CRACK GROWTH IN METALS AFFECTED BY HYDROGEN

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ABSTRACT

A theoretical model of the crack growth is proposed in terms of physical mechanics of a real crystal with provision for the hydrogen environment effect on metals, microfracturing peculiarities, physical aspects of hydrogen interaction with atoms of the crystal lattice and crystal structure imperfections, real elasto-plastic situation at the macrocrack interface.

KEYWORDS

Hydrogen embrittlement; mechanism of fracture; crack growth.

INTRODUCTION

The problem of hydrogen effect on fracture resistance of metals is a matter of scientific interest of different specialists: physicists, material scientists, engineers, designers, - all those who work to ensure serviceability of machinery and equipment. The needs of contemporary practice and future prospects in development of technology contribute to this interest. The reason for this is the development of "hydrogen economy" which is supposed to solve a number of technical, economic and ecological problems as it allows to produce, store, transport and consume energy with the aid of hydrogen.

Among hydrogen effects on various mechanical properties of metals - tensile strength, plasticity, fatigue characteristics, etc. - the initiation and propagation of cracks induced by hydrogen in deformed metals is worth a most profound interest. This proceeds from a well known fact, that in machine parts and structures it is impossible to guarantee absolute absence of cracklike defects or imperfections likely to cause cracks in the process of operation. Due to the hydrogen influence the defects, usually negligible, may become dangerous and cause accidental brittle failure of machine parts. Hydrofen affects metals in such way that strength of solids becomes dependent primarily on the crack growth behaviour in a given material. So, the studying of the hydrogen effect on the crack propagation process in metals becomes a problem of paramount importance.

The problem of the hydrogen-induced crack growth in metals requires a complex of approaches, which allows to obtain solutions of a series of fundamental and specific problems, studied by respective sciences. Basing on a general sequence of processes and events concerned in the metal - environment system (Moroz, Chechurin, 1967; Nelson, 1974), the following problems should be pointed out as of paramount importance:

- environmental reactions of hydrogen production and transport to metals;
- surface interaction and hydrogen entry into metal;
- state and behaviour of hydrogen inside metal;
- hydrogen effect on fracture initiation and propagation in metals.

The last problem has certain crosspoints with the problem of sufacial interactions in terms of the metal - environment system. But, the surface processes affect the fracture processes through the formation and development of deformed structures, but not involving their intrinsic properties and limiting characteristics. The hydrogen effects in the core of fracture on the formation of fracture pilots and their limit equilibrium state are concerned within this case.

The material strength science has acquired numerous data on the strength of materials by now. A series of hypotheses and concepts of the mechanism of hydrogen effect on the fracture process has been put forward. All these concepts explain the hydrogen induced fracture of materials by one (or several) of the following factors: 1)molecular hydrogen pressure in microcavities; 2)decohesion in the crystal lattice of metal; 3)interactions with dislocations; 4)formation of hydrogen-containing phases (hydrides, etc.); 5)surfacial influence (chemisorption).

Many scientists contributed to the development of this problem: Bernstein, Cherepanov, Johnson, Karpenko, Kolachev, Marichev, Oriani, Rice, Tetelman, Thompson, Troiano, Wei, Williams and others. Such a number of hypotheses proposed is accounted for both by a complicated character of hydrogen - metals interaction and complications in the very process of fracture. Each of the hypotheses usually explains the embrittlement by one only of the named factors and it is very often in such cases that very important results in physics and mechanics of deformation and fracture are not taken into account.

The stage of preceeding investigations of the problem may be described as analytic one, for it includes the designation of basic hydrogen effects on metals and each of the effects was investigated separately. Recently, this approach gives way to a synthetic one in studying the hydrogen induced fracture, when the factors of embrittlement are considered not separately but in their interconnection with the fracture process as a whole.

Here we shall illucidate the problem as a whole, for it is too manysided to be described in one report, we shall concern ourselves with only some of its aspects.

ANALYSIS OF THE HYDROGEN-INDUCED CRACK GROWTH BEHAVIOUR IN METALS ON THE BASIS OF THE BRITTLE FRACTURE CONCEPT

The hydrogen-induced crack growth behaviour in metals is conventionally studied basing on the fracture mechanics results. In such case it is usually accepted the concept of the stress intensity factors (SIF) taken as parameters unanimously determining the material mechanical state in the fracture process zone at the crack front, regardless of the mode of loading and geometry of a cracked solid. Analysing the phenomenology of the hydrogen effect on fracture in metals it is not difficult to arrive at some conclusions (Nelson, 1974) which seem to be so common that are assumed as axioms belonging to the theory of the hydrogen-induced crack growth in metals. They lead to the general concept that hydrogen-assisted crack growth in metals is controlled not only by the properties of the materials, but also by the processes of transportation and collection of hydrogen in local areas of the fracture process zone.

It follows from what has been stated, that for the case of the hydrogen-induced crack growth in metals the Griffith-Irwin brittle fracture theory, being under real conditions a basic concept for the macrocrack development study, does not fit the described process adequately. This is determined by the fact, that such model is based on the concept of only two crack states - propagating and non-propagating - and correspondingly of a single critical parameter, which marks the interface between these two states. In the case of hydrogen embrittlemet many authors already distinguish between three crack states and correspondingly, three SIF K_1 ranges (Nelson, 1974; Williams, 1973). We speak of the first state, when the physico-chemical characteristic of a system at a given load level do not provide conditions sufficient for the crack growth to start. This state is accompanied with a corresponding SIF range $K_1 < K_{1th}$, where K_{1th} is the thrshold SIF value. The second state is characterized by hydrogen transport controlled subcritical crack growth at $K_{1th} < K_1 < K_{1c}$, when the crack growth is delayed by the processes of the hydrogen transportation into the fracture core. And, finally the third one is the state of the post-critical crack growth at $K_1 \geqslant K_{1c}$, when the crack propagation at a given type of hydrogen distribution in the system is assisted by a purely mechanical factor i.e. the loading level, there is no need for any hydrogen redistribution. This crack state is similar to the crack state in testing under static loads and conventional conditions. The corresponding critical parameter is usually the same as the conventional crack propagation resistance (fracture toughness) K_{1c} (Johnson, 1976; Chaplja and others, 1979; Kobayashi and others, 1981).

