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LETTER TO THE EDITOR

The electron–nuclear system of the E-cell

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Abstract. Processes in a radiation defect (called the E-cell) of a crystal lattice of hydrides A_XH_Y (the ordering number Z and the mass number N of the element A must be equal to one of the following pairs of numbers: (2,3), (3,6), (4,7) or (5,10)), formed by the capture of a thermal neutron in a crystal, are considered. As a result of this capture, one of the lattice cells has a surplus of electrons forming the electronic shell of atom A. The phenomena in E-cells are mainly characterised by the following features: (i) the average density of free electrons in the central region of the E-cell exceeds 10^{25} cm^{-3}; (ii) H-nuclei rearrangement to a distance <0.1 Å leads to an energy gain in the electron–nuclear E-cell system; and (iii) the probability of H-nuclei tunnelling, determined as $\exp(-W)$, is characterised by $W = 20$–30.

The electrons are stably confined in the E-cell if the pressure in the crystal is in the Mbar range.

We consider a defect cell of a crystal lattice of a hydride A_XH_Y formed by an element A whose ordering number Z and mass number N are equal to one of the following configurations: (2,3), (3,6), (4,7) or (5,10). It is known that such a defect cell can be formed as a result of the thermal neutron induced fission of an atom A (see, e.g., [1]). Fission products leave the defect cell in a time $\sim 10^{-17}$ s, which is much shorter than the reconstruction time of the electron system ($\simeq 10^{-8}$–10^{-12} s). If the pressure in the crystal is of the order ~10 Mbar or greater, almost all the electrons constituting the electronic shell of the atom A remain confined in the defect cell. This effect has the following explanation: in order to leave the defect cell, the electron must first join the electronic shell of one of the atoms surrounding the defect cell and then it can leave the cell from the external side of the cell boundary. This process is accompanied by an increase in the total energy of the atom which can be interpreted as the height of the electron potential barrier.

The total energy of the electronic shell of the atom and (after electron precipitation) of the negative ion was estimated using the Thomas–Fermi (TF) model [2, 3]. In this framework it is supposed that the atom is squeezed to size X (where $X = R/d$ is a dimensionless radius, $d = 0.468$ Å is the length scale of the TF model) and the pressure needed for this is determined [2]. Calculations were carried out for $Z = 3$ and $Z = 5$, and the results obtained are shown in table 1.

It is reasonable to compare the height of the potential barrier ΔE with the average energy $\sim 16Z^{4/3}$ eV of electrons which remain in the cell after the fission products of the

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Table 1. Pressure and energy values for various X, R.

		$Z = 3$		$Z = 5$	
X	R (Å)	P (mbar)	ΔE (eV)	P (mbar)	ΔE (eV)
1.50	0.70	17.7	60.1	34.0	72.6
1.75	0.82	7.82	44.2	14.2	52.5
2.00	0.94	3.90	33.7	6.76	39.5
2.25	1.05	2.18	26.7	3.54	30.8
2.50	1.17	1.33	21.6	2.01	24.7
2.75	1.29	0.87	17.9	1.21	20.3
3.00	1.40	0.59	15.1	0.77	16.8
3.25	1.52	0.43	12.9	0.51	13.3
3.50	1.64	0.32	11.1	0.35	12.2
3.75	1.76	0.25	9.89	0.24	10.6
4.00	1.87	0.19	8.64	0.17	9.38

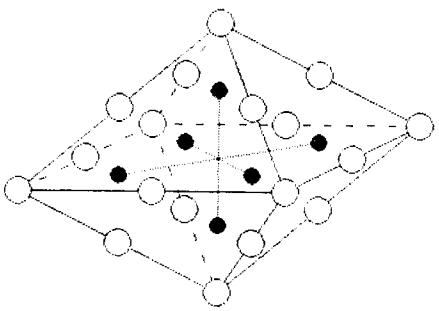

Figure 1. Geometry of the E-cell. The open circles are the Li atoms, the full ones are H atoms.

atom A nucleus leave it. This implies the use of the above mentioned estimate of the pressure needed for the confinement of the electron in the defect cell.

