GLIDE PLANE DECOHESION IN HYDROGEN INDUCED CRACKING

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Abstract. A dislocation theory of the mechanism of hydrogen induced fracture is developed in this paper. The Stroh-type model of cleavage in blocked array of dislocations is advanced to consider possible separation along the shear plane, too. The cores of densely placed dislocations in a coarse slip band of multiple plain pileups are taken into account as the nuclei of both probable traverse and longitudinal cleavages in a band. The equations of equilibrium of this dislocation population in stress field are built up and fracture criteria are derived as the limit conditions for stability of band equilibrium. The role of hydrogen is associated with its effect on lattice cohesion (interatomic potential) just in dislocation cores, which allows one to explain peculiarities of hydrogen assisted fracture of metals.

Resumen. En este artículo se desarrolla una teoría dislocacional del mecanismo de fractura inducida por hidrógeno. El modelo de Stroh de clivaje en alineamientos bloqueados de dislocaciones es mejorado para incluir también la separación a lo largo del plano de deslizamiento. Los núcleos de dislocaciones densamente poblados en una banda de deslizamiento consistente en apilamientos planos múltiples se tienen en cuenta como embriones de clivaje tanto longitudinal como tranversal a lo largo de una banda. Se formulan las ecuaciones de equilibrio del conjunto de dislocaciones en el campo tensional, y se derivan criterios de fractura como condiciones límite para la estabilidad del equilibrio de la banda. El papel del hidrógeno se asocia con su efecto sobre la cohesión de la red (potencial interatómico) precisamente en los núcleos de dislocaciones, lo que permite explicar las peculiaridades de la fractura inducida por hidrógeno en metales.

1. INTRODUCTION

Significant amount of observations of hydrogen assisted damage in iron- and nickel-base alloys implies that hydrogen affected fracture is a plasticity enhanced phenomenon [1-3]. Depending on the particular circumstances, e.g., on hydrogen content in metal, temperature, etc., fracture proceeds apparently by microcracks opening either *traversely* to blocked shear planes (t-cracks), or by *longitudinal* separation of intense slip bands (l-cracks) localised along characteristic slip traces [3-6],as shown in Fig. 1. Interactions of dislocations in slip bands immersed in macroscopic external stress field σ_{xx}^*, σ_{yy}^* and τ_{xy}^* (Fig. 1) are supposed to be responsible for the background mechanism of these manifestations.

The objective of this work is to develop mathematically the model for elucidation of related dislocation reactions towards a better understanding of hydrogen effects on materials. The model to be presented below was inspired by the previous studies [7,8] which involved dislocation core in analysis of fracture micromechanisms.

2. MODEL BACKGROUNDS

Apart from hydrogen effects, it is now commonly recognised that (micro)plastic shear is a necessary prerequisite and an inevitable attribute of fracture in crystalline solids which have favourable density and mobility of dislocations, such as the majoriyt of metals and alloys. Under sufficiently fine examination this seems to be always observable, even in rather brittle macroscopic manifestations of fracture [2,9].

The dislocational nature of the microscopic *deformation-and-fracture* event has been well proved and has received ample theoretical elaboration [10]. Evolution of dense dislocation arrays in stress fields was shown to be the common way of nucleation and growth (at least, initial) of microcracks. Peculiarities of the particular array configuration —e.g., if it is a Stroh-shape blocked plain pileup or a Cottrell-type couple of two intersecting ones or other [9,10]— have minor importance. With independence of specific array structures, interaction of closely spaced dislocations and their coalescence produce cleavage microcracks in unrelaxed pileups.