Let us now consider the problem of the crack growth resistance of materials characterization in the presence of hydrogen and try to point out the parameters permitting to connect the laboratory specimens behaviour under testing and behaviour of materials in real-size structures. We shall discuss this problem in terms of the previously outlined crack growth behaviour.

Concerning quantitative characteristic of the hydrogen-affected crack growth resistance of metals, numerous authors (Alymov and others, 1976; Capeletti, 1976; Kolachev, Mal'kov, Sedov, 1975; Jablonskii, 1979) used a short-term fracture toughness parameter obtained with a standard procedure (ASTM standard, British standard, Soviet standard and other similar procedures (Panasyuk, Andrejkiv, Kovchik, 1977a; Srawley, 1977), writing K_{1c} for this parameter on analogy with the conventional fracture toughness parameter. In this paper let K_{1QH} denote this parameter with provision for its principal difference from the critical characteristic K_{1c}. A great sensitivity of the K_{1QH} parameter to hydrogen was stressed and it was assumed to be the measure of the hydrogenation sensitivity of the materials.

It should be mentioned that conventional concept (i.e. Griffith-Irwin concept) used in brittle fracture mechanics do not satisfy the demands of the study of the considered effect in case of hydrogen embrittlement of metals and do not allow to obtain the parameter characterizing the behaviour of the material, but not of a manufactured specimen. A study contributing to this concept and treating the origin and properties of the parameter K_{1QH} as those of the invariant characteristic of the material, was performed within our Institute by Chaplja and others (1979). Namely, the comparative fracture tests were carried out under normal conditions and in gaseous hydrogen environment with a conventional procedure of fracture toughness evaluation. The typical test results are given in Fig. 1. The tests were carried out in parallel with fractographic analysis of the specimens. For testing in hydrogen environment the "load - displacement" diagram proves to be nonlinear. The 5% secant line procedure was applied to obtain the K_{1QH} value. The K_{1A} value corresponding to the slow-to-unstable fracture transition denoted with a point A in diagram $P-\Delta$ and with the interface line A at the fracture surface was also obtained. It comes out in this case, that the value of K_{1A} equals the SIF critical value K_{1c}, obtained in the absence of hydrogen. Besides, the K_{1QH} value was proved to be only one of the SIF values from the $K_{1th} < K_1 < K_{1c_1}$ range, corresponding to the stage of the slow crack growth[1]. In this case it determines only the behaviour of a certain cracked specimen, but can hardly demand to be a parameter characterizing the behaviour of material under given conditions. In fact, the K_{1QH} value, determined by the 5% secant line procedure, i.e. by 2% increment in the crack length (Srawley, 1977), is dependent not only on the loading conditions (the SIF value alteration rate $\overset{\circ}{K}_1$) the average crack growth rate V_{av} in the interval from ℓ_0 to $\ell_0+\Delta\ell$ (ℓ_0 is the initial crack length), but on the calculated crack increment value $\Delta\ell = 0.02\ell_0$ i.e. on the specimen dimensions and even on the initial crack length in it. Such dependence in the first approximation is expressed by

$$K_{1QH} = K_{1th} + \overset{\circ}{K}_1 (0.02\ell_0 / V_{av}) . \tag{1}$$

This causes doubt about the comparability of the data obtained in the described way and limits the possibilities of their comparative application in evaluating the quality of the materials and predicting the crack behaviour in structures.

In recent studies of the hydrogen assisted crack growth characteristics in metals an approach based on the crack growth rate $V = d\ell/dt$ dependence on the SIF value have been widely

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[1] A similar study was later performed by Japanese researchers on internal hydrogen embrittlement (Kobayashi and others, 1981).

used. This dependence may be plotted on diagrams giving the most comparable and complete information on the crack growth resistance properties of materials affected by hydrogen and consequently used to evaluate growth of cracks in structures (Johnson, 1976; Wei, 1967). It is obvious, that all the experimentally obtained parameters and dependencies characteristic of fracture resistance of any "metal - hydrogen" system, are either included into these kinetic diagrams as K_{1th}, K_{1c} or may be calculated on their basis, as e.g. the diagrams of delayed failure in the coordinates of "applied load (the initial SIF value K_{1i}) versus time to failure t_f "(Wei, 1967).

It explains the great interest to their theoretical investigation and development of the diagrams in terms of certain theoretical concepts. Considerable success has been achieved in this sphere due to the studies conducted by Cherepanov (1974), Gerberich, Chen, John (1975), van Leeuwen (1974a, 1974b, 1975), Fishgoit, Kolachev (1981), see also review Andrejkiv, Panasyuk, Kharin (1978).

But known theoretical concepts of the hydrogen assisted main crack propagation in metals are, to our mind, somewhat schematic as they include, in full measure, neither the results of studying of elementary effects of interaction of hydrogen in deformed metals with atoms of the crystal lattice and structural imperfections, nor the achievements in physics of microscopic processes of deformation and fracture. These being phenomenological in origin do not present a description of the crack growth kinetics in materials in closed form. That is why it has become prospective to develop a theory of the hydrogen-induced crack propagation in metals with provision for the true elasto-plastic situation at the macrocrack contour, physical microscopic effects of hydrogen interactions with defects of metals structure and fracture origins, following macroprocesses.

