BORON - IMPURITY TRAP IN ELECTROCHEMICAL NICKEL SYSTEMS FOR THE HYDROGEN ATOMS

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Abstract: The main objective of this work is to study the influence of boron during the processes of hydrogen permeation of electrochemical systems based on nickel. In this regard, the experimental results of the behavior of hydrogen in electrochemical nickel systems in the course of their boron doping are considered. The introduction of the boron concentration in excess of 5 nuclear percent in electrochemical nickel helps to increase the amount of occluded hydrogen. A possible reason for this behavior is the presence of impurity and structural traps for atoms of hydrogen. Boron atoms as impurity traps are considered. Concentration of hydrogen in the electrochemical system is defined as the probability of the formation of defective structures in the metal and is a random variable. The probability density of distribution of defects in the electrochemical system is a function of the parameters of electrolysis. However, the main factor is the current density and chemical composition of electrolyte (presence amorphizator - boron). Amorphous alloys based on aluminum or nickel may be used as drives of hydrogen. Mathematical modelings of the interaction of hydrogen atoms together with the structural traps were performed. The kinetics of capture hydrogen atoms by structural traps was also defined. The physical model of formation of tensile stresses in the vicinity of the boron atoms was proposed additionally. Hydrogen atoms are deployed in places where there are defects of the crystal lattice, forming a connection with nickel and boron. Hydrogen atoms are located near the defects of crystal lattice, thus forming a connection with nickel and boron. Tensile stress occurs in the vicinity of boron atoms. It provides the interaction of boron atoms with hydrogen and the formation of impurity traps for atoms of hydrogen.

Key words: boron, alloying, system of nickel-boron-hydrogen, structural defects, dislocation, declination, the top of microcracks, hydrogen, hydrogenation, octapores, tetrapores, battery hydrogen metal hydride, trap hydrogen atoms.

Nomenclature

a - half-length of microcracks;

b - modulus of the Burgers vector of an edge dislocation;

B_1, B_2 and B_3 - constants depending on the material;

C_0 - average concentration of hydrogen atoms;

C_p^1 - the equilibrium concentration of hydrogen atoms at the inner radius of a structural defect environment;

C_p^2 - the equilibrium concentration of hydrogen atoms at the outer boundary of structural defects environment;

D - diffusion coefficient of hydrogen atoms;

D_c - diffusion coefficient of the impurity atom;

D_k - diffusion coefficient of the complex;

DH - diffusion coefficient of the hydrogen atom;

ΔE – the binding energy of the complex;

k - Boltzmann constant;

$N(\tau)$ - value of the time dependence of the number of captured hydrogen atoms;

r – radial component of polar coordinate system;

r_0 - inner radius characterizing structural defects;

R - the average half-distance between defects (outer radius surrounding the declination);

T - absolute temperature;

V - interaction potential of the hydrogen atom with the stress field of structural defects.

Greek letters

$\delta\upsilon$ - the volume change of the metal when placing the hydrogen atom;

θ - angular component of polar coordinate system;

μ - shear modulus;

σ - external stress;

σ_{ll} - the first invariant of the stress tensor of the structural defects;

υ - Poisson factor;

τ - the dimensionless time;

ω – magnitude of turning of disclination vector.

1. Introduction.

It is known that in the foreign and domestic literature, for example [1-6], there is information about the possible use of hydrogen compounds of metals for safe energy-efficient way to store hydrogen. However, the literature generally describes the behavior of metals and alloys obtained by metallurgical method. As for the possibility of using electrochemical systems of storage of hydrogen, this theme in the literature is almost absent. Basically the development of this direction is carried out by scientists in Russia and Ukraine. It should be noted, that the basic attention in scientific publications of galvanizing, for example, [7, 8] is given to the problem of the removal of hydrogen from electrochemical systems (metals and alloys) as a component causing the deterioration of physical and mechanical properties (the appearance of hydrogen embitterment).

The materials of this article are submitted for consideration of the problems of application of electrochemical systems for hydrogen storage, which was developed in the Russian scientific schools.