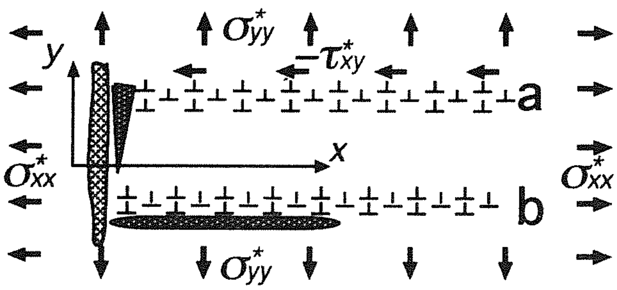

Fig. 1. Two modes of microcracking in unrelaxed coarse slip bands blocked at an impenetrable obstacle (a — t-cleavage, b — l-separation)

Minute analysis of a dislocations [11,12] revealed that, apart from the leading term of its stress field responsible for interaction between dislocations at long distance r with the force $F \propto r^{-1}$, there is a series of the opposite sign terms which dominate the short range components of the force as $F \propto -r^{-(2i+1)}$ (i = 1,...). The latter ones are due to the dislocation core effects and are quite essential for interaction of closely spaced dislocations, breakdown of interatomic bonds and nucleation of dislocational cracks in pileups [7,12]. This implies the key role of a dislocation core in the initiation of microscopic fracture processes.

Drastic effects of hydrogen on mechanical behaviour of metals are habitual for certain macroscopically averaged hydrogen content, e.g., in BCC ferrous alloys, about few ppm by weight [13] which corresponds to 10^{-5}—10^{-4} in atomic fractions H/Fe [14]. This should argue the incredible impact of each hydrogen atom on metal lattice as far as it must be of enormous intensity and long span to be able to cause observable macroscopic effects, if hydrogen is assumed to be uniformly distributed in metal. Meanwhile, more precise studies proved that nearly all the hydrogen in metal at moderate temperatures $T \lesssim 400$ K segregates on dislocations [15], namely, in their adjacent Cottrell clouds and in cores, where its atomic concentration can exceed unity [15,16]. This saturation level seems to be able to induce significant changes in the dislocation core.

Combination of the last notion and the previous one on the role of dislocation cores in microfracture implies the auspicious way to explanation of mechanisms of hydrogen assisted damage. To follow it, advancement of dislocation models of fracture is desired with attention to the dislocation core. Moreover, stress field produced by plain edge dislocation has no tensile component $\sigma_{yy} \neq 0$ able to facilitate cracking along its own glide plane (l-cleavage) as is depicted in Fig. 2 in accordance with known formulae for stresses [17]

$$\sigma_{xx} = -Mby\frac{3x^2+y^2}{r^4}, \quad \sigma_{yy} = Mby\frac{x^2-y^2}{r^4},$$

$$\tau_{xy} = Mbx\frac{x^2-y^2}{r^4} \quad \left(M = \frac{E}{4\pi(1-\mu^2)}\right) \qquad (1)$$

where $r^2 = x^2 + y^2$, b is the length of the Burgers vector of a dislocation, E is the Young modulus, μ is the Poisson coefficient, and Cartesian coordinates x and y are fixed as in Fig. 2. Only dislocation cores can provide tensile stresses to promote l-cleavage in slip plane of a single pileup [8], which makes their incorporation not only advantageous but necessary to analyse this mode of fracture in a slip band.

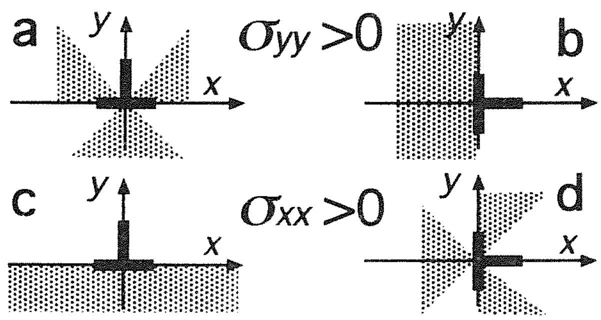

Fig. 2. Stress-fields of edge dislocations (a, b — stress σ_{yy}, c,d — stress σ_{xx}). Areas of positive (tensile) stresses are shadowed and on borders between sectors the correspondent stresses are zero.