ON THE THEORY OF THE HYDROGEN-INDUCED CRACK GROWTH IN METALS

The problem of the critical condition (fracture criterion) is the basic one for the theory of the hydrogen-induced crack growth in metals. In terms of this problem the intensity of mechanical effect on the macrocrack front in metal (determined by the SIF value) must be associated with the quantity of the hydrogen collected in the core of fracture at the moment, when the limit of the stable deformation of the material in the vicinity of the crack tip is reached.

The length of the potential fracture initiation zone is comparable with the crack tip opening displacement δ_t . To obtain it one may use the formula of the type (Cherepanov, 1974: McMeeking 1977):

$$\delta_t = \alpha K_1^2/(E\sigma_y) , \qquad (2)$$

where E is Young's modulus, σ_y -yield strength of the material, α -numerical coefficient ($\sim$1). In accordance with the available data on the SIF values at which the hydrogen-induced crack growth in various steels with different ultimate strength values is observed (e.g. data of McIntyre, Walker (1978) and Loginov. Phelps (1975)) the dimentions of the fracture initiation zone have the order of magnitude of 1 - 100μm. At intervals of such length in the vicinity of the crack tip the distribution of hydrogen may have a rather non-uniform character. The dimensions of the fracture origin may be evaluated by the dislocational microcrack size, which has the order of 0.01 - 0.1μm for metals (Grigor'jeva, Popov, Nosyreva, 1969; Vladimirov, 1976). Thus, it follows that the fracture initiation is associated with the peculiarities of the hydrogen distribution in the fracture zone. Meanwhile, the available experimental techniques to analyze the local hydrogen content allow to determine its total amount only in regions with a 100 - 300 μm diameter (Dikii and others, 1981: Smiyan, 1980). Thus, it is rather difficult at present to obtain the desired criterial relation experimentally. This problem calls for a more detailed theoretical study and development of techniques for indirect evaluation of the criterion in terms of available experimental data.

In this connection may the following be noted. The potential fracture zone limit state criterion should be selected with

provision for the condition, that depending on the hydrogen distribution the points of the given zone become differently related to the fracture causing stress - strain state and almost any of them may become the critical one. This criterion should be formulated as condition when hydrogen concentration C reaches its critical value C_{cr} in point X . The critical values are determined by the stress σ_{ij} and strain ε_{ij} components, which are the functions of K_1 and the point location. The generalized form of the fracture criterion is:

$$C(X) = C_{cr}(K_1, X) \quad \text{or} \quad K_{1cr} = K_{1cr}(C, X). \qquad (3)$$

It is assumed, that the stable deformation limit of the material at the crack tip is reached in case, when condition (3) has been realized in any point of the fracture process zone.

The phenomenological approach does not allow the right-hand part of the criterial equation (3) to be defined concretely. It is possible to solve this problem basing on the determination of relations between hydrogen and metal interaction and reaction of materials to mechanical actions. In this case it is needed to use some additional physical results and ideas, which constitute the model of the hydrogen-induced fracture mechanism for metals.

For almost forty years of intensive studies on the problem of hydrogen affected fracture of metals, beginning with the studies by Zapffe, a great number of models for the mechanism of this phenomenon has been proposed (they have been widely discussed by Kolachev (1966), Moroz, Chechulin (1967), Pokhmurskii Shved, Yaremchenko (1977), Smialovski (1962) and others). Some of these studies go only as far as qualitative explanation of some effects of hydrogen embrittlement in metals, the other studies present theoretic concepts proved by quantitative analysis. But common theoretic concepts are usually limited to only some of the "embrittling " factors (decohesive hydrogen effect, hydrogen dislocation interactions or others) which are considered without provision for the real sequence of events in the core of fracture. In this report the model of hydrogen-induced fracture is formulated as a component of the theory of macroscopic crack growth in metal.

Qualitative Model of Hydrogen-Induced Macrocrack Growth in Metals

The case of crack propagation in rather plastic metals, subjected to hydrogen-containing environments is considered. We assume the metal to be practically free of hydrogen. We do not consider conditions and materials with a possible hydrogen-induced degradation of metal of chemical origin (hydrogen corrosion, hydride brittleness, etc.).

As far as hydrogen-induced macrocrack in metal is concerned, it is possible to state, that its tip zone structure does not differ from the case, when there is no hydrogenation. The characteristics of the macrocrack in the given cases are the following:

1. The profile of the macroscopic crack is formed through shear, the stress value in the vicinity of the inevitably blunted crack tip are in all cases substantially smaller, than the ideal lattice strength (Vladimirov, 1976; Vladimirov and others, 1981; McMeeking, 1977; Yemaletdinov, Khananov, 1977).

2. The crack tip is surrounded with the zone of plastic deformation of a considerable inhomogeneity caused by its discrete dislocation nature. This is a source of local overstresses in the precracking zone. Besides, at the crack tip there is an adjoining region free from dislocational discontinuities and overstresses (Vladimirov, 1976; Vladimirov and others, 1981).

What has been stated means, that the overcoming of the occuring barriers is the determinative stage of the macrocrack propagation. The process of such a crack propagation is unlikely to be associated with the surfacial sharp microcrack initiation at the blunt macrocrack tip. This process may be caused by the fact, that due to hydrogen the lattice cohesive strength in the surfacial layer of the metal at the blunted crack tip decreases up to the level of mechanical stresses observed in this place. Thus, the given type of the macrocrack propagation depends on the hydrogen ability to cause a considerable reduction in cohesive strength of the metallic lattice (by some orders of magnitude (McMahon, Briant, Banerji, 1978). The available experimental data (Au, Birnbaum, 1978; Flis, Smialovski, 1979; Kamdar, 1974) show, that hydrogen does not affect the fracture of metals even under extreme conditions of their interaction, but only if in metals there exists no factor that could cause microlocalization of plastic deformation.

Taking into account what has been set forth above together with some general physical concepts (Finkel', 1970; Vladimirov, 1973, 1976) it is possible to represent the qualitative aspects of the macrocrack growth in metals, affected by hydrogen-containing environments, in the following way (Fig. 2).