Electrolytic metals and alloys, unlike metallurgical, have a different mechanism. Firstly: hydrogen on the electrode (cathode) is allocated together with the formed atoms of metal according to equations:

$$Me^{n+} + ne \rightarrow Me^0$$
$$H^+ + e \rightarrow H^0$$
$$H^0 + H^0 \rightarrow H_2$$
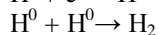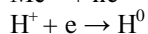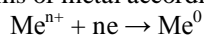
Secondly: the presence of atomic hydrogen (chemical reaction 2) increases the probability of interaction of metal with hydrogen.

And, finally, the third: the formation of structural defects, which has a higher potential in comparison with usual atom, becomes possible in case of electric crystallization of metals. The interaction of a hydrogen atom is most likely if such defects are.

Therefore, the process of hydrogenation of electrochemical systems differs from the interaction of hydrogen with materials of metallurgical production. In connection with the peculiarities of formation of structure of electrolytic coatings problem occurs due to the different nature of creating links metal-hydrogen and different strength of the link Me–H. That is why the question about the stoichiometry of the formed compounds of the metal-hydrogen is highly uncertain because dispersion of the energy of coupling for different types of defects is large enough.

According to the said previously, the concentration of hydrogen in electrolytic metals and alloys on their various areas can be very different, and this in turn will determine the kinetics of diffusion processes.

Many works are devoted to the diffusion of hydrogen in electrolytic metals and alloys; however applied classic methods of diffusion research do not give comparable results due to a number of reasons. At the same time, indirect methods for determination of hydrogen content in the studied sites (in galvanic coatings) provides only an integral picture of the contents of hydrogen in the sample.

Firstly, diffusion processes in electrolytic metals have a number of features that differentiate them from structures received by metallurgical method. Secondly, the hydrogen as the main research goal is logged badly by radiographic and spectrophotometric method.

And finally, the known isotope mass-spectroscopic methods can be applied to the study of these processes with a large limitation of the validity of the results.

The main feature of electrolytic coatings is the presence in the metal structure of a large number of defects, their density distribution in the bulk is a random feature. Therefore, the determination of the concentration of defects on the surface of the electrode becomes impossible.

At the same time, indirect methods for determination of hydrogen content in the studied objects (electroplating) allow you to see only the integral picture of the contents of hydrogen in the sample.

A distinctive feature of electroplating compared with compact metals is their specific behavior during heat treatment. In particular the amount of the hydrogen absorbed by galvanic metals and alloys is abnormally great in comparison with typical metals.

High concentration of defects in electrochemical systems allows attributing them to amorphous structures.

Number of defective structures is in direct ratio to the volume of absorbed hydrogen.

On the basis of this interrelation it is possible to consider electroplated coatings as the disorder structures inclined to interaction with hydrogen on borders, having high potential energy.

Since the number of crystallization centers in the galvanic processes depends on the current density, it can be assumed that the irregularity of the local values i_c will determine the active centers of the formation of compounds of the metal-hydrogen. According to the equation of classical electrochemistry [9] the cathode current is equal to:

$$i_c = i_0 \left[e^{\frac{\alpha ZF}{RT}} \cdot \eta - e^{\frac{(1-\alpha)ZF}{RT}} \cdot \eta \right]. \qquad (1)$$

From a formula (1) it follows that value of cathode current depends first of all on current of an exchange (i_0) in system electrolyte metal-solution. Ideally amorphous system should be such a structure at which

there is no crystal, and between atoms there are only electronic connections, i.e. in the conditions of electrochemical structure the number of the centers of formation of germs in system would strive for infinity. In real conditions the number of centers of crystallization is determined by the formula:

$$N = N_0 \cdot e^{\frac{A_3}{\kappa T}} \qquad (2)$$

Thus, preceding from the formula (2) the number of the centers of the formation of nucleuses will increase with the reduction of work on formation of a single nucleus. On the other hand, the density of a current is directly proportional to the number of nucleation centers. It follows that the extremely high current densities should be formed coating greater degree of amorphization. Apparently, similar processes occur in nickel alloys, where boron is used (as amorphizator) as an alloying element [10].

