## Kirkinskii V.A., Novikov Yu.A. Interaction of hydrogen isotopes in crystalline compounds according to the numerical experiments related to the problem of natural nucleation

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Experimental data of the last 12 years persuasively show the possibility of nuclear interaction of heavy hydrogen isotopes in palladium deuteride during electrolysis and other chemico-physical processes (see reviews in 1-5). However, because of significant difference in ratio of reaction products at low and high energies, non-satisfactory reproduction of effects and inconsistency with the theoretical estimations of reaction rates on the basis of common ideas, the possibility of low-temperature nuclear synthesis is open to question until now.

The authors worked out the original theoretical model of the mechanism of the interaction of hydrogen isotopes in metals [5, 6]. New approach to the estimation based on the dynamical consideration of deformation of electron shells during diffusion of hydrogen atoms in metallic crystalline structures and on their surface. Programs are constructed, and a computer modeling of the kinetics of interaction for different hydrogen isotopes in the wide temperature interval is carried out. On the basis of the obtained data, a conclusion on possibility of nuclear synthesis in some geochemical processes is made [7]. In the present study, the results on the numerical estimations of the rates of nuclear interactions of hydrogen isotopes in palladium and α and γ-Fe are presented.

The computer modeling of nuclear reaction in palladium deuteride was carried out in order to compare with the results of the experiments on the release of the excess heat in order to check the reliability of the theoretical approach.

A release of the excess heat during sorption-desorption of deuterium in finely grained palladium, measured in our laboratory, was 1 Wt per gram of $PdD_{0.6}$ [9]. Values, similar in order of magnitude, were measured in the number of studies on the electrolysis of $D_2O$-based solutions using palladium cathode (see reviews [4, 9] and the series of papers [10]). It is shown in [9, 10] that the energy release is correlated with the amount of helium forming during the experiment according to the predominant reaction $D+D\rightarrow{}^4He+23.8$ MeV. Lesser amounts of $^3He$ form by $D+D\rightarrow{}^3He+n$ and $D+D\rightarrow T+p$ followed by tritium decay $T\rightarrow{}^3He+\beta$. The measured ratio $^3He/^4He \approx 4$ in the reaction products excludes the possibility of contamination by helium from air, where this ration differs by 5 orders of magnitude [10].
palladium deuteride corresponds to the experimental values. That proves the reliability of the theoretical model.

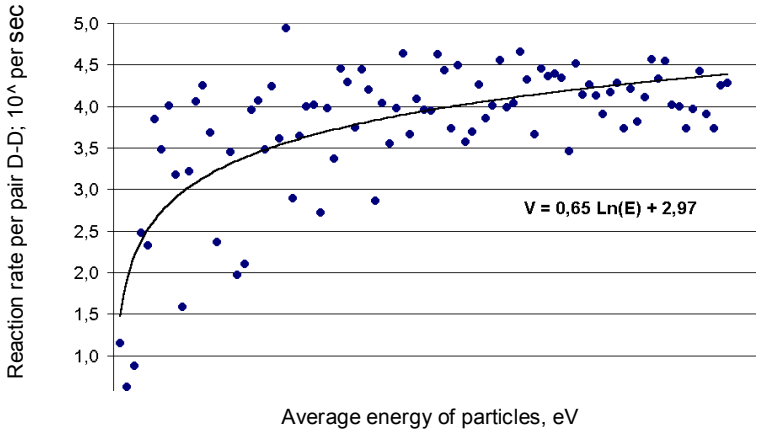


**Fig. 1.** Dependence of the average reaction rate D-D in PdD on deutron energy.

Thus, the order of magnitude of the excess energy calculated form the rate of nuclear interaction of deutrons in

In order to estimate the natural nuclear synthesis, it is interesting to model the interaction of hydrogen isotopes in the crystalline structures of α- and γ-iron as the most common natural metal.