When loading a solid with a macroscopic blunt crack, a zone of intensive plastic deformation is formed in the vicinity of the crack tip long before the limit equilibrium state is reached at $K_1 = K_{1c}$. This plastic zone exhibits local non-uniformity, which gives rise to excessive dislocation groups of the same sign. Being interlocked with obstacles (grain boundaries, phase boundaries, etc.), they form retarded dislocation arrays, cause high local overstresses and create structures, which may lead to dislocational cracks. These possible fracture nucleations may occur at a distance from the crack tip, which is not smaller than the one depending on the dislocation structure parameters, such as the size of the dislocation source, etc. (Vladimirov, Khannanov, 1970). Hydrogen, entering the metal has no time to pile up in the potential fracture zone during load rising in the quantity sufficient to affect the fracture pilots nucleation considerably. After a period of time, if the process of loading is continued, the stability of the dislocations arrays in the precracking zone is disturbed. A dislocational microcrack, coming from the opposite direction occurs, and is absorbed by the main crack, thus permitting the main crack growth to be continued. This occurs when the stress intensity factor reaches the K_{1c} value.

If the loading is limited by the $K_1 < K_{1c}$ level equilibrium dislocation arrays occur in the precracking zone before the collected hydrogen amount is enough to produce any practically significant effect. As hydrogen enters the metal this equilibrium may be disturbed and the relaxation of the dislocation configuration may occur, i.e. its transformation into a dislocational microcrack. This happens due to the microscopic effects caused by the hydrogen presence in metals (alteration of the interatomic bonds or effects of the hydrogen interactions with dislocations, or others). The growth of the macrocrack by joining with microcrack is arrested some distance away from the initial position of the crack tip, where the metal is not sufficiently saturated with hydrogen. In the vicinity of the newly formed crack tip a precracking zone appears again preceded by dislocational fracture pilots. Hydrogenation of metal is repeated through the surface at the opened crack tip and so on. Thus, the macrocrack growth occurs in the form of successive jumps. The average period Δt of the "pilot appearing - hydrogen accumulation - relaxation of the nonequilibrium dislocational configuration" cycle is the time of the jumps repetition and together with the jumps average length $\Delta \ell$ determines the average macroscopic macrocrack growth rate $V = \Delta \ell / \Delta t$.

The proposed concept is quite realistic, which is proved by the facts verifying the basic principle of the model, consisting in disturbance of the fracture pilots - dislocation arrays equilibrium by the hydrogen entry into metal, which makes the dislocation array fall into dislocational cracks. Such facts are observed by Oriani and Josephic (1979, 1981): splash-like acceleration of the stress relaxation in a deformed specimen or creep in a loaded specimen at ambient temperature during hydrogenation which could be explained by a shift of the formerly retarded dislocation arrays. The consequence of the assumed disturbance of the dislocation arrays and their shift as hydrogen enters the metal, should be delayed local plastic deformarion. This effect have been really observed experimentally in the vicinity of the crack tip in the metal subjected to hydrogen containing environments (Chu, Hsiao, Li, 1979). Finally, numerous experimental results show that plasticity localization is the factor affecting the hydrogen sensitivity property of metals, and the most brittle fracture modes, when studied in detail, proved to be bound up with local plastic deformation outbursts (Thompson, 1978; Thompson, Bernstein, 1978).

Fracture Model and Criterion of Local Instability in a Hydrogenated Material near the Macrocrack Tip

To describe the process of nucleation and development of fracture in overstressed elements of a solid it is necessary to consider both the structure of the leading dislocation core and the discretness of the heading part of the dislocation array. In this respect let us consider a combined discrete - continuous model of a blocked dislocation array presented in Fig. 3.

Let the dislocations array contain n number of dislocations of Burgers vector b, let it be located in the normal stress field σ_n and let stress τ_t press it to some barrier. In this array two leading dislocations are considered to be discrete and the rest of the array is considered in continuum manner. For the first two dislocations we introduce a core model similar to a mechanical model of cohesive forces adopted in the microscopic crack concept (Panasyuk, 1968). The core is treated as a wedge shape cavity, located in elastic continuum with its sides contracted by forces of atomic planes interaction and the stresses at the wedge tip are equal to the ideal lattice strength g_m. Without going into details of the performed analysis we shall note the following (Panasyuk, Andreikiv, Kharin, 1982; 1983).

The dislocation core structure appreciably affects the dislocations interaction force. Proceeding from the assumed dislocation core structure, we arrive at a conclusion that, with small L values of distance between dislocations, the force appreciably differs from the classical dependence of 1/L type (dashed line in Fig. 4). In particular, the mutual repulsive force F_{12} for dislocations B_1 and B_2 grows to some extreme value as they approach each other, but then this force decreases rapidly due to dislocation cores interaction (solid line in Fig. 4). This causes the situation, when the repulsive force F_{12} cannot prevent the dislocations from being brought together, which leads to the instability of the B_2 dislocation with its further joining with heading dislocation B_1 of the array, i.e. the mergence of the dislocations with the following formation of a super dislocation of the Burgers vector of 2b value. For this case the instability condition for dislocational structure will take the form (Panasyuk, Andreikiv, Kharin, 1982; 1983):

$$n(\tau_t - \tau_i) = 0.308\,(g^* - \sigma_n), \qquad (4)$$

where τ_i is the resistance of lattice to the slip of dislocation, $g^* = \varkappa\, g_m$, where $\varkappa$ is the coefficient of the atomic interaction forces dying down, $3/4 \leq \varkappa \leq 1$.

Note, that there is no interaction between the sides of a superdislocation with Burgers vector 2b in iron, according to computations of Altynbayev, Khannanov (1977) i.e. a superdislocation may be assumed to be a nucleation of a microcrack. Thus, condition (4) becomes a condition for a nucleation of fracture at the head of the dislocations array.

