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NUMERICAL CALCULATIONS OF COLD FUSION RATES IN METAL DEUTERIDES

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ABSTRACT

An original model of a nuclear fusion mechanism in metal crystal structures at low energies is developed. It uses a new approach for estimation of electron screening in metals, which is based on account of dynamic deformation of outer metal electronic orbitals during counter motion of two deuterons near their sites boundary [1-3]. Computer simulation of deuterium behavior in the palladium deuteride crystal lattice has shown that the calculated rate of nuclear reactions agrees in order of magnitude with the values deduced from experimental data on excess heat output and helium generation.

Computer simulations confirmed our initial hypothesis that the main cause of cold fusion could be dynamic screening of hydrogen isotopes nuclei by the electrons of the atomic outer shells in metal crystal lattice [1,2]. Owing to a non-uniformity of distribution of electron density in the crystal lattice, there are local regions, which are the most favorable for screening. In turn, chaotically moving ions of hydrogen isotopes at their approaching one another create some kind of potential holes, promoting rearrangement of electrons on outer shells of metal atoms, which reinforce the screening.

In this report a new model for simulation of cold fusion is presented. In more details it is considered in the book [3]. The model is based on following postulates:

- the Coulomb potential describes the interaction of all charged particles - electrons, deuterons, nuclei of metal atoms;
- the electron and deuterons (protons) motion is described by the equations of motion:

$$m_e \frac{d}{dt^2} \vec{r}_{\{e_i,D_j\}}(t) = \sum_k (1-\delta_{k\{e_i,D_j\}}) \vec{F}_{k\{e_i,D_j\}}(\vec{r}_k(t), \vec{r}_{\{e_i,D_j\}}(t)), \quad (1)$$

where $\vec{r}_{\{e_i,D_j\}}(t)$ means the coordinate of i-*th* electron or of j-*th* deuteron in time t, $\delta_{k\{e_i,D_j\}}$ - the Kronekker symbol, the factor $(1-\delta_{k\{e_i,D_j\}})$ eliminates an action of a particle on itself, $\vec{F}_{k\{e_i,D_j\}}(\vec{r}_k(t), \vec{r}_{\{e_i,D_j\}}(t))$ - force operating on i-*th* electron (j-*th* a deuteron) from k-*th* charged particle (electron, deuteron or metal atom core):

$$\vec{F}_{k\{e_i,D_j\}}(\vec{r}_k(t), \vec{r}_{\{e_i,D_j\}}(t)) = \frac{Z_k Z_{\{e_i,D_j\}}}{\left|\vec{r}_{\{e_i,D_j\}}(t) - \vec{r}_k(t)\right|^3} \left(\vec{r}_{\{e_i,D_j\}}(t) - \vec{r}_k(t)\right). \quad (2)$$

- trajectories of electrons in atoms are randomly distorted under the action of electrons and nuclei of neighboring atoms and also exterior fields. The probability of detecting an electron in a volume $d\Omega$ (corresponding to the value of the integral on $d\Omega$ from quadrate of the module of electron wave function ψ) is equal to the limit of the ratio of residence time of an electron in this volume over all time of observation T:

$$\int_{d\Omega} d\mathbf{r}\ |\psi(\mathbf{r})|^2 = \lim_{T\to\infty} \frac{\sum \Delta t(\psi(\mathbf{r},t)) : \mathbf{r}\in d\Omega}{T}. \quad (3)$$

Integrating the set of equations (1) on time under different initial conditions (that is, values of coordinates $\vec{\mathbf{r}}^{\,0}_{\{i,j\}} = \vec{\mathbf{r}}_{\{e_i,D_j\}}(0)$ and velocities of electrons and deuterons $\vec{\mathbf{v}}^{\,0}_{\{i,j\}} = \vec{\mathbf{v}}_{\{e_i,D_j\}}(0)$ in zero time $t = 0$), we receive minimum distances of two deuterons approaching - r_{min}.