The non-compensated electric charge arising in the defect cell implies the attraction of neighbouring atoms and, therefore, the effective decrease of the cell volume (by approximately a factor three). This is accompanied by the growth of the average density of electrons to about $\sim 10^{25}$ cm^{-3}. Supposing that the electron gas in the defect cell is degenerate, we find that the Fermi energy is ~ 100 eV, and that the average electron kinetic energy is of the same order.

A feature of the processes occurring in the defect cell is the formation of a common electron–nuclear system, in which displacements of hydrogen nuclei induce a change in the total energy of the electron subsystem. This circumstance allows us to consider the defect cell as a new physical object called the 'E-cell'.

Let us clarify the idea of the E-cell. Let us consider for instance the cubic crystal structure of the NaCl-type lattice (e.g. LiH has such a structure). Suppose that the centre of the E-cell is located at the site of the fission nucleus and that the centres of the neighbouring metal atoms are connected by straight lines. The border of the E-cell formed by these lines is octahedral (see figure 1). Six H atoms together with their own electrons and the Z electrons forming the electron shells of the central atom are located inside the E-cell. We also attribute to the E-cell system a part of those electrons which

belong to boundary atoms. Using the considerations of [4] about charge distribution between cells in a crystal lattice, we infer that the number of these electrons is equal to $4Z$. Therefore the total number of electrons in the E-cell is $N_e = 5Z + 6$.

Exact quantum mechanical calculations for a system with such a number of particles are impossible. But here we can use statistical methods or even, due to the comparatively large size of the E-cell, the quasiclassical approximation of these methods, which is known as the TF model [2].

To simplify the mathematical part of the problem we use the spherical model of the E-cell, i.e. we replace the boundary octahedron by a sphere with the same volume. The radius R_c of the sphere is related to the crystal lattice constant, L, via the equation $R_c = Ln^{-3/2}$. We suppose that the $4Ze$ contribution of the boundary nuclear charge is uniformly distributed along the sphere surface, while the charge of the N_e electrons and $N_H = 6$ hydrogen nuclei is continuously distributed in the E-cell space according to the electrical potential (U) distribution.

Let us now consider the problem of the collective interaction in the electron–nuclear system of the E-cell. Let us suppose that two H nuclei are located at the points $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$. As in the TF model, the distribution of the electron density, n, is consistent with the distribution of the electrical potential U. The equation for U has the form

$$\Delta U = 4ne(n(U) - \delta(\boldsymbol{r} - \boldsymbol{r}_1) - \delta(\boldsymbol{r} - \boldsymbol{r}_2)). \tag{1}$$

It is solved numerically and then the kinetic and potential energies of the electron system as functions of the distance between H nuclei and the cell centre (under the assumption $\boldsymbol{r}_1 - \boldsymbol{r}_2$; $|\boldsymbol{r}_1| = r = dx$) are found. The results for $Z = 3$ are depicted in figure 2: curves 1, 2 and 3 correspond respectively to the kinetic, potential and total energy of the electron system, while curve 4 corresponds to the total energy E of the electron–ion system (including the potential energy of the Coulomb interaction of H nuclei). These results imply that the electron subsystem tends to bring together the nuclei; the mutual repulsion of the latter becomes important only at the distances less than 10^{-9} cm.

The equilibrium position of nuclei corresponds to $X_0 = 0.185$. Knowledge of the function $E(r)$ makes it possible to calculate the probability of nuclear tunnelling. In the quasiclassical approximation, this probability is determined by the exponent $\exp(-W)$, where [3]

$$W = 2\sqrt{2M}\int_0^{R_0} \mathrm{d}r \frac{\sqrt{E(r) - E}}{h}. \tag{2}$$

Here M is a reduced mass of H nuclei, E is their initial energy, and R_0 is the back point of their classical motion. If E is supposed to be equal to the maximal depth of the potential (i.e. the nuclei are assumed to tunnel from the equilibrium state), then $W = 27$. One may suppose, however, that the nuclei have the same average kinetic energy as the electrons have (i.e. about 100 eV). In this case $R_0 \sim 3 \times 10^{-10}$ cm, while the tunnelling probability is determined by the quantity $W = 17$.