Considering in the same way the dislocation configuration formed after condition (4) is satisfied, with provision for the superdislocation (crack) properties we obtain the condition for the nucleational crack growth due to the dislocations of the array joining the crack (Panasyuk, Andreikiv, Kharin, 1983):

$$n(\tau_t - \tau_i) = 3.35\,(1 - 0.501\sigma_n E/g_m^2)(g_m^2/E - \sigma_n). \qquad (5)$$

It is interesting to note, that the instability of the dislocation which is nearest to the leading superdislocation (crack) constitutes the condition for instability of the whole array (Vladimirov, 1973; Vladimirov, Khannanov, 1969), which slips after condition (5) is fulfilled, into an expanding dislocational crack.

Now the time has come to analyze the hydrogen effect. Hydrogen facilitates fracture in an array of dislocations, as it reaches the array. There are two ways for this process to occur: either the reduction of the friction resistance of the lattice τ_i, or the reduction of the cohesive properties of the lattice in the dislocation core, i.e. g_m-value reduction. As far as the first factor is concerned, the controversy in numerous results (Bernstein, 1974; Cornet, Talbot-Besnard, 1977, 1978; Matsumoto, Eastman, Birnbaum, 1981; Pokhmurskii, Shved, Yaremchenko, 1977; Shved, 1981) leads to the conclusion that the given factor influence may be refered to the specific properties of particular alloys, both to those promoting and impeding fracture of the type under consideration. Comparing these facts with knowledge that hydrogen causes harmful effects of a universal character, one feels doubtful about the decisive role of the given factor in hydrogen environment embrittlement.

As for the hydrogen-affected reduction of the cohesion in the dislocation core zone, it is now a well grounded phenomenon and there is no doubt in decohesion of the electronic nature (i.e. associated with alterations of the electronic structure of metals due to hydrogen presence) (Losch, 1979; Troiano, 1960; Watanabe, 1977). With due regard for the fact, that the dislocation core zone is the region of the most likely hydrogen atoms localization, it is possible to speak of the core as the center of cluster formation and of possible (Walker J., Walker T., Kelly, 1972) metal-hydrogen hydride-type bonding localization. Both of these effects may be taken for sources of specific decohesion which is associated with individual alongation of some particular metal-metal bonds (Fujita, 1976; Gehlen, Markworth, Kahn, 1976) with reduction of the corresponding interaction forces. Thus, as for the dislocation core, it is only natural to speak of effective decohesion as a sum of three previously denoted effects of electronic, hydride and cluster origin. It is obvious, that the total decohesive effect is more universal than each of the components. With this in mind the further discussion of the mechanism of hydrogen effect on fracture will be based on the concept of effective decohesion in the dislocation core zone. This dislocation-decohesion concept of hydrogen embrittlement will, thus, generalize the conventional decohesive Troiano-Oriani concept (Troiano, 1960; Oriani, 1972).

In terms of this concept we describe the following sequence of events for an array previously free of hydrogen. The hydrogen, entering the metal, collects first of all in places most sufficient in terms of binding energy. Dislocation cores, with hydrogen atomic concentration reaching unit or even excessing it also belong to such places (Heady, 1978; Hirth, 1980). This is accompanied by reduction of the effective core cohesion parameter, which is the function of the hydrogen amount in the dislocation core zone $g^*_H(N_\perp)$ ($N_\perp$ is the number of hydrogen atoms per the distance of the lattice parameter along the dislocation line. On account of lack of more precise information we take it as is usually done (Oriani, Josephic, 1974) in linear form

$$g^*_H(N_\perp) = g^* - k_g N_\perp \, . \tag{6}$$

With provision for equation (6) the hydrogen-assisted fracture nucleation criterion takes the form of

$$n(\tau_t - \tau_i) = 0.308\,(g_* - k_g N_\perp - \sigma_n) \tag{7}$$

and the dislocational crack propagation criterion is presented by:

$$n(\tau_t - \tau_i) = 3.35[1 - 0.501\sigma_n E/(g_m - k_g N_t)^2][(g_m - k_g N_t)^2/E - \sigma_n], \tag{8}$$

where N_t determines the number of hydrogen atoms associated with the atomically sharp microcrack tip.

Values $N_\perp$ and N_t are associated with equilibrium hydrogen concentration in a regular lattice of metal C. This relation is expressed with a well known linear dependence containing a proportionality factor of the $\exp(V_b/kT)$ type, where V_b is binding energy of a hydrogen atom with the corresponding defect, k is the Boltzman constant. The value of V_b for an atomically sharp microcrack is unknown, though it is possible to assume that it is located between the binding energies of the hydrogen atom with the dislocation core and the free metal surface. Taking into account, that the described values do not differ appreciably (Hirth, 1980), we may say, that $V_{bt} = V_{b\perp}$ and, consequently, $N_t = N_\perp = N_0$.

In Fig. 5 with provision for the latter equality the criterial conditions for the microcrack initiation and propagation (7), (8) are represented. In this case it is interesting to note, that the latter is the evaluation from above for a real condition, including the pressure effect of the gaseous hydrogen, entering a microcrack with dislocations. But, basing on calculations (Panasyuk, Andrejkiv, Kharin, 1982), the gaseous H_2 pressure in a defect may be neglected for the hydrogen content in metal of order of several ppm, causing no harm to a precise process description.