In general, the amount of dissolved hydrogen in metal can be determined from the expression:

$$V_{H_2} \equiv (m_{Me}/\rho_{Me}) \cdot N_A , \qquad (3)$$

$$V_{H_2} \equiv V_{Me} \cdot N_A \cdot k_L \cdot k_d \cdot k_i \; , \qquad (4)$$

where N_A - Avogadro constant; k_L - coefficient depending on the effects of external fields on the process of formation of compounds Me-H; k_d - coefficient of defects, taking into account the number of generated defects per unit volume; k_i - coefficient of conversion of metal volume in atomic weight in accordance with the number of N_A (how many grams of - atoms occupy the bulk of metal).

To use such formula for analytical definition of amount of the dissolved hydrogen is quite difficult. At the same time, it reflects all the phenomenology of process of interaction of hydrogen with metal at its electrochemical restoration. Earlier in [10] it was shown that the content of hydrogen electrochemical coatings type on the basis of alloy Ni-B depends on a number of factors: V_{H_2} = f (C boron additives, i_C, $t_{el\text{-}lyte}$, $\tau_{el\text{-}lyte}$). Detailed study of this process showed that the concentration of boron in the system is one of the determining factors influencing the content of hydrogen in the electrolytic alloy Ni-B.

The aim of this work was to study the impact of boron on structural changes and processes of interaction with hydrogen in electrochemical systems on the basis of nickel.

In this article attempts of carrying out complex researches of features of some elements possessing properties of metal structures, for the purpose of their use as the main electrode materials for hydrogen accumulators were made.

2. The experimental procedure

The content of hydrogen determined by a method of vacuum extraction. When determining the content of hydrogen in Ni - B alloys it was supposed that hydrogen is in solution in the form of gas inclusions (discontinuities, filled with hydrogen).There are several methods for determination of hydrogen content in the alloys. Currently the vacuum extraction method for determination of content of hydrogen is the most developed and accurate.

Its principle is based on heating of an analyzed sample in vacuum up to the temperature at which there is rather intensive diffusion of hydrogen from a sample. The volume of the emitted gas determine by change of pressure in system at its constant volume.

Concentration of hydrogen (cm^3/100g of metal), containing in a sample, is defined under a condition if its mass is known. For this purpose a sample placed in the quartz camera in which the vacuum about 10^{-5} mm Hg is created. The sample was heated to a temperature of 500 degrees C. Then pressure was measured before heating and after heating the sample respectively. The hydrogen volume was determined by calculating the difference of pressure. The hydrogen volume is calculated by the difference of pressure before and after heating by the formula:

$$V_{H2} = 205 \cdot \Delta P/m, \quad cм^3/100 \, g, \qquad (5)$$

where ΔP - is the pressure difference, mm. Hg;
m - mass of the sample, g; coefficient 205 defined constructive characteristics of the measuring equipment.

This study was carried out in sulfamate electrolyte for nickel – plating, by using boron compounds of class of higher polyhedral borates $Na_2B_{10}H_{10}$ [11].

Characteristics of the electrolysis process: the current density, i_C = 0.5 to 4.0 A/dm²; the temperature of the electrolyte $t_{el\text{-}lyte}$ = 30 – 50 °C; pH = 3.5 – 4.5. Nickel was used as the anode, copper brand M-1 - as the cathode. Spectrophotometric method was used to determine the content of boron in the system Ni-B [11]. The electronic microscope of УЭМВ – 100 AK was applied to research of structure of coverings of Ni-B. For research of phase structure of samples the x-ray difractometer ДРОН – 2.0 was used.

3. Experimental results and their discussion

The relative content of boron alloy Ni-B is 0.5-1 %. However, the proportion of alloying component increases to about 6-10 atm. %, if it is recalculated using the atomic mass. It means that, 1 atom of boron on each 10-15 atoms of nickel are formed the phases of introduction in total. The influence of concentration of boron additives on hydrogen permeation of the system Ni-B is shown in figure 1.

