum effects predicts the formation of non-stationary particles consisting of protons (deuterons) with an electron rotating around them in orbits close to elliptical, with an apogee of $\sim 10^{-11}$ cm and a perigee of $\sim 10^{-12}$ cm. These "mini-hydrogen atoms", which vary in size and shape, are up to 3-4 orders of magnitude smaller than ordinary hydrogen atoms, but 1-2 orders of magnitude larger than neutrons. They can exist and move in the environment of free electrons of metals, and, like neutrons, approach the nuclei of isotopes of hydrogen or other elements at a distance at which, due to the tunneling effect, nuclear reactions of synthesis or

transmutation of elements are possible. The formation of such atoms increases the previously calculated rate of nuclear reactions in metals[1-6] by 5-6 orders of magnitude, that is, to values corresponding to experimental data.

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