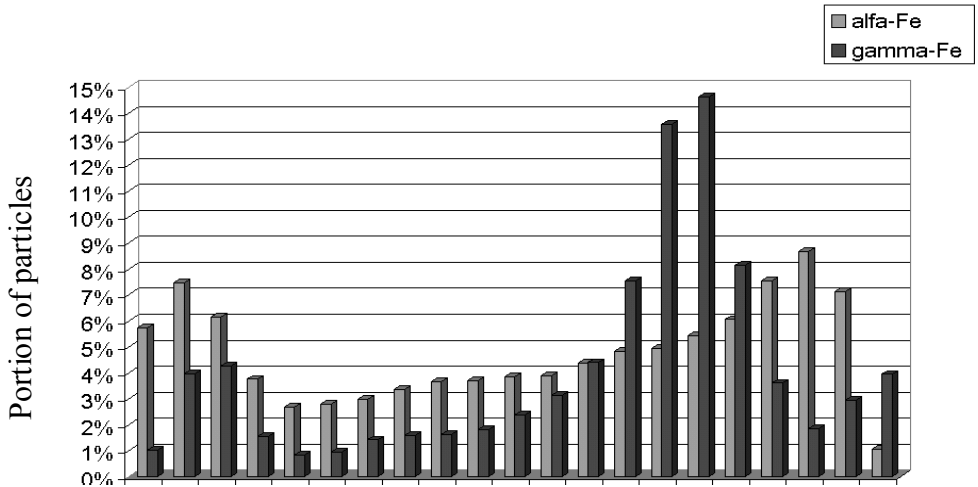

**Fig. 2.** Portion of close particles in α- and γ-Fe for different ranges of rapprochement of particles.

In the first series (5100 numerical experiments), we calculated the probability of rapprochement for the random initial conditions, then energies of approaching deutrons were fixed in the range 0.23±0.005 eV (that corresponds to the potential barrier for diffusion of particles). An average distance of the rapprochement was 0.68 Å, that corresponds, within the accuracy, to the average distance in D-D molecule. However, about 19 % of all experimental values (968) showed the rapprochement less than 0.1 Å. The reaction rate for the each case of the rapprochement was calculated by the shifted Coulombian potential with an energy of shift equal to the energy of shielding. If the reaction rate is calculated from the each variant of rapprochement, being subsequently averaged, then the reaction rate will be $10^{6.4}$ $sec^{-1}$ $DD^{-1}$. The most favorable initial conditions were chosen in order to optimize the calculations. Taking to account the peculiarities of the synthesis in real conditions, the conclusion about a significant additional decrease of the reaction rate by the correction coefficient ~$10^{-16}$-$10^{-18}$. This coefficient regards the real mobility and concentration of hydrogen atoms in palladium and the factor, which regards the probability of a realization of the initial conditions of rapprochement, used in the model. In this case, the reaction rate would be $10^{-10}$-$10^{-12}$ $sec^{-1}$ per the D-D pair, that corresponds to the energy release of 1-100 Wt per gram of palladium deuteride.

In the second series (2500 numerical experiments), in addition to the conditions of the first series, the stochastic disturbance of shielding electrons was introduced. It corresponds to the model proposed by us previously [5]. The results show that the stochastic disturbance practically does not influence on the total result of the dynamic shielding by electrons of deutrons brought together in the frame of the suggested model.

In the third series (25500 numerical experiments), the modeling of the dependence of rapprochement distance on energy in the range 0.001-9.0 eV. The obtained data show a slow decrease of an average distance of rapprochement with the energy of particles. The tendency (Fig. 1) show that the reaction rate rapidly increases in the range 0-1 eV and becomes slow at higher energies. That corresponds to the decrease of contribution of the dynamic shielding in rapprochement for high-speed particles.

Hydrogen isotopes, occupying the tetrahedral sites (TS) in α-Fe, move along three probable trajectories: 1) through the octahedral sites (OS) in the direction (100), 2) TS-TS in the direction (110), 3) TS-TS in the direction (111). In this experimental series (27800 numerical experiments), the probability of rapprochement for the random initial conditions, when energies of electrons were in the range 0.01±0.005 eV (that corresponds to the height of the potential barrier for diffusion in α-Fe), was computed. The reaction rate was calculated for each experimental value by the shifted Coulombian potential with the shift energy equal to the energy of shielding.

The series includes 27780 numerical experiments. An average distance of rapprochement in the while series was 1.094 Angstrom. That is significantly larger than an average distance in the D-D molecule. However, about 5.7 % of all experimental values showed the rapprochement less than 0.1 Angstrom (Fig. 2). The reaction rate was calculated as a mean value of the reaction rates of each variant of rapprochement, and was $10^{1.5}$ $sec^{-1}$ $DD^{-1}$. That is by four orders of magnitude lower, than the value for palladium deuteride. Estimations show that regarding the high mobility of deutrons and hydrogen solubility in α-Fe about $10^{-5}$, the value of the correction coefficient would be about $10^{-17}$. Slight difference of the coefficient in comparison to PdD (despite low hydrogen concentration) is related to the high mobility of deutrons. Taking to account the concentration of deuterium in natural hydrogen ($1.5*10^{-4}$), the reaction rate in α-Fe is about $10^{-21}$ $sec^{-1}$.

In γ-Fe, where hydrogen atoms occupy octahedral sites, the conditions of their rapprochement are less favorable. From 17800 experimental values, about 1.0 % of cases show the rapprochement less than 0.1 Angstrom (Fig. 2). The average reaction rate is $10^{-3.0}$ $sec^{-1}$ $DD^{-1}$. At normal temperature, the mobility of deutrons in γ-Fe is extremely low, but the hydrogen solubility is higher than in α-Fe, and the correction coefficient is about $10^{-23}$. Respectively, the reaction rate is about $10^{-26}$ $sec^{-1}$ $DD^{-1}$ or $10^{-32}$ $sec^{-1}$ per pair of atoms of natural hydrogen. Nethertheless, owing to the high solubility of hydrogen at high pressures and temperatures (up to the composition $FeH_{0.7}$ at 70 kbar [11]), the probability of nuclear interaction at high temperatures is higher than for α-Fe. For instance, at temperature 1200 K, the reaction rate (regarding the extreme concentration of hydrogen) is about $10^{-23}$ $sec^{-1}$ $DD^{-1}$. The extreme reaction rate (at 100 % of filling of the octahedral sites by hydrogen atoms and their perfect mobility) is about $10^{-19}$ $sec^{-1}$ $DD^{-1}$. That corresponds to the energy release about $10^{-7}$ – $10^{-8}$ Wt per gram of FeH.

Thus, the results of the numerical modeling unambiguously show the principal possibility of nuclear synthesis of helium isotopes from natural hydrogen in the crystalline structures of α- and γ-Fe under Earth's conditions. It is known that iron is the major component of the Earth's core, and native iron is found in some basalts as well. If this iron contains hydrogen admixture, the nuclear reactions could be the additional source of thermal energy in the Earth, whose significance must be estimated further.

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