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Procedia Structural Integrity 16 (2019) 252–259

Structural Integrity Procedia

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6th International Conference "Fracture Mechanics of Materials and Structural Integrity"

Microcrack under internal pressure at dislocation defect

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Abstract

By solving the problem of the theory of elasticity for a boundary dislocation with a cavity on its continuation, a stress-strain state in a solid crystalline body is determined. The correlation for calculating the energy of a body with a dislocation crack under pressure is obtained. The geometric parameters of a crack-like dislocation cavity are calculated. The values of equilibrium and non-equilibrium crack lengths are established on this basis. Also the value of the critical pressure at which the dislocation crack start begins is received. Stress intensity factors for the dislocation crack are obtained and calculated. Physical essence of fracture toughness is established using stress intensity factors.

Peer-review under responsibility of the 6th International Conference "Fracture Mechanics of Materials and Structural Integrity" organizers.

Keywords: Fracture mechanics, dislocation crack, internal pressure, energy of deformation; stress intensity factor.

1. Introduction

Study of the material fracture process is topical. Here the forecasts/predictions from the position of fracture mechanics are very important. The prediction of fracture becomes effective on the basis of theoretical foundations of the theory of dislocations. Although the principles of this theory are not new at present the renewal of its theoretical foundations is intensively carried out by modern researchers. It is also confirmed by the use of dislocation approaches to other different investigations necessary in materials science, fracture mechanics, theory of crystals etc.

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2452-3216 © 2019 The Authors. Published by Elsevier B.V.
Peer-review under responsibility of the 6th International Conference "Fracture Mechanics of Materials and Structural Integrity" organizers.
10.1016/j.prostr.2019.07.049

Dislocation fracture mechanisms are widely developed today by well-known scientists. Dislocation motion, as a rule, initiates the material plasticization. Enough number of impeded dislocation planes leads to the materials fracture by macrocracks formation. Such fracture is partially expected due to atomic hydrogen in the material. Fulfillment of the formed microcracks by hydrogen is accompanied by molecule formation of hydrogen atoms $H^+ + H^+ = H_2$ and corresponding internal pressure. So the investigations about the influence of hydrogen pressure in such a cavity on its propagation are relevant. It is practically important both for the development of hydrogen technologies and widening of fracture mechanics use.

2. Problem principal and key equations

Dislocation crack being a component of edge dislocation has practical importance for the solution of a number of fracture mechanics problems. After the investigation of the dislocation crack it becomes possible to analyze the influence of hydrogen on the materials embrittlement using Stashchuk and Dorosh (2016) in conformity with the energy of hollow nucleus. The attempt of such nucleus examination in certain approximation is presented by Friedel (1964) and by Fan (1994), Fan and Xiao (1997), Chen (2004). The dislocation crack with plastic zones was studied by Hoh et al (2012). Let us consider n number of inserted atomic half-planes in a crystalline body (Fig. 1). Such type defect of crystalline body is considered as an edge dislocation by Eshelby (1954), Friedel (1964), Cottrell (1964), Hirth and Lothe (1968). It induces internal stress-strain state in crystal, and also changes its internal energy. According to Eshelby (1954), Friedel (1964), Cottrell (1964) the edge of the inserted half-plane and the cavity formed in its vicinity is called the nucleus that breaks the regular structure of the crystal. The cavity on the continuation of the inserted extraplane is considered as a crack of l length (Fig. 1).

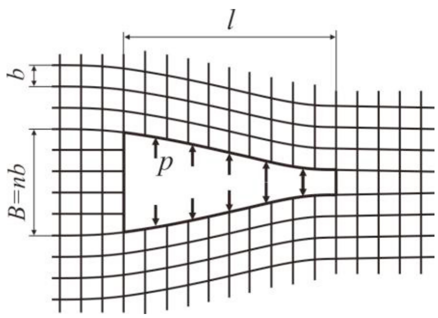

Fig. 1. The scheme of edge dislocation with the cavity under internal pressure.

In one of the crack tips, where the atomic insert ends, the dislocation discontinuity is equal to Burgers vector $\vec{B} = n\vec{b}$ (Eshelby (1954), Friedel (1964), Cottrell (1964), Hirth and Lothe (1968)), where $|\vec{b}| = b$ – distance between atomic planes. In the other crack tip, where the crystal structure ends, the crack edges close. Let us assume that pressure in the dislocation crack equals p. It is necessary to establish the influence of internal pressure in the cavity on stresses in the crystal body with such defect, and to estimate the strength of the body material. The form of the dislocation crack surface, stresses in the crystal with the dislocation, components of vector dislocations, volume of nucleus cavity and the energy of the material with such defect are already known and described by Stashchuk and Dorosh (2015, 2016). Estimation of the microcrack critical length that foregoes dislocation half-plane was deciding. Transformation of equilibrium dislocation crack to non-equilibrium was discovered under loading. Results of such type are very important for investigation of hydrogenated materials. Here the top priority task is to estimate the stress-strain state of the body with the dislocation crack under pressure p.

Let us bind dislocation crack-like defect with the Cartesian coordinate system xOy. Axis Ox is overlapped with the axis of defect symmetry, and centre O with the final atom of the inserted atomic half-plane B (Fig. 2).

It is supposed that along the defect with the inserted half-plane, that is on the $x \in (-\infty, 0]$ beam, the displacements $\upsilon^+ = -\upsilon^+ = B/2$ are given at upper (+) and lower (-) edges accordingly. These displacements are stipulated by internal stresses formed by the inserted half-plane. The internal pressure p is set on the crack edges.