Hirth [8] analysed stress concentration from core fields in the Stroh-type blocked pileup of edge dislocations assuming the cores to be the centres of dilatation. They give rise only to tensile stress components of each dislocation, in particular, to $\sigma_{yy} \propto r^{-2}$, and thus can not affect neither interaction between dislocations being carried through shear stress component τ_{xy} nor dislocation spacing and their coalescence in arrays to form crack nuclei, consequently. To fill in this deficiency the mechanistic model [7,12] served well where the core was treated as a V-shape wedge cavity (Fig. 3a) represented by a distribution in a domain $-h \leq y \leq 0$ (i.e., h being the core size) of infinitesimal dislocations with density $\eta(y)$ so that its width is

$$u(y) = \int_{-h}^{y} \eta(\xi)\, d\xi \qquad (2)$$

and opposite faces attract each other as atomic planes in crystal do with the interatomic force intensity $g = g(u)$, Fig. 3a. In addition, the preservation condition for Burgers vector must be obeyed:

$$\int_{-h}^{0} \eta(\xi)\, d\xi = b \qquad (3)$$

This model quantitatively agrees with more refined physical studies and is able to explicate the way how the Stroh-type t-crack arises in a pileup, including the role of hydrogen (cf. [7,12,14]). To adopt the model for consideration of the l-cracking in a pileup it is natural to introduce there the carrier of this sort of cleavage as it has been done for the t-one, i.e., to consider a T-shape dislocation core as in Fig. 3b. It is represented by the same t-part (2) and (3) together with the l-component of a core given by a density of infinitesimal dislocations $\zeta(x)$ at $-a \leq x \leq a$ so that the l-opening is

$$v(x) = \int_{-a}^{x} \zeta(\xi)\, d\xi \qquad (4)$$

with the complementary condition of Burgers vector preservation

$$\int_{-a}^{a} \zeta(\xi)\, d\xi = 0 \qquad (5)$$

Again, according to common approach of cohesive forces, the opposite faces of this core element attract each other with the intensity $g = g(v)$, see Fig. 3b.

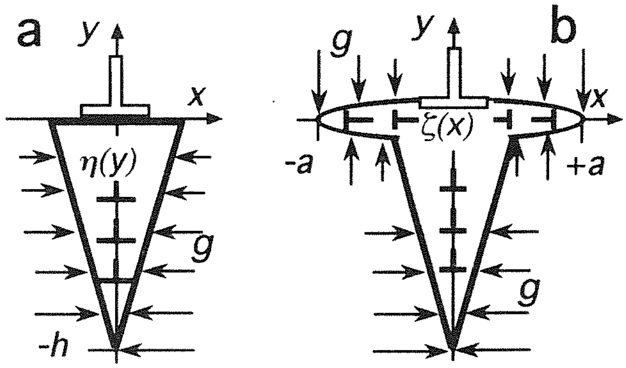

Fig. 3. Cohesive-forces models of the core of an edge dislocation: (a) — the V-shape wedge-like core; (b) — the triple wedge T-shape one.

The relation between traction g and separation δ between core faces, $g = g(\delta)$, is specified by the maximum attraction $g_m = max_\delta g(\delta)$ corresponding to the ideal lattice strength and by the span of interatomic forces efficacy δ_c, so that

$$g(\delta) = 0 \text{ when } \delta \geq \delta_c \qquad (6)$$

In general, these two parameters are the functions of hydrogen content in a core C^*:

$$g_m = g_m(C^*) \text{ and } \delta_c = \delta_c(C^*) \qquad (7)$$

With this core model the two types of potential cleavage in a pileup may be studied as is used to do in fracture mechanics of cohesive cracks. The criterion of crack initiation will spring from the limit equilibrium of the whole dislocational configuration which bears all the forces: external resolved stresses and interactions between pileup constituents (cf. [7,12]).