For estimation of the possible nuclear fusion rate at such approaching together of two deuterons we can model their interaction potential $U_{D\text{-}D}$ as the Coulomb potential, diminished by the magnitude of energy of screening $E_{screening}$:

$$U_{D-D} = \frac{e^2}{r} - E_{screening}$$
$$E_{screening} = \frac{e^2}{r_{min}} - \frac{m_D}{2}(|\vec{\mathbf{v}}^{\,0}_{D1}|^2 + |\vec{\mathbf{v}}^{\,0}_{D2}|^2) \quad (4)$$

For the potential obtained in such a way, a probable rate of nuclear reactions λ was calculated by the formula:

$$\lambda = \sqrt{\frac{n_1 n_2}{\mu}} \int_0^{+\infty} d\varepsilon\ f(\varepsilon)\,\sigma(\varepsilon)\,\sqrt{\varepsilon}\ , \quad (5)$$

where n_1, n_2 - densities, μ - the reduced mass of isotopes, ε - the kinetic energy of approaching pairs, $f(\varepsilon)$ - energy distribution function of approaching pairs (here we use Boltzmann distribution function), cross-section $\sigma(\varepsilon) = (S_0/\varepsilon)P(\varepsilon)$, S_0 denotes the usual S-factor for the corresponding reaction type [4,5], $P(\varepsilon)$ is the barrier penetration factor.

$$P(\varepsilon) = \exp\left[-\frac{2}{\hbar}\int_{r_n}^{r_0} dr\,\sqrt{2\mu(V(r)-\varepsilon)}\right], \quad (6)$$

where r_0 corresponds to the classical turning point for model potential V(r) at energy ε, r_n is a radius of nuclear force action.

The computer realization of the model was carried out on an example of palladium deuteride. According preliminary simulation, the most favorable conditions for two deuterons coming together in palladium crystal lattice take place on the boundary of two octahedral sites (O-sites). Two palladium atoms placed between two neighboring O-sites and two deuterons in O-sites centers were considered for simulation. The initial trajectory of a palladium 4d-electron was set as an ellipse, in one of its focal points a nucleus of palladium atom with an efficient charge Z_{Pd} is located. The large and small axes of the ellipse can be defined proceeding from a potential of ionization and the condition that the maximum of an electron density weighted-mean on time corresponds to the maximum of the radial density of Pd d-orbital. The position of this maximum was found from [6].

The computer simulation was carried out both for the most probable initial positions of electron orbits and for the possible deviation from them. For approaching deuterons the initial conditions were set symmetric concerning boundary of O-sites. Movement of particles begins simultaneously. The deuterons originally are posed in the centers of neighboring O-sites and are moving with equal velocity directed strictly towards each other, electrons - on some random positions on the appropriate elliptic orbits, and the initial positions of the first and second electrons are antisymmetric.

The initial estimations of the possibility of deuterons coming together were carried out both for fixed electron orbits (without account of influence on electrons by the neighboring electrons and deuterons), and with account of all interactions between considered charged particles. As simulation shows, screening of approaching deuterons by electrons, which orbits are located in the in a plane <||>, is much weaker.

The evaluation of the most favorable initial condition were performed for initial orbits located in the plane <⊥> for initial energies of deuterons 5 eV, 1 eV and 0.23 eV. Besides, the calculations were carried out to evaluate an influence of the following factors on the obtained results: 1) deviations of the electron orbits plane from <⊥> up to $\pm 3^o$; 2) deviations of the initial positions of deuterons from symmetric up to ±0.04 nm.

After evaluation of the most favorable initial condition for D-D approaching three main series for calculation of D-D reaction rate in palladium deuteride were carried out.

In the first series the probability of atoms drawing together was calculated under random initial conditions, when the energies of approaching deuterons are given in the range of 0.23±0.005 eV (this corresponds to the height of a potential barrier for diffusion of particles). The average distance of atoms approaching one another in the whole series is 0.68 angstrom; this corresponds to the average distance in a *D-D* molecule within the accuracy of the experiment. However, more than 20% of all experimental values show that the distance of approach is less than 0.1 angstrom (fig. 1). The rate of the reaction for every case of particle approach was calculated according to the shifted Coulomb potential (4) with the energy of shift equal to the energy of screening.