The relative content of hydrogen $V_{H_{2,Ni}}$ =104 sm³/100 g cathode current density i_C = 2A/dm²; acidity

of pH = 4,0; electrolyte temperature t $_{el\text{-}te}$ = 40 ^{0}C). The degree of hydrogenation of Ni-B with increasing boron content of 0.35 to 1.33% increases.   Analysis of experimental data shows that the hydrogen content in the Ni-B system is less than in the same mode for Ni electrolysis at the same electrolysis regimes.
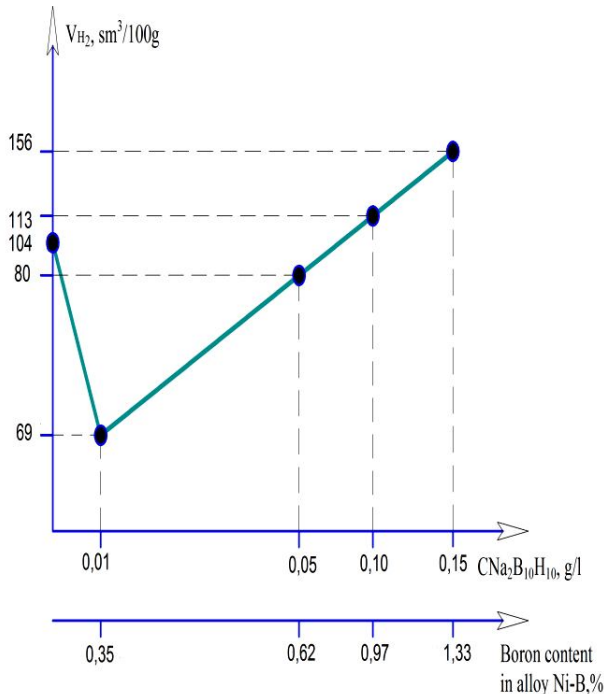

Fig. 1. The dependence of the hydrogenation of Ni-B on the concentration of boron-containing additives in the electrolyte. Electrolysis mode: i$_C$ = 2 A/dm^2, t$_{el\text{-}te}$ = 40 ^{0}C, pH = 4.0, the sample thickness d = 4 mm, base - copper brand M-1.

For example, the hydrogen content in nickel $V_{H_{2,Ni}}$ = 104 sm^3/100 g, and $V_{H_{2,Ni}}$ = 80 sm^3/100 g - in the system Ni-B (electrolysis mode: i$_C$ = 2 A / dm^2; pH = 4,0; t$_{el\text{-}te}$ = 40 ^{0}C) at a concentration in the electrolyte Na$_2$B$_{10}$H$_{10}$ of 0,05 g/l. A further increase in the electrolyte Na$_2$B$_{10}$H$_{10}$ concentration above 0.1 g/l leads to increased levels of boron and hydrogen in Ni-B system. In the system of Ni-B volume of hydrogen is greater than in an ordinary Ni - alloy. Thus, when the concentration of boron-containing additives in the electrolyte C$_B$ = 0.15 g/l; $V_{H_{2,Ni}}$ = 156 sm^3/100 g, (electrolysis mode: i$_C$ = 2 A / dm^2; pH = 4.0; t$_{el\text{-}te}$ = 40 ^{0}C), the sample thickness d = 4 mm.

This phenomenon is correlated with the structural changes in the nickel system in the presence of boron. Firm solution of boron and hydrogen is formed in nickel at an alloying of electrochemical nickel systems by boron to 1%. In the course of crystallization there is a formation of a face-centered crystal lattice (FCC) of nickel [11]. This is proved by x-ray and electron microscopic analysis of the studied samples.

Data on the effect of boron concentration in the Ni-B coatings on the internal tension (σ), hydrogenation

($V_{H_{2,Ni}}$), phase composition, texture are presented in the table. Inclusion of an alloying component – boron in a lattice of nickel increases dispersivity of received coverings (fig. 2A, B).
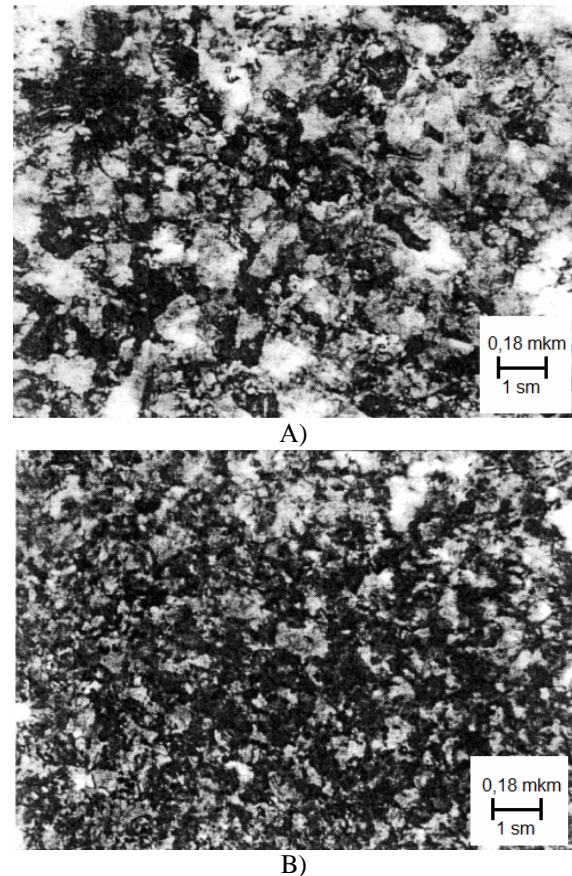

