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Calculations Of Nuclear Reactions Probability In A Crystal Lattice Of Titanium Deuteride

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For calculations of probability of nuclear reactions of hydrogen isotopes in the crystal lattice of titanium deuteride the model offered earlier for palladium deuteride was used. In a series of experiments the probability of D-D approach for random initial conditions was calculated, when initial energies of approaching deuterons were set in the range of energies 0.01-0.51 eV. For each experimental value of D-D approach the reaction rate was calculated on the shifted Coulomb potential with the shift energy, which equals to the energy of screening. The mean distance of D-D approach on all series equals 0.97 angstroms, that exceeds the mean distance in a molecule D-D. However, more than 14% of all experimental values show an approach of deuterons for a distance less than 0.1 angstroms. The general reaction rate for the given set of the initial conditions will make $10^{1.91}$ DD^{-1} s^{-1}. It is 4 orders of magnitude less, than the analogous rate calculated earlier for palladium deuteride. For optimization of calculations the most favorable initial conditions were selected. As a result the rate of the reaction calculated according to the above model should be additionally multiplied by a correction factor, which allows for the probability of the occurrence of these favorable conditions. In our case it equals 10^{-16} - 10^{-18}; the rate of the nuclear fusion reaction of deuterons in titanium deuteride should be 3-4 orders lower, than the earlier calculated rate for palladium deuteride and equals 10^{-14} - 10^{-16} DD^{-1} s^{-1}.

The titanium was the second metal after palladium, for which anomalous phenomena were detected at electrolysis in solutions of some electrolytes in heavy water and during adsorption and desorption of deuterium gas [1,2]. These anomalous phenomena were interpreted as nuclear reactions at low energies. In connection with the much lower cost of titanium it is interesting to evaluate theoretically probable rates of a nuclear fusion in this metal.

Many authors in more than 100 works proposed various hypotheses and suggested theoretical models to explain the anomalous experimental data. The models are elaborated to a various degree. Some authors make very rough estimations, the other ones tried to provide quantitative calculations (see reviews in [3,4]). In the first theoretical works it has been presented the probabilities of the nuclear reactions at low energies calculated by standard quantum-mechanical methods. The calculated rates of the nuclear fusion turned to be minor, i.e. significantly much lower to be possibly determined by the modern methods. What is the reason of the discrepancy between theoretical and experimental data? We suppose that it is related to the fact that the standard quantum-mechanical methods of calculation are first elaborated for the stationary states, wherein the averaging of the interaction of particles in time and space is used. The analysis of the experimental data shows that nuclear reactions occur under very nonequilibrium conditions. This causes great fluctuations in approaching of particles with equal energies. The fluctuations result from a specific place of interaction of the particles in a crystal structure and from the conditions of the dynamic screening effect of the approaching particles by the electrons of the outer shells of the atoms of solid bodies.

Earlier we have proposed a model, which makes it possible to evaluate the significant role of deformation of the metal electron shells for deuteron screening [5]. The probabilities of the nuclear interaction of deuterons, calculated by this model, correspond in the order of magnitude of the energy yield to those observed experimentally. In the present paper we will evaluate the dynamic deformation of the electron orbitals basing on a new approach, which includes the elements of quantum and classic mechanics.

According to the usual quantum mechanics concept, electrons, inhered in the shell of an atom, are described by the multiparticle wave function Ψ (r), and the probability of finding an electron in any region of space $d\Omega$ is determined by the following formula:

$$\int_{d\Omega} d\mathbf{r} |\Psi(\mathbf{r})\Psi^*(\mathbf{r})|$$

The simplified interpretation of electrons in an atom as electron "spread" in space (n (**r**) = | Ψ (**r**) Ψ * (**r**) |) is also used quite often. Such an approach is sometimes in a good agreement with theoretically calculated and practically measured results for some classes of physical tasks (for example, in solid state physics, atomic and molecular physics, interaction of ionic radiation with solids, Thomas-Fermi model of atom etc.).