Apparently a common attribute of hydrogen affected fracture is that it happens by localisation of plastic strain, also promoted by hydrogen, when slip bands become extremely coarse and widely spaced [6]. In average, these bands of the width H_B are supposed to be formed by the N-floors heap of identical plain pileups of n dislocations in each one (Fig. 4a), so that cumulative Burgers vector of a band is $B = nNb$. Coarsening of shear especially favours the l-cleavage in the bottom-floor slip line of the shear band because at $y = 0$ a cumulative non-zero tensile stress σ_{yy} acts (cf. Fig. 2a) from a closely adjacent body B_B of dislocations of a remainder pileups situated above, i.e., at $y > 0$. Slip localisation urges pull apart of the planes of atoms along this single pileup of a heap.

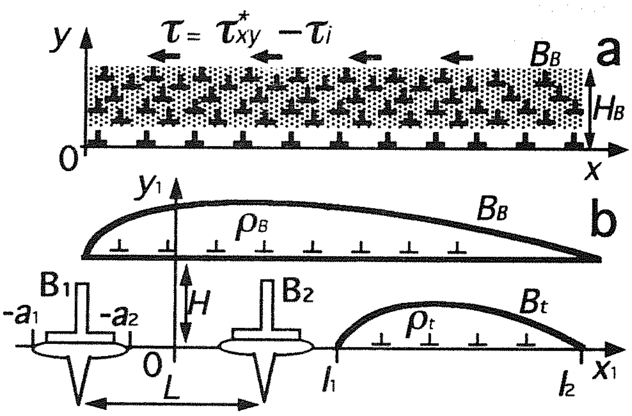

Fig. 4. The scheme (a) and the basic model (b) of a coarse shear band as a scene for development t- and l-decohesion cracking. The assemblage B_B of the upper-floor pileups of a band is shadowed in (a).

From previous analyses of stress fields and dislocation interactions in arrays (cf. [7-10,12]) it may be assumed that in the band under consideration the stress concentration from all its dislocations is the most severe just in the vicinity of the head of the bottom pileup. In addition, the head dislocations B_1 and B_2 separated by the distance L (Fig. 4b) are the most closely spaced in the whole set, so that the core interactions are there the strongest whereas the role of the remainder dislocations is dominated by their long-range stress fields according to equations (1) for each one. Thus, the only two dislocations B_1 and B_2 are worthy of minute treatment with attention to their cores whereas consideration of all the others as the classical elastic ones will be a proper approximation to the analysis of cleavage nucleation. These ordinary dislocations form two arrays: the super-array B_B which comprises the main body of the band, and the tail B_t of the bottom pileup (Fig. 4b).

3. BASIC EQUATIONS

To evaluate interactions and equilibrium in the shear band, the two arrays B_t and B_B of ordinary elastic dislocations are described by continuous dislocation densities, correspondingly, $\rho_t(x)$ and $\rho_B(x)$ situated along certain portions $l_1 \leq x \leq l_2$ and $0 \leq x \leq L_B$ of their slip lines $y = 0$ and $y = H$, where L_B is the length and H is the effective width of the shear band. These densities are constrained to preserve the cumulative Burgers vectors of the arrays as follows:

$$\int_{l_1}^{l_2} \rho_t(x)dx = B_t \quad (B_t = (n-2)b \approx nb \text{ at } n >> 1) \quad (8)$$

$$\int_{0}^{L_B} \rho_B(x)dx = B_B \; (B_B = n(N-1)b \approx nNb \text{ at } N >>1) \quad (9)$$