The specially developed averaging procedure (Panasyuk, Andrejkiv, Kharin, 1983) allows transition from microscopic to macroscopic variables in terms of criterial dependencies (7) and (8). As a result we obtain the fracture initiation and propagation criterion in the material point subjected to hydrogen effect in terms of continuum (macro-) mechanics of elastic-plastic solids

$$A\varepsilon_i(\tau_{max} - \tau_i) = g^* - K_g C - \sigma_n^{max}, \tag{9}$$

$$A'\varepsilon_i(\tau_{max} - \tau_i) = [1 - 0.501\sigma_n^{max} E/(g_m - K_g C)^2][(g_m - K_g C)^2/E - \sigma_n^{max}], \tag{10}$$

where ε_i - equivalent plastic strain, $\tau_{max}, \sigma_n^{max}$ - maximum shear and tensile stresses. In this case A, A', K_g are phenomenological constants in a certain way associated with corresponding microscopic parameters (the graphic representation of the described conditions is obtained from a microscopic analogue with the corresponding alteration of the scale in coordinate axes, Fig. 5).

With due regard for the fact, that the ε_i is associated with reduction in area of a smooth specimen ψ , it becomes obvious, that in Fig. 5 the section of the criterial surface with the $\sigma_f = \sigma_f(C)$ surface (σ_f being macroscopic true fracture stress) represents the main characteristic properties of the experimentally obtained dependence $\psi = \psi(C)$ (Moroz, Chechurin, 1967; Pokhmurskii, Shved, Yaremchenko, 1977; Smialovski, 1962). This suggests the possibility to use the experimentally obtained using uniformly stressed and hydrogenated specimens dependencies $\sigma_f = \sigma_f(C)$ and $\psi = \psi(C)$ to determine the parameters of criterial equations for given material (though, in this case some error can be achieved due to complications, associated with the necessity to provide uniform hydrogen distribution in a specimen, etc.). In principle, together with the data on the stress and strain distribution in the vicinity of the crack tip in an elasto-plastic material, the dependencies (9), (10) determine the criterion (3) of the limit equilibrium state of the material in the vicinity of the crack tip. In this case it is necessary to use the solutions expressing the peculiarities of the stress-strain state of the fracture initiation zone with maximum truth. These are solutions in terms of geometrically nonlinear models of elasto-plastic media, and such is the solution by McMeeking (1977).

Kinetics of Hydrogen Accumulation in the Fracture Process Zone

As it follows from the stated above, the potential fracture nucleation zone is located inside the metal, in front of the macrocrack. For this reason the analysis of the hydrogen entry into the fracture nuclei should be based on the study of the hydrogen diffusion in the stress field at the macrocrack front. We attempt to analyze this problem in such a way taking into account the peculiarities of the real stress-strain state of the solid in the vicinity of the crack tip.

If we approximate the numerically obtained by McMeeking (1977) stress distribution in the crack plane with a piece-wise-linear dependence, the equation of hydrogen diffusion in the stress field is reduced in our study (Panasyuk, Andrejkiv, Kharin, 1981) to an equation with piece-wise-continuous coefficients

$$\partial C/\partial t = D\partial^2 C/\partial x^2 - H(x_m - x)DV_h(\sigma_m - \sigma_0)(RTx_m)^{-1}\partial C/\partial x \quad (11)$$

with the conditions of the hydrogen concentration and flux continuity at $X = X_m$. Here X-coordinate is the distance from the crack tip into the metal; X_m is the abscissa of the hydrostatic stress σ maximum point; D and V_h - diffusion coefficient and partial molar volume of hydrogen in metal; $\sigma_m = \sigma(x_m)$, $\sigma_0 = \sigma(0)$ H(•) is the Heavyside function.

For a zero initial condition and boundary conditions of constant concentration at the surface of the metal at the crack tip $C|_{x=0} = C_s$, the problem was reduced to a procedure of the Laplace transform inversion. A closed approximated solution was obtained with the method of asymptotically equivalent functions in the form of (Andrejkiv, Kharin, 1982):

$$C = C_s e^{m\eta}\left[\mathrm{erfc}\left(\frac{\xi}{2\sqrt{\tau}}\right) + (e^{-m\eta} - 1)e^{\lambda\xi + \lambda^2\tau}\mathrm{erfc}\left(\frac{\xi}{2\sqrt{\tau}} + \lambda\sqrt{\tau}\right)\right], \quad \eta = 1 - (1-\xi)H(1-\xi), \quad (12)$$

where $\xi = x/x_m$, $\tau = Dt/x_m^2$, $m = \frac{V_h(\sigma_m - \sigma_0)}{2RT}$, λ is the parameter of asymptotic equivalency obtained from the solution of some minimax problem. Fig. 6 shows the hydrogen concentration distribution at the

macrocrack tip region, calculated using formula (12) with the parameters values, corresponding to steels: V_H = 1.96 cm^3/mol (Beck, Subramanyan, Williams, 1971), σ_y = 869 MPa(steel 4147) and σ_y = 1450 MPa (steel 4340) at T = 295K (such steels were tested by McIntyre, Walker (1978) and by Loginov, Phelps (1975). Therewith to evaluate the real timescale the t scale is given at $X_m = 1.2\ K_1^2 / (E\,\sigma_y)$ (McMeeking, 1977) for K_1 = 40 MPa$\sqrt{m}$, $D = 10^{-10}$ m^2/s, E = 201 GPa, σ_y = 1450 MPa.