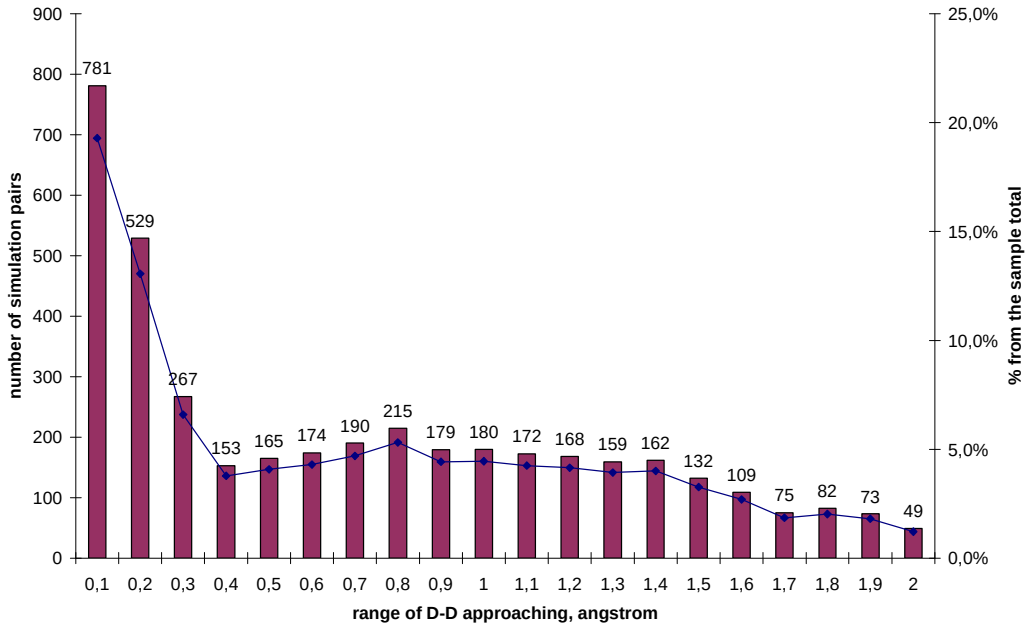

Fig. 1. Distribution of reaction D-D pairs on their range of minimal approaching to one another for the first series.

In the second series stochastic disturbances of screening electrons were added to the calculations of the first series; this corresponds to the model we have previously suggested [1,3]. The results of modeling demonstrate that in the framework of the proposed model stochastic effects in the mean do not influence the total result of dynamic screening of approaching deuterons by electrons.

In the third series, modeling of energy dependence of the distance of approach in the range from 0.001 to 9.0 eV was carried out in addition to the calculations of the second series. The obtained data demonstrate a slow decrease in the average distance of approach with the increase of energy of approaching particles. As seen from the trend line (fig. 2) the rate of reaction rapidly increases in the range of energies 0–1 eV and is retarded at higher energy values. This fact is the evidence that the influence of dynamic screening on coming together of high-speed particles is reduced.

The results of the calculations performed according to the suggested model show that near the boundaries of octahedral sites deuterons can approach one another sometimes up to the distances equal or even less then 0.001 nm. Fusion rate was calculated for every variation in deuteron approaching using formula (5) and then was averaged over the sample.

The following prerequisites for the simulation were selected: 100% occupation of O-sites by deuterium atoms, Maxwell distribution at temperature T = 300 K, full mobility of all deuterium atoms.

For estimation of actually possible rates of nuclear reactions in the crystal lattice of palladium deuteride it is necessary: to take into account the influence of deviations from symmetry of initial approaching conditions of deuterons to O-sites boundary; to estimate the correction on increase in minimum distance of approaching at arbitrary positions of the orbits plane of Pd 4d-electrons which take part in screening; to make a correction for mobility of particle.