The results obtained make it possible to estimate the time t which characterises the reaction of hydrogen nuclei fusion in the E-cell. If n_H ($\sim 4 \times 10^{24}$ cm^{-3}) is the density of nuclei, v ($\sim 10^7$ cm s^{-1}) is their velocity, and S_{eff} is the effective cross-section of the reaction, then

$$t = 1/n_H v S_{eff} = 2.5 \times 10^{-8}/S_{eff} \quad \text{s}. \tag{3}$$

Here S_{eff} must be expressed in barns. To calculate S_{eff} we assume that it is the nuclei D and T that participate in the reaction and use the results of measurements of S_{mes} (see,

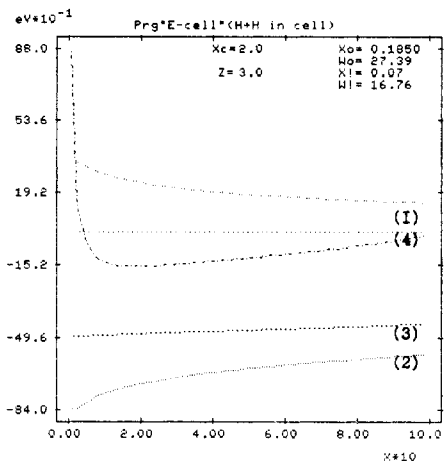

Figure 2. The dependences of the energy components of the E-cell electron–nuclear system on the distances between H nuclei.

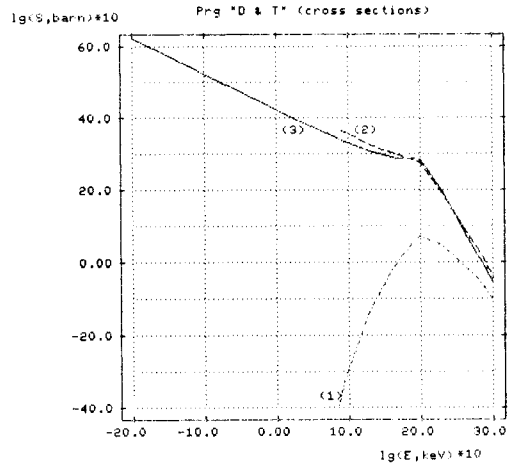

Figure 3. Energy dependence of the nuclear fusion cross-section.

e.g., [5]). The difference between S_{mes} and S_{eff} is caused by the difference between the Coulomb interaction of nuclei D and T in the measurement process (one may assume that they interact in vacuum) and in the E-cell. Taking into account the tunnelling probability, we may determine the section S_{nuc} of nuclear interactions from the known S_{mes}. Assuming that the interaction is of a resonant nature (this conjecture is justified by the form of the dependence of S_{nuc} on the energy) and interpolating the function S_{nuc} with the help of the Breit–Wigner formula, we can extrapolate the function S_{nuc} up to argument values ~100 eV.

The results of this calculation are depicted in figure 3: curves 1, 2 and 3 correspond respectively to S_{mes}, S_{nuc} and S_{ext}. These results imply that $S_{nuc} \simeq 1$ Mbarn for a H nuclei energy of 10–100 eV. Substituting these quantities into (3), we obtain

$$t = 2.5 \times 10^{-14} \exp(W) \quad \text{s.} \tag{4}$$

If $W = 27$, we have $t = 10^{-1}$ s. For the most favourable case $W = 17$ and $t = 10^{-5}$ s.

Our main result is the depiction of a new physical object called the 'E-cell', in which displacements of hydrogen nuclei induce a change of the total energy of the electron subsystem. The phenomena in the E-cell are mainly characterised by the following features:

(i) the average density of free electrons in the central region of the E-cell exceeds 10^{25} cm^{-3};

(ii) H-nuclei rearrangement to a distance <0.1 Å leads to an energy gain in the electron–nuclear E-cell system; and

(iii) the probability of H-nuclei tunnelling, determined as $\exp(-W)$, is characterised by $W = 20$–30.

The electrons are stably confined in the E-cell if the pressure in the crystal is in the Mbar range.

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