Mathematical Description of the Macrocrack Growth Kinetics

In accordance with general qualitative concepts of the hydrogen-associated macrocrack growth in metals on the basis of developed mathematical relations the system of equations of the subcritical crack kinetics may be obtained in the following way. The condition for fracture to occur in some crtical point $X = X_c$ is:

$$C(\xi = x_c/x_m,\ \tau = D\Delta l/(x_m^2 V)) = C_{cr}(K_1, x_c) \quad (13)$$

(it is taken into consideration, that $t = \Delta l / V$).
The critical point itself is determined by the critical fracture condition satisfied for the first time i.e.

$$C'_x(\xi = x_c/x_m,\ \tau = D\Delta l/(x_m^2 V)) = C'_{cr,x}(K_1, x_c). \quad (14)$$

Finally, the length of the crack jump Δl is determined by the extent of the overhydrogenated (compared with concentration level at X_c) region:

$$C(\xi = \Delta l/x_m,\ \tau = D\Delta l/(x_m^2 V)) = C_{cr}(K_1, x_c). \quad (15)$$

The system of equations (13) - (15) gives a closed description of the subcritical crack growth in metals due to hydrogen effect (here to the right- and left-hand parts correspond the functions (3) and (12) respectively). In some cases, depending on particular alloy properties the precracking zone critical state may be caused either by a critical strain or stress value and this may lead to considerable simplification of equations (13) - (15). For alloys of not too low plasticity, such as numerous steels, the first possibility is preferable. In this case the critical point position becomes determined apriori, and it allows to exclude equation (14) and to present the right-hand parts of the remaining equations through function $C_{cr} = C_{cr}(K_1)$. The critical conditions (9), (10) were already pointed out to be associated with the dependencies of mechanical characteristics of smooth specimens on uniform hydrogen concentration in them. With consideration for this fact, the relations between common mechanical characteristics and the crack propagation resistance parameters, determined in terms of known continuum - structural models (see review by Romaniv, Tkach (1977)), allow the direct transition from criterial conditions expressed with (9), (10) to a dependence of type $C_{cr} = C_{cr}(K_1)$ to occur.

Applying the dependence (Panasyuk, Andrejkiv, Kovchik,1977b) between the local strain at the crack front, SIF value and deformation at a smooth specimen fracturing, $\varepsilon_f = \ln(1-\varphi)^{-1}$, it is possible to express the criterial condition in the following way:

$$K_{1cr}(C)=\sqrt{dE\sigma_y e_f(C)}=\sqrt{dE\sigma_y \ln[1-\varphi(C)]^{-1}}, \qquad (16)$$

where d is the parameter determined by the material structure and constraint in the stress - strain state at the crack tip. As a result we obtain an equation of the crack growth rate on the SIF value dependence:

$$C(\delta_t/X_m,\ DE\sigma_y/(\alpha K_1^2 V))=C_{cr}(K_1), \qquad (17)$$

where the solution of the equation of the hydrogen diffusion in a stressed field (12) constitutes the left-hand part and the inverse function to the one, expressed by equation (16) constitutes the right-hand part.

Relations (12), (16), (17) through mechanical characteristics of material (E,σ_y), constants of hydrogen permeation and other type interactions with metal (D, V_H, C_s) allow to simulate a kinetic diagram for metal cracking, in case the dependence for reduction in area of a previously uniformly hydrogenated specimen on the hydrogen concentration at the smallest cross section at the moment of failure $\varphi(C)$ is obtained experimentally. The above mentioned concentration in general differs from the concentration of hydrogen uniformly distributed in the metal after precharging, and it is rahter difficult to give it an equivalent determination. As for utilizing the hydrogenated specimen plasticity dependence on the initial average hydrogen concentration in the specimen for the theoretical description

of the crack growth kinetics, it is clear, that in the given case the calculated crack growth values should be in some but not so large error as compared with those, that could be obtained with the true dependence of plasticity on the amount of hydrogen in the failured cross section.

The performed calculations (Andrejkiv, Kharin, 1981; Panasyuk, Andrejkiv, Kharin, 1981; 1982; 1983) in terms of the described concepts demonstrated, that the structure and character of the criterial relations allow to obtain a result perfectly reflecting the essential characteristics of the experimentally obtained dependencies (see Fig. 7). Due to lack of the necessary data on the governing characteristics of the process it is impossible to compare the calculated curves with the experimentally obtained results. That is why we may speak only of the qualitative conformity between the stated theoretical concepts and practice.

CONCLUSIONS

Considering the case of the hydrogen containing environment effect on the propagation of macrocracks in metals a theoretical model of the phenomenon is proposed with provision for certain microscopic fracture processes, physical effects of interaction of hydrogen with atoms of crystal lattice and crystal structure defects and peculiarities of elasto-plastic deformation at the macrocrack front. A dislocation - decohesion concept is formulated for the hydrogen influence on mechanical behaviour of metals, which brings about an association of the hydrogen effect on fracture of metals with its influence on the dislocations core structure in blocked dislocation arrays. This allows, in particular a more precise formulation in terms of the solid state physics of the problem of the hydrogen role in fracture initiation with provision for dislocation peculiarities in atomic configuration and electronic structure. The problem of hydrogen diffusion in a stress field at the macrocrack tip is given a solution with consideration of the stress state characteristics at large strains. A closed system of equations is deduced to describe the kinetics of the macrocrack growth.

Although, at present no success has been achieved in obtaining a complete set of governing parameters from the available experimental data to characterize conditions of fracture initiation and propagation quantitatively, a proper qualitative conformity between theoretical concepts and experimentally obtained results has been achieved. This enables us to believe the given description of the phenomenon to be a realistic one.

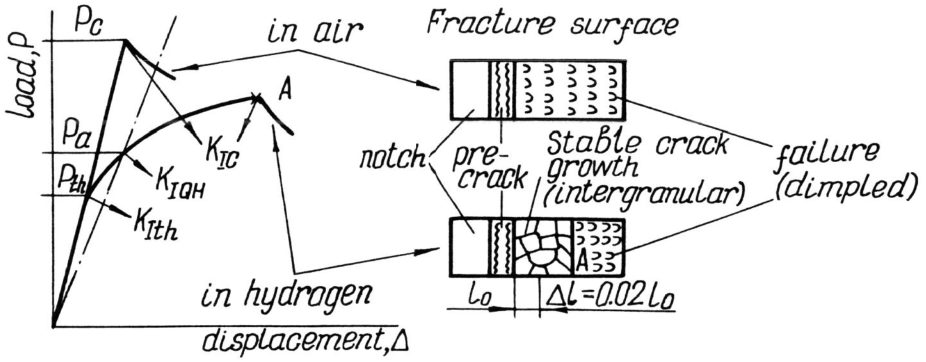

Fig. 1. Typical fracture toughness tests results.