The exact configurations of these arrays are to be found from the equations of equilibrium of dislocations under *glide* forces defined by the cumulative shear stress τ_{xy} [17]. They are as follows (cf. [7,12]):

$$\int_{l_1}^{l_2} \frac{\rho_t(\xi)}{\xi - x} d\xi = \frac{b}{x} + \frac{b}{x - L} +$$
$$+ \int_0^{L_B} \rho_B(\xi)(x-\xi)\frac{(x-\xi)^2 - H^2}{[(x-\xi)^2 + H^2]^2} d\xi - \frac{\tau}{M} \qquad (10)$$

$$\int_0^{L_B} \frac{\rho_B(\xi)}{\xi - x} d\xi =$$
$$= bx\frac{x^2 - H^2}{[x^2 + H^2]^2} + b(x-L)\frac{(x-L)^2 - H^2}{[(x-L)^2 + H^2]^2} +$$
$$+ \int_{l_1}^{l_2} \rho_t(\xi)(x-\xi)\frac{(x-\xi)^2 - H^2}{\left[(x-\xi)^2 + H^2\right]^2} d\xi - \frac{\tau}{M} \qquad (11)$$

where resolved shear stress $\tau = \tau_{xy}{}^* - \tau_i$ accounts for lattice resistance (friction) against dislocation glide τ_i.

The structure of the core of each dislocation B_i (i = 1,2) is not frozen but depends on stress field in the dislocation site taking there the equilibrium configuration of densities $\eta(y)$ and $\zeta(x)$ under cumulative stresses, correspondingly, σ_{xx} and σ_{yy}, opposed by lattice cohesive forces $g(u)$ and $g(v)$. Following the same route as in previous studies of the t-cleavage in a single pileup [7,12], two cores of B_i are supposed to be identical and symmetrical with respect to the axis y_1 of new coordinate system (x_1,y_1) with the origin pinned at $x = L/2$, $y = 0$ (Fig. 4b). Then, the cores B_1 and B_2 occupy the intervals $[-a_1,-a_2]$ and $[a_2,a_1]$ of the x_1-axis, correspondingly. It is convenient to continue analysis in this new coordinates. Because the spacing L is small comparing with all other characteristic dimensions of the shear band (i.e., H, L_B, l_1 and l_2), this shift of coordinate system may cause only insignificant alterations of the equations describing the heavy components of the shear band. For this reason we do not discriminate below between the two coordinate systems while considering the long-range stress fields.

Closeness of B_1 and B_2 allows one to neglect the x-variation of stress field in the region of their location assuming it to be approximately the same as at $x = 0$. Then, for the t-cleavage components of both cores the equation of equilibrium may be derived as it was done before [7,12], calculating the stresses $\sigma_{xx}(x{=}0,y)$ on the wedge faces from all constituents of the band, i.e., long-range stress on the core B_i from its neighbour B_j (i,j = 1 or 2, $i \neq j$), pileup tail B_t and band body B_B, and from the l-cleavage component $\zeta(x)$ of the core itself, sequentially. Equilibrating them with external stress $\sigma_{xx}{}^*$ and cohesive forces $g(u)$ gives:

$$\int_{-h}^{0} \frac{\eta(\xi)}{\xi - y} d\xi = by\frac{3L^2 + y^2}{[L^2 + y^2]^2} +$$
$$+ y\int_{l_1}^{l_2} \rho_t(\xi)\frac{3\xi^2 + y^2}{[\xi^2 + y^2]^2} d\xi +$$
$$+ (y - H)\int_0^{L_B} \rho_B(\xi)\frac{3\xi^2 + (y-H)^2}{[\xi^2 + (y-H)^2]^2} d\xi +$$
$$+ \int_{-a_1}^{-a_2} \zeta(\xi)\frac{\xi(y^2 - \xi^2)}{[\xi^2 + y^2]^2} d\xi + \frac{g(u) - \sigma_{xx}{}^*}{M} \qquad (12)$$

Using the same technique, the equilibrium equation for the l-pulled portion of the i-th core comprises the $\sigma_{yy}(x,y{=}0)$ stresses from the symmetric counterpart of the j-th one, from its own t-cleavage part represented by the density $\eta(y)$, the long-range stress of the super-pileup B_B (the tail B_t does not contribute to σ_{yy} stress), and the external field component $\sigma_{yy}{}^*$, all them opposed by the cohesive force intensity $g(v)$. Explicitly this yields the following:

$$\int_{-a_1}^{-a_2} \zeta(\xi)\left[\frac{1}{\xi - x} - \frac{1}{\xi + x}\right] d\xi =$$
$$= \int_{-h}^{0} \xi\eta(\xi)\frac{(x + L/2)^2 - \xi^2}{\left[(x + L/2)^2 + \xi^2\right]^2} d\xi +$$
$$+ H\int_0^{L_B} \rho_B(\xi)\frac{\xi^2 - H^2}{[\xi^2 + H^2]^2} d\xi + \frac{g(u) - \sigma_{yy}{}^*}{M} \qquad (13)$$