Fig. 2. Microstructure of Ni (A) and Ni-B (B) precipitation. Electrolysis mode: boron content in the coating Ni-B - 0,5%; i$_C$ = 2 A/dm^2; pH = 4,0; t$_{el\text{-}te}$ = 40 ^{0}C;

For nickel films, obtained at electrolysis mode: i$_c$ = 2 A/dm^2; pH = 4,0; t$_{el\text{-}te}$ = 40 ^{0}C, the predominant number of grains (68%) is in the limits of sizes from 0 to 400 A so that the texture thus obtained can be attributed to the fine-grained, and the form of grains - as equiaxed one (Fig. 2A). For Ni-B film with a boron content of 0.5%, for the regime of electrolysis: i$_c$ = 2 A/dm^2; pH = 4,0; t$_{el\text{-}te}$ = 40 ^{0}C, the predominant number of grains (93%) is in the limits from 0 to 400 A, and their resulting structure also is equiaxed form (fig. 2B). Thus, the share of large blocks, typical for pure nickel, decreases with increasing concentration of boron in the system Ni-B, and the share of small blocks increases. This impairs the perfection texture, causes deformation and increased distortion of the nickel crystal lattice and the reduction in the lattice period and the interlinear distance.

Internal tension increases approximately at 4 times if content of boron increases almost to 1% (table) while the parameter of a crystal lattice decreases so: on

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0,0003 Å - at concentration of boron of 0,62 % and - on 0,0009 Å - at concentration of boron of 0,97 %.

Increasing the concentration of boron in the system Ni-B causes an increase in the hydrogen content, compared with the nickel system. Probably, this process occurs by the capture of hydrogen into encirclement of boron, and, thanks to their more intensive interaction, in comparison with interaction of hydrogen with nickel. Atoms of hydrogen are deployed in places of defects of a crystal lattice, forming connection with nickel and boron. The number of defects in nickel-boron alloy surpasses their quantity in the samples with pure nickel. It is possible as boron replaces impurity with a small nuclear radius therefore reduction of parameters of a crystal lattice is observed at a nickel alloying by boron.

The tensile stress occurs in the vicinity of boron, which leads to the interaction of boron atoms with hydrogen and the formation of impurity traps for hydrogen atoms. Such a shift can be modeled using the internal stress fields in the vicinity of the boron atoms (radius of a nickel atom $r_{Ni} = 0.124$ nm, radius of the boron atom $r_B = 0.091$ nm; radius of a hydrogen atom $r_H = 0.046$ nm). The displacement of nickel atoms in the vicinity of the boron impurity is shown in figure 3. Distinction of nuclear radiuses is the reason of displacement of Ni atoms into the vicinity of the boron atom (atom substitution), which is the admixture. In contrast to boron, hydrogen is an implanted impurity, so it increases parameters of the nickel lattice. Hydrogen is localized in defective structures of a nickel alloy.