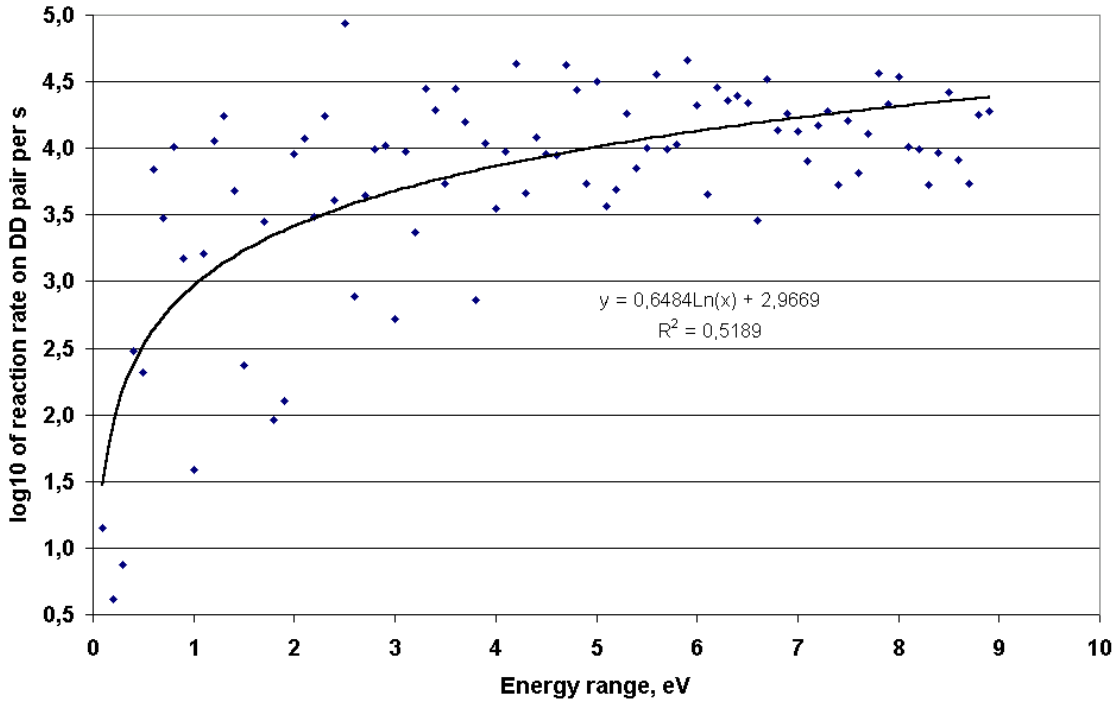

Fig. 2. Energy dependence of D-D reaction rate in palladium deuteride according the model simulation for the third series.

Taking into account these corrections one obtain that the rate of D+D reaction is 10^{-10}-10^{-12} per second per DD pair. It corresponds to the release of the energy 1-100 Watt per gram of palladium deuteride. This value agrees with the results of the experiments on excess heat output and helium generation [7-12]. The rate of p+D reaction is 2-3 order of magnitude lower and for p+p reaction is significantly - 17-18 order of magnitude - lower than for D+D nuclear reaction.

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REFERENCES

1. Kirkinskii V.A., Novikov Yu.A., "Theoretical modeling of CF", Novosibirsk, 48 p. (1998), in Russian.
2. Kirkinskii V.A., Novikov Yu.A., Europhysics Letters, v. 46, No 4, p. 448 (1999).
3. Kirkinskii V.A., Novikov Yu.A., "Theoretical modeling of cold fusion", Novosibirsk, 105 p. (2002)
4. Brown R.E., Jarme N., Phys. Rev. C, v. 41, No 4, p. 1391 (1990).
5. Bahcall J.N., Ulrich R.K., Rev. Mod. Phys., v. 60, p. 297 (1988).
6. Waber J.T., Cromer D.T., J. Chem. Phys., v. 42, p. 4116 (1965).
7. Storms E., J. Sci. Expl., v. 10, p. 185 (1996).
8. McKubre M., Crouch-Baker S. et al., in Proceedings of ICCF-8, 2000, Lerici, Italy, p. 455 (2001).
9. Arata Y. and Zhang Yue-Chang, Proc. Japan Acad., v. 70B, p. 106 (1994); Proc. Japan Acad., v. 72B, p. 179 (1996); Proc. Japan Acad., v. 73B, p. 1 (1997); Proc. Japan Acad., v. 74, p. 155 (1998); Proc. Japan Acad., v. 75B, p. 281 (1999); Proc. Japan Acad., v. 75B, p. 76 (1999); Japan J. Appl. Phys., v. 38, p. L774 (1999); Japan J. Appl. Phys., v. 37, p. L1274 (1999).
10. Miles M.H., Bush B.F., Jonson K.B., Infinite Energy, v. 15-16, p. 35 (1997).
11. Kirkinskii V.A., Drebushchak V.A., Khmelnikov A.I., Europhysics Letters, v.58, No 3, p. 462 (2002).
12. Kirkinskii V.A., Drebushchak V.A., Khmelnikov A.I., J. Thermal Analysis and Calorimetry, to be published.