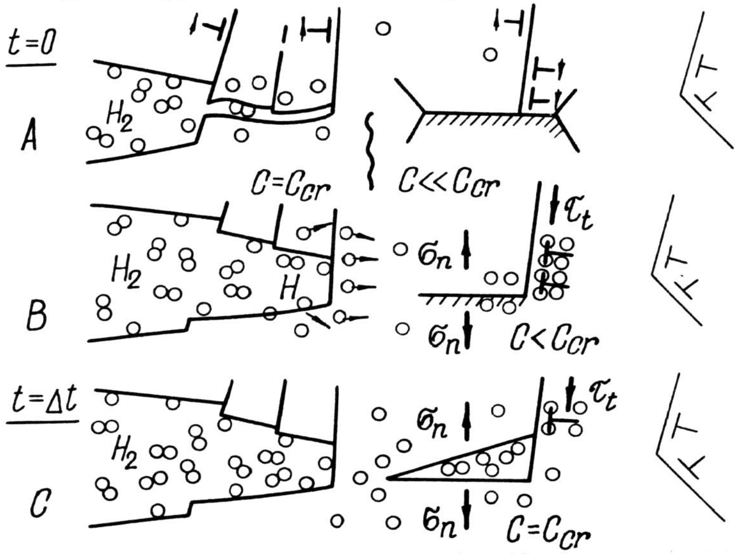

Fig. 2. Schematic diagram of the sequence of events at the crack tip.

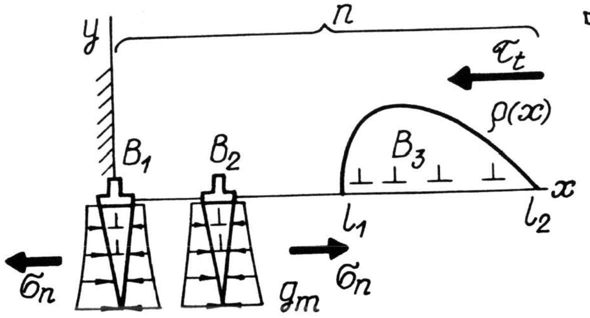

Fig. 3. Combined discrete – continuum model of the blocked dislocation array.

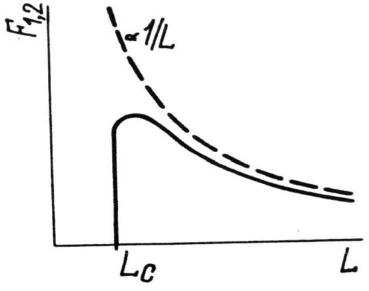

Fig. 4. Interaction force (repulsive) between dislocations B_1 and B_2 of the array.

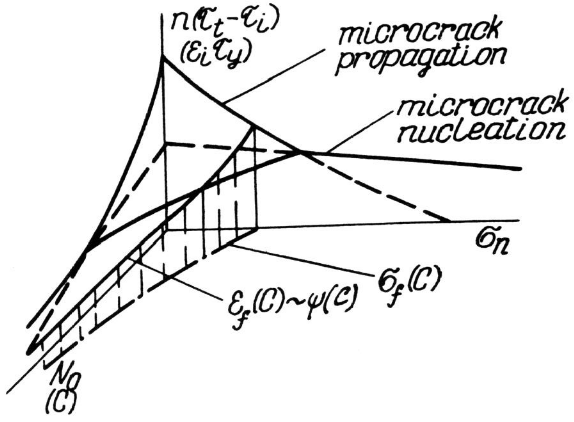

Fig. 5. Schematic diagram of the conditions for fracture initiation and propagation in terms of micro(macro) variables.

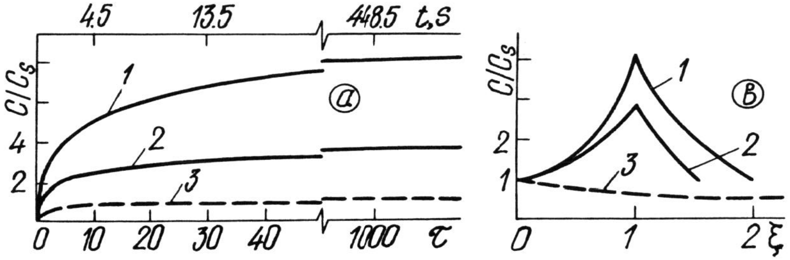

Fig. 6. Hydrogen concentration alteration (a) at $\xi = 1 (x = x_m)$ and (b) at $\tau = 5.0$ (1 - 4340 steel, 2 - 4147 steel, 3 - diffusion equation solution with no provision for mechanical stress effect).

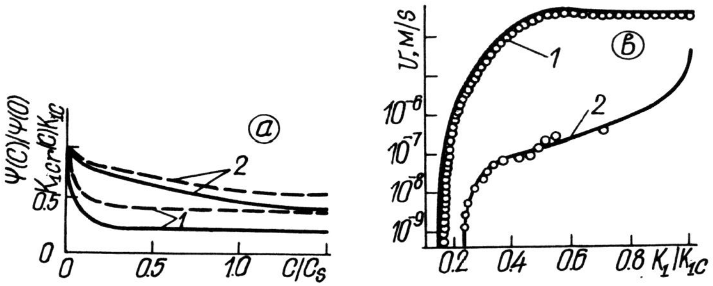

Fig. 7. Theoretical simulation of kinetic diagram for metal cracking: a - criterial curve $\psi = \psi$ (C) (solid line) and dependence (16) (dotted line); b - kinetic diagrams for metal cracking for 4340 (1) and 4147 (2) steels (circles - experimental data of McIntyre, Walker (1978) and Loginov, Phelps (1975)).

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