Joint sedimentation even in small amounts of boron (6 at. the %) with nickel from solutions of dekagidroborator of sodium leads to change of nature of emergence and growth of particles, and also density of their distribution. When nickel-boron systems are forming the speed of origin (emergence) of germs exceeds the speed of their growth therefore, unlike pure nickel, formation of new grains goes continuously in the process of passivating of a surface of growing sediment. It causes the reduction of the size of the crystallites being formed and increases their concentration on surfaces. On the one hand it testifies about possibility of formation of structures with the greatest number of defects in unit of volume of the metal due to existence in them structural and impurity traps. On the other hand,

introduction of boron promotes the formation of implicitly expressed crystal structure with transition to amorphous structures. As it is known, the metals which are in an amorphous state accumulated on ~ 40% of hydrogen are more, than crystal structures [3].
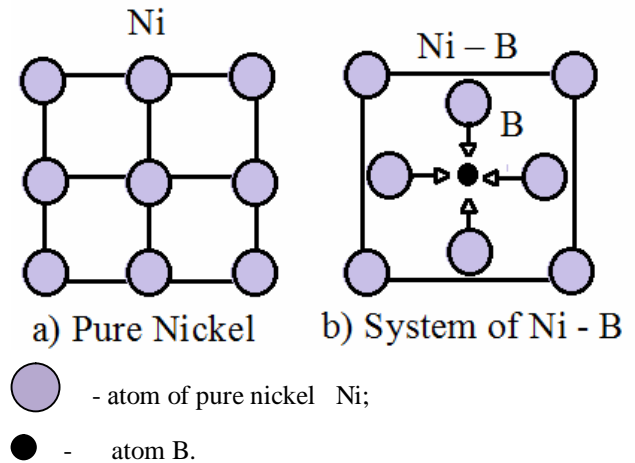

- atom of pure nickel Ni;

- atom B.

Fig. 3. The displacement of nickel atoms in the vicinity of the boron impurity

When electric crystallization of nickel in the presence of boron formed different structural defects that change the kinetics of hydrogen absorption, as well as its content per unit volume.

Possibilities of electrochemical systems on the basis of nickel on reversible sorption of hydrogen, taking into account the fields of tension created by structural defects, are considered. The main types of structural defects are edge dislocation, tops of microcracks and wedge

Positive wedge isclinations. Atoms of hydrogen interact with fields of tension of the listed defects. The content of hydrogen is increasing in the unit of volume of metal. For the description of diffusive processes, in the presence of impurity atoms, the model is chosen in the form of cylindrical covers (hollow cylinders) and process diffusion of atoms of hydrogen through a cylindrical cover with impurity and structural traps is shown [12].

Table 1

Internal stress, texture, phase composition and hydrogenation of Ni-B coatings with different boron content. Electrolysis mode: $i_c = 2$ A/dm^2, pH = 4.0, $t_{el-te} = 40$ °C

B content in the alloy, % A. weight	Phase composition	d_{311} A	a_{av} A	Grain size, μm	Texture axis	σ, MPa	V_{H_2} cm^3/100 g
0	FCC lattice of Ni	1,0624	3,5236	0,06-0,20	<111>	75,7	80
0,35	One phase: solid solution of B in FCC lattice of Ni	-	- 3,5233	-	<111>	50	43
0,62		1,0623		0,02-0,12	<111>	135	60
0,97		1,0621	3,5227	-	weak no	308	88

4. Mathematical modeling of the experimental results

Structural and impurity traps for hydrogen atoms were considered for the mathematical modeling of the experimental results. Diffusive migration of hydrogen atoms in the volume of metal and the subsequent appearance of impurity segregation and the hydride phases depend on the formation of structural and impurity traps. Defects in the crystal structure: dislocations, disclamations, grain boundaries are understood as structural traps. Substitution impurities having a small atomic radius, compared to the base metal (boron impurity in nickel, for example), form a so-called impurity traps. Different types of traps interact with hydrogen atoms. Types of interaction have their own characteristics. Structural traps (edge dislocations, for example) provide the seizure and retention of hydrogen atoms for a long time due to hydrogen segregation or hydride phases. With the help of impurity traps for some time there is a seizure of atoms of hydrogen with the formation of inactive complexes. After some time (especially temperature rise) complexes disintegrate and free hydrogen atom meets new impurity trap in the form of impurity substitution small ionic radius. The slowdown of the process of diffusion is observed as a macroscopic phenomenon. Slowing the diffusion process is observed as a macroscopic phenomenon. The diffusion coefficient of the complex is determined by the expression (6) [13]:

$$Dk = (DH \cdot Dc/(DH +Dc) \cdot exp (\Delta E / k \cdot \Delta T), \qquad (6)$$

where Dk - the diffusion coefficient of the complex, DH - the diffusion coefficient of the hydrogen atom, Dc - diffusion coefficient of the impurity atom, ΔE – the binding energy of the complex, k - Boltzmann constant, T - absolute temperature.
If DH >> Dc, then (6) takes the form:

$$Dk = Dc \cdot exp (\Delta E/k \cdot \Delta T). \qquad (7)$$

The above inequality (7) is always satisfied for the hydrogen atoms (especially at low temperatures). Therefore, the diffusion coefficient of the complex "a hydrogen atom - a small atomic radius of substitution impurity" depends only on the binding energy of the two atoms. The definition of this energy is the separate task and is not discussed in this article.