Finally, to close the system of equations describing the structure of the localised shear band the equation to define equilibrium position of the dislocation B_2, i.e., the spacing L between B_1 and B_2, must be derived. It consists of the forces of interaction of the element B_2

with B_1, B_t, and B_B, summarising which we have the following:

$$L\int_{-h}^{0}\int_{-h}^{0}\eta(\xi)\,\eta(y)\,\frac{L^2-(y-\xi)^2}{[L^2+(y-\xi)^2]^2}\,d\xi dy\;+$$
$$+\,b\int_{l_1}^{l_2}\frac{\rho_t(x)}{L-x}\,dx\;+$$
$$+\,b\int_{0}^{L_B}\rho_B(x)(L-x)\frac{(L-x)^2-H^2}{[(L-x)^2+H^2]^2}\,dx-\frac{b\tau}{M}=0$$

(14)

Singular integral equations (10)-(13) with respect to correspondent densities of infinitesimal dislocations accompanied with equation (14) regarding equilibrium location of the dislocation B_2, and supplemented with norm conditions (3), (5) and (8), (9) form the closed system of equations to define equilibrium of the slip band and evaluate its stability in external stress field — microfracture criteria— provided the lattice cohesive properties (7) are known as functions of hydrogen content in dislocation core C^*.

4. DISCUSSION

Two possible forms of microfracture nucleation in a shear band are obvious: (i) cleavage of the dislocation B_1 spreading as a brittle cohesive crack along negative y-semiaxis — t-cleavage; (ii) breakthrough of the l-parts of neighbour cores B_1 and B_2 towards each other to produce another brittle cohesive crack of the length $2c \geq (2a_1 + L)$ on the x-axis — l-cleavage or glide plane decohesion. These events are governed by the common criteria of the fracture mechanics of cohesive cracks [10] with account for local stress from all available sources, i.e., dislocations of the shear band.

In addition, the third less evident form of the stability loss exists in the pileup: instability of the position, firstly, of the dislocation B_2, and afterwards of the whole tail B_t so that they drop down to the pileup head B_1 and coalesce there producing a superdislocation with Burgers vector $B_c >> B_1 + B_2 = 2b$, probably up to $B_c = B_t$ [7,12]. The opposite faces of this superdislocation do not attract each other and it really forms the wedge-like brittle crack. The origin of this instability is in the interaction of the closely spaced dislocations B_1 and B_2 with account for the role of their cores. Namely, the first integral-term in equation (14) represents the force $F(B_1,B_2)$ between two dislocations. Applying Taylor's series expansion with respect to $|(y-\xi)/L| \leq h/L < 1$ to the integrand this force can be calculated as follows:

$$F(B_1B_2)=\frac{Mb^2}{L}\left[1\;-\;\frac{3}{L^2}\int_{-h}^{0}\int_{-h}^{0}\mathrm{F}(\eta(\xi)\eta(y)(\xi-y)^2;b^2)\,dyd\xi\;-\;\mathrm{O}\!\left(\frac{h^4}{L^4}\right)\right] \qquad (15)$$

Positive force corresponds here to repulsive interaction of dislocations B_1 and B_2. As distinct from the classical formula of dislocations theory, in (15) appears the term in brackets which reflects the role of cores. These latter give rise to attraction of dislocations which dominates at short distance L between them. In general, the cores attraction is controlled by the their structures, mainly by correspondent densities $\eta(y)$, which, in turn, depend on stresses in dislocations location produced by external forces and adjacent elements of the shear band.