At the same time it is thought that the electrons are in constant rotary motions with velocities two orders of magnitude less than the light speed (~ 1/137 for ground states of hydrogen atoms and a little bit greater for inner shells of other atoms). It is reasonable to suggest that this motion is not a perpetual series of tunnel jumping from one point in space to another, but happens on randomly threaded trajectories, thus fulfilling (for the system as a whole) fundamental conservation laws of energy and angular momentum (the latter one due to the central character of interaction forces between the particles composing the system). As a result of interaction with electrons of other atoms and exterior fields, the trajectory of each electron is distorted, and over long time intervals it will appear in different space regions in the neighborhood of the atom core. Thus, the time spent by an electron in a certain space region is proportional to the probability of detecting the electron in this particular region according to distribution of an electron probability density ($|\Psi(\mathbf{r})\Psi^*(\mathbf{r})|$). Thus, the proposed model does not contradict to the formal quantum mechanics descriptions of atomic systems.

The analysis of the particle interaction using the classic approach with regard to the random outer actions on the charged particles is not an artificial calculation method. It is developed from the interpretation of quantum mechanics on the basis of the stochastic Markov processes (see 6, 7 and references in these articles) and non-linear dynamics [8]. We believe that the proposed EODD model (electron orbital deformation dynamic model [4,9,10]) reflects a physical reality, which is important to realize some fast processes, the nuclear fusion reactions at lower energies, in particular. This approach to solve the problem of screening of the ion charges of hydrogen isotopes in the palladium crystal structure is given below as an example. More general problem on the relevancy of the above interpretation of quantum mechanics is beyond the scope of present article and requires special consideration.

According to the physical nature, the interaction potential obtained based on the solution of quantum-mechanical equations is the result of averaging over all possible distances of approaching for each values of particles energy. The possible approaching forms a kind of distribution with the average and most probable distance of approach, which corresponds to the point of the interaction potential. It can be reasonably presumed that the probability of this "spread" around the average distance greatly increases with the presence of the nonequilibrium situation and strong outer effects. However, since the rate of the reaction depends not linearly but exponentially on the distance of particle approaching, the use of the average values of approaching to calculate probable rate of the reaction results in considerably understated values of the probability of fusion reactions.

The peculiarity of our model is consideration of dynamic screening of deuterons by electrons of the outer shells of the metal atoms near the boundary of their two neighboring positions in the crystal structure.

For calculations of probability of nuclear reactions of hydrogen isotopes in the crystal lattice of titanium deuteride the model offered earlier for palladium deuteride was used [4,9]. The hydrogen isotopes predominantly occupy tetrahedral sites in the face-centered cubic lattice of titanium hydride. A symmetrical position of deuterium atoms concerning the edge connecting two adjacent tetrahedral sites in titanium was selected as initial conditions for calculations. In a series of numerical experiments the probability of D-D approach for random initial conditions was calculated, when initial energies of approaching deuterons were set in the range of energies 0.01-0.51 eV (the potential barrier for diffusion of deuterium atoms in titanium is 0.51 eV). For each experimental value of D-D approach the reaction rate was calculated on the shifted Coulomb potential with the shift energy, which equals to the energy of screening [4,9].