The main types of structural traps for hydrogen atoms must be considered. The main types of structural defects are edge dislocations, the top microcracks and wedge disclamation. They differ from each other by a singularity. The main characteristic of the structural traps is the interaction potential (binding energy) of the hydrogen atom with the stress field of structural defect.

Potential of interaction of atom of hydrogen with a field of tension of structural defects is defined by a known ratio (8) [14]:

$$V = - \frac{\sigma_{ll}}{3} \delta \upsilon , \qquad (8)$$

where σ_{ll} - the first invariant of the stress tensor of the structural defects;
$\delta\upsilon$ - change the volume of the metal when placing the hydrogen atom.

This value is a constant value for all metals and is $\delta\upsilon$ = 3•10-30 m3 [15]. For σ_{ll} > O (positive dilatation), and $\delta\upsilon$ > 0 (the hydrogen atom increases the lattice parameter), the potential V takes a negative value. This corresponds to the attraction of a hydrogen atom to the area surrounding the structural defect.

The potential V is its dependence on the coordinates for each of the structural defect (edge dislocations, the top cracks and wedge declinations) [12, 15]:

$$V_1 = -A_1 \frac{sin\,\theta}{r}, \qquad A_1 = \frac{\mu b(1+v)}{3\pi(1-v)}\delta\upsilon$$
(Edge dislocation)

$$V_2 = -A_2 \frac{cos\dfrac{\theta}{2}}{\sqrt{r}}, \qquad A_2 = \frac{2\sqrt{a}\sigma(1+v)}{3\sqrt{2}}\delta\upsilon$$
(Top of microcracks)

$$V_3 = -A_3 ln\frac{r}{R}, \qquad A_3 = \frac{\mu\omega(1+v)}{3\pi(1-v)}\delta\upsilon$$
(Wedge declination) $\qquad (9)$

where r и θ - polar coordinates, μ - shear modulus , b - modulus of the Burgers vector of an edge dislocation , υ - Poisson factor , ω – magnitude turning vector of the declination, a - half-length of microcracks , σ - external stress, R - outer radius surrounding the declination, $\delta\upsilon$ - changes in the volume of the metal when placing the hydrogen atom.

Singularity of (9) at r → 0 is eliminated by introduction a neighborhood into the origin of coordinates. The size of the field (for example, the core of an edge dislocation) occupies the space of a few interatomic distances in the vicinity of structural defects (equation (9)) impurity segregation of hydrogen atoms and the metal hydride formed when the solubility limit is reached. These structural defects are traps for hydrogen atoms. They are called structural traps.

Kinetics of segregation of hydrogen in the vicinity of structural defects is described by the diffusion

equation of parabolic type with the corresponding initial and boundary conditions:

$$\frac{1}{D}\frac{\partial C}{\partial t} = \Delta C + \frac{\nabla(C\nabla V)}{kT}, \tag{10}$$

provided that $r0 < r < R$, $C(r, 0) = C0$,

$$C(r0, t) = C_p^1, \quad C(R, t) = C_p^2,$$

where D - diffusion coefficient of hydrogen atoms, k - Boltzmann constant, T - absolute temperature, r0 - a characteristic inner radius of a structural defect, 2R - the average distance between defects, C0 - average concentration of hydrogen atoms, C_p^1 and C_p^1 - the equilibrium concentration of hydrogen atoms at the boundaries of structural defects environment.