Therefore, in addition to the two mentioned above fracture mechanics-type criteria, the following condition of the limit of the stable equilibrium of the shear band must be evaluated, too:

$$\frac{\partial F(B_1B_2)}{\partial L}=0 \qquad (16)$$

The criterion (16) determines nucleation of t-cleavage in single Stroh-type pileup which occupies unique slip line because the alternative criterion of cohesive crack extension is more difficult to fulfil [7,12]. This is unlikely to be changed with respect to t-crack in a shear band, too. What about initiation of the l-cleavage, it also seems to be less probable in single pileup due to insufficient tensile stress concentration. However, in a localised intense shear band the opposite may happen, i.e., l-cleavage may be easier. The main reason for this is that the body B_B produces tensile stress, roughly, $\sigma_{yy} \sim MB_B/H$ (cf. formulae (1)) which promotes slip band decohesion. Beside, shear stresses produced by B_B on the bottom pileup at $y = 0$ may be unfavourable for t-cleavage in accordance with instability criterion (16) as far as they push the tail B_t away from the pileup head and thus assist repulsion of the dislocations B_1 and B_2. Although, this repulsion of B_2 may compete with attractive action on this dislocation of the very head portion of the body B_B, i.e., of its density $\rho_B(x)$, situated at $0 \leq x \leq x_0 < L$, $y = H$, if the "cap" of its negative stress τ_{xy} covered the location of the element B_2. This probability, and finally, the possibility of t-cleavage, increases with rising of the ratio of H/L, i.e., for more thicker shear bands (less localised plasticity). On contrary, narrowing of the shear bands, e.g., due to hydrogen, promotes l-cleavage.

The central idea of the presented model concerning the role of hydrogen associates microfracture facilitation with diminishing of lattice cohesion properties (decohesion) just in dislocation cores, cf. (7). The effect of hydrogen on decrease of interatomic forces in metal now is well grounded (cf. [12]). On the other hand, lattice friction stress τ_i also was confirmed to depend strongly on interatomic potential [18], which surely affects the whole structure of the core, i.e., relations between its *t*- and *l*-components, and the Peierls one [17] not taken into account herein as apparently less relevant directly. This way by which the core-decohesive action of hydrogen can provoke shear localisation [6] is the predecessor for decohesion fracture itself, and promotes the *l*-cleavage in shear band, in particular, through narrowing of the band width *H*. On the other hand, apparent increase of lattice friction due to pinning dislocation to hydrogen [6] amplifies even more the susceptibility to *l*-cleavage as it follows from the presented model because greater τ_i prevents the external stress τ_{xy}^* to bring dislocations of the blocked arrays more close and nucleate the wedge-like *t*-crack. All that suggests interactive roles of hydrogen in both shear localisation and cleavage, the two having their origins in hydrogenous disturbance of interatomic potential just in dislocation cores. However, to assess the effective contribution of these anticipated influences of hydrogen on deformation and fracture needs further quantitative elaboration of the dislocation model of shear band evolution.

5. CONCLUSIONS

A dislocation model is developed towards elucidation of underlying mechanisms of hydrogen induced fracture. The earlier discrete-continuum model of Stroh-type cracking going traversely to slip plane of blocked array of edge dislocations is advanced to make it possible the consideration of the shear plane separation, too. The interactions of dislocations in a narrow shear band containing a number of plain arrays are considered with attention to the dislocation cores role. This latter is shown to be essential for microfracture initiation in dense dislocation configurations. Accounting for the effect of hydrogen on interatomic potential in a dislocation core which must be strong because of segregation of hydrogen on dislocations, this provides a reasonable description of mechanism of hydrogen affected fracture (embrittlement) as a plasticity-related phenomenon. Further development of the proposed model, expectedly, will allow establishing correlations between hydrogen effect on material and microstructural parameters such as grain size or inclusions spacing, slip band width and localisation (spacing).

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