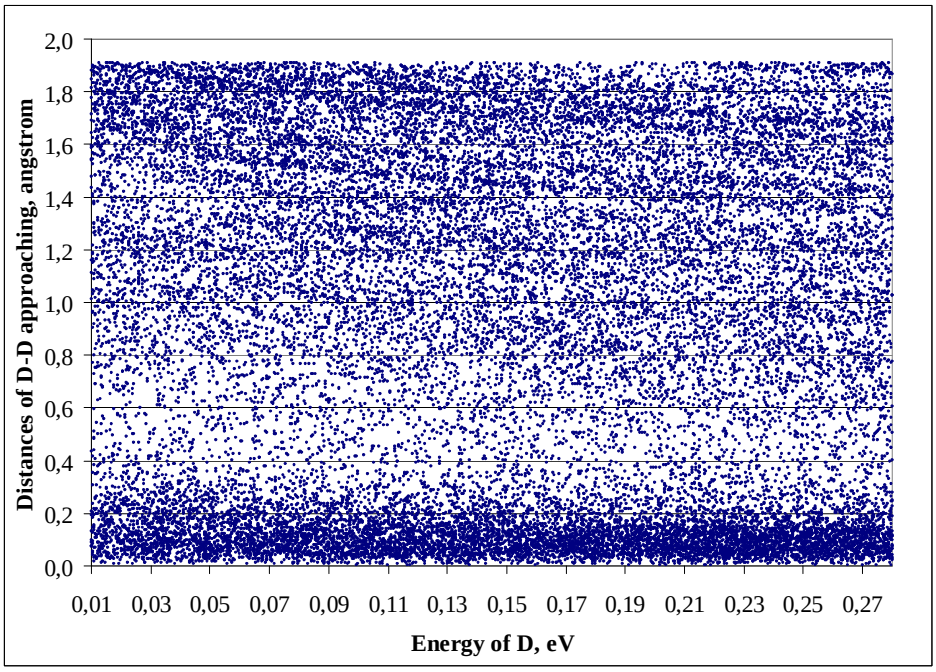

Fig. 1. Distribution of minimal distances of D-D approaching during their counter motions on the boundary of the neighbor T-sites in titanium deuteride vs their started kinetic energy.

The series consists of 34660 experimental values (fig. 1). The mean distance of D-D approach on all series equals 0.97 angstroms, that exceeds the mean distance in a molecule D-D. However, more than 14% of all experimental values show an approach of deuterons for a distance less than 0.1 angstroms (fig. 2). If one considers the reaction rate at each case of approach, and then averages as a whole on the entire sample, the general reaction rate for the given set of the initial conditions will make $10^{1.91}$ DD^{-1} s^{-1}. It is 4 orders of magnitude less, than the analogous rate calculated earlier for palladium deuteride [9]. For optimization of calculations the most favorable initial conditions were selected. As a result the rate of the reaction calculated according to the above model should be additionally multiplied by a correction factor, which allows for the probability of the occurrence of these favorable conditions. In our case it equals 10^{-16} - 10^{-18}. Thus, the rate of the nuclear fusion reaction of deuterons in titanium deuteride should be 3-4 orders lower, than the earlier calculated rate for palladium deuteride [9] and equals 10^{-14} - 10^{-16} DD^{-1} s^{-1}.

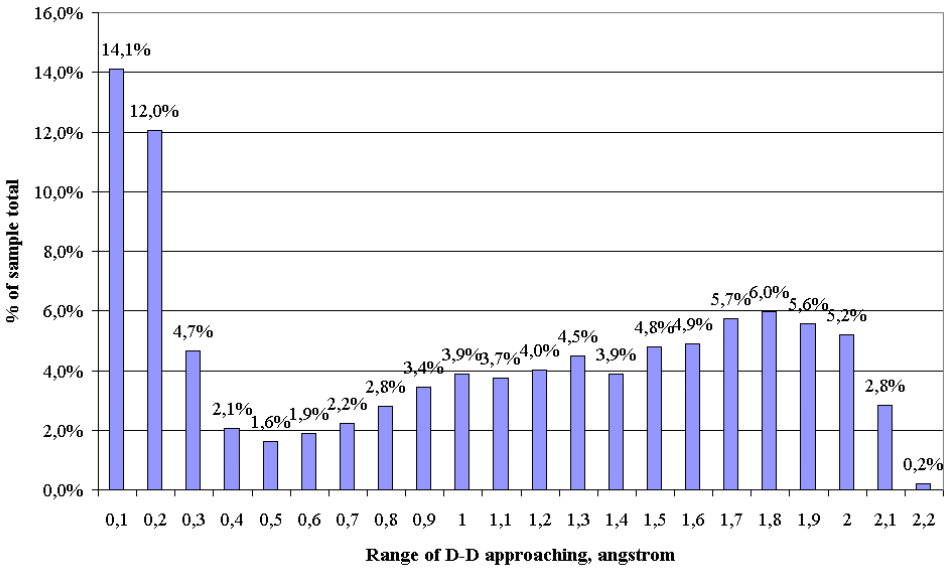

Fig. 2. Distribution of reaction D-D pairs on their range of minimal approaching to one another in titanium.

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