The exact analytical solution of the problem (10) exists only for a defect wedge disclamation with the use of the potential of interaction of hydrogen atoms with the stress field of structural defects. In this case, the interaction potential is determined by the logarithmic coordinate dependence. Solution of the problem using the expressions (9) calls the mathematical difficulties for other structural defects. Therefore, various approximate methods must be used. The most famous of them - using only the gradient of the interaction potential in the diffusion flux of hydrogen atoms. So, for example, only the second member of the right side is taken into account in the equation of diffusion. It is fair to describe the kinetics of segregation near a structural defect where the decisive contribution to the kinetics of the process is making the gradient of the stress field. The initial stage of the kinetics of formation of impurity segregation is subject to the following relationships in this approximation:

$$N_1(\tau) = B_1\tau^{2/3}$$
(Edge dislocation)

$$N_2(\tau) = B_2\tau^{4/5}$$
(Top of microcracks)

$$N_3(\tau) = B_3\tau \tag{11}$$
(Wedge disclamation),

$$\tau = \frac{Dt}{r_0^2}$$

where $\frac{Dt}{r_0^2}$ - the dimensionless time, B1, B2 and B3 - constants depending on the material, r0 - characteristic size of the region to avoid singularities in the interaction potentials.

The quantity N(t) is the dependence of the number of trapped atoms of hydrogen from the time [12]. It is proportional to the square of the characteristic dimension (cross sectional area) segregation of the hydrogen atoms which are formed from structural defects. The given ratios show ability of various defects to capture atoms of hydrogen from firm solution. Wedge disclination carries out this process in a linear (linear dependence of the dimensionless time). Kinetics of hydrogen segregation is slower for the top of the microcracks and edge dislocation. It means that atoms of hydrogen from firm solution are captured by means of structural defects (type of wedge disclinations) faster. To other structural imperfections at distribution of atoms of hydrogen remains less.

Impurity traps for atoms are substitution impurities of small atomic radius in relation to the size of the atoms of the base metal. Therefore, in the vicinity of such impurities tensile stresses are formed and the hydrogen atom is energetically preferable to form a complex with the impurity atom As a result, the diffusion mobility of hydrogen atom decreases. The effective diffusion coefficient of hydrogen atoms is introduced in the description of diffusion processes in these conditions, if the impurity traps are present.

Ceteris paribus, this is true. In the macroscopic scale the decrease of the diffusion coefficient of hydrogen atoms is observed.

In the macroscopic scale the decrease of the diffusion coefficient of hydrogen atoms is observed. Thus, structural and impurity traps reduce the hydrogen permeability of metal. If structural and impurity traps for hydrogen atoms are placed in the coating of structural elements, such coatings extend the operational period of the production of advanced equipment.

5. Conclusions

1. Experimental results on the behavior of hydrogen in electrochemical systems based on nickel at its doping boron atoms are considered. The introduction of a certain concentration of boron into the electrochemical nickel increases the number of absorbed hydrogen. The introduction of a certain concentration of boron into the electrochemical nickel increases the number of absorbed hydrogen. A possible reason for this behavior is the presence of impurities and structural traps for hydrogen atoms. It is necessary to consider atoms of boron as impurity traps.

2. Concentration of hydrogen in electrochemical system has casual character and is defined by probability of formation of defective structures in metal.

3. The energy of the metal-hydrogen depends on the potential of the defect and, presumably, it is spread over a sufficiently wide range. This fact determines the temperature of the extraction of hydrogen from the metal structure.

4. The probability density distribution of defects in an electrochemical system is a function of the parameters of electrolysis. However, the decisive factor is the current density and chemical composition of the electrolyte (the presence of amorfizator - boron).

5. Mathematical modeling of the interaction of hydrogen atoms with structural traps was performed. It is shown that the edge dislocations, microcracks top sand wedge disclination are structural traps. The kinetics of hydrogen atoms of capture by structural traps is determined.

6. The physical model of formation of the tension of stretching in a vicinity of atoms of boron is offered. Their emergence is caused by displacement of atoms of nickel in a vicinity of impurity of boron.

7. Structural and impurity traps reduce the hydrogen permeability of the metal.

Thus, to improve specific capacity in the drive requires the presence of structural defects as traps hydrogen. The composition of the alloy is regulated, and is chosen so that it has provided the required elasticity of dissociation of hydrogen [16].
Amorphous alloys based on aluminum or nickel can be used as such drives (abcorbat of hydrogen). Beryllium, boron, niobium, and rare earth elements can be alloying components.

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