The stress-strain state of the body with the dislocation crack is determined by Muskhelishvili (1977):

$$\sigma_x+\sigma_y=2\left[\Phi(z)+\overline{\Phi(z)}\right],\ \sigma_y-i\tau_{xy}=\Phi(z)+\Phi(\bar{z})+(z-\bar{z})\overline{\Phi'(z)}. \tag{1}$$

$$2\mu(u'+i\upsilon')=\chi\Phi(z)-\Phi(\bar{z})-(z-\bar{z})\overline{\Phi(z)}. \tag{2}$$

where $z = x+iy$, $i^2=-1$; u and v – components of displacement, $u' = \partial u/\partial x$, $\upsilon' = \partial\upsilon/\partial x$.

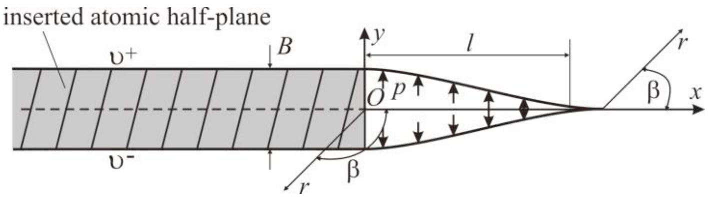

Fig. 2. The scheme dislocation crack under internal pressure.

Using the results of Stashchuk and Dorosh (2016) the complex potentials for the discussed defect are:

$$\Phi(z)=\Omega(z)=\frac{\mu B}{4\pi(1-\nu)}\frac{1}{\sqrt{z}\sqrt{z-l}}+\frac{p}{2}\left(\frac{2z-l}{2\sqrt{z}\sqrt{z-l}}-1\right). \tag{3}$$

Here μ – modulus of shear.

The crack length l is determined from the known balance equation (Griffith (1920, 1924)):

$$\frac{\partial U}{\partial l}+\frac{\partial F}{\partial l}=0 \tag{4}$$

where U – elastic energy of deformation for a crystal body with the dislocation crack under internal pressure, and F – work spent for the formation of the dislocation crack free surfaces.

Elastic energy of deformation U from (4) is found by Timoshenko and Goodyear (1970) using the known Clapeyron's theorem, according which the work of deformation (elastic energy of deformation) in the absence of volume forces equals to half the work A of internal forces on the initiated displacements

$$U=\frac{1}{2}A=\frac{1}{2}\iint_S t_i u_i\,ds=-\int_{-\infty}^{l}\sigma_y^+(x,0)\,\upsilon^+(x,0)\,dx. \tag{5}$$

where t_i – surface forces; u_i – components of displacements.

Expression of stress distributions →$\sigma_y(x,0)$ on the edges of inserted atomic half-plane in (5) according to (1) – (2) and (3) is:

$$\sigma_y(x,0)=\sigma(x)=-\frac{\mu B}{2\pi(1-\nu)}\frac{1}{\sqrt{(x-l)x}}-p\left(1+\frac{2x-l}{2\sqrt{x(x-l)}}\right).\ \ x\in(-\infty,0]. \tag{6}$$

According to (2), complex potentials (3) and with the account that $\upsilon(0,0)$=0,5B, the displacement of dislocation crack edge is:

$$\upsilon(x,0)=\upsilon(x)=\frac{B}{2\pi}\arccos\frac{2x-l}{l}+p\frac{1-\nu}{\mu}\sqrt{x(l-x)}. \tag{7}$$

Using the equations (6), (7) and expression (5) we get according to Stashchuk and Dorosh (2016):

$$U\approx\frac{\mu B^2}{4\pi(1-\nu)}\ln\left(\frac{4R}{l}\right)-\frac{Bpl}{2}-\frac{\pi(1-\nu)}{8\mu}p^2l^2. \tag{8}$$

Correlation (8) is the generalization of the plastic energy of deformation for classical dislocation. When p = 0, the known formula (Stashchuk and Dorosh (2015)) for body energy with edge dislocation follows from here. The work in (4) is spent for the formation of new surfaces of the dislocation crack in the presence of residual half-unlimited insert in crystal body (Fig. 2) is calculated by Griffith (1920, 1924):

$$F=2\gamma l. \tag{9}$$

where γ – specific surface energy.

After substitutions of (8) and (9) into (4) the equation for the estimation of dislocation crack length l is received:

$$-\frac{\mu B^2}{4\pi(1-\nu)l}-\frac{Bp}{2}-\frac{(1-\nu)\pi}{4\mu}p^2l+2\gamma=0. \tag{10}$$

Solution of (10) gives two correlations for crack length estimation:

$$l_{eq}=\frac{\pi\mu}{\pi^2p^2(1-\nu)}\left(4\gamma-Bp-2\sqrt{4\gamma^2-2Bp\gamma}\right).$$

$$l_{cr}=\frac{\pi\mu}{\pi^2p^2(1-\nu)}\left(4\gamma-Bp+2\sqrt{4\gamma^2-2Bp\gamma}\right). \tag{11}$$

The first correlation corresponds to the value of equilibrium crack length, second – to value of nonequilibrium dislocation crack length.

Let us note that it was obtained by Stashchuk and Dorosh (2015) that in the absence of pressure in the dislocation crack its length is determined by (10) when $p = 0$:

$$l_{eq}=\frac{\mu B^2}{8\pi(1-\nu)\gamma}\nu=\frac{EB^2}{16\pi(1-\nu^2)\gamma}.$$

For the criteria of the dislocation crack spontaneous propagation let us assume the condition for equation fulfillment

$$l_{eq}=l_{cr}. \tag{12}$$

Equation (12) is realized if $4\gamma^2 - 2Bp\gamma = 0$. Thus, the value of critical pressure is:

$$p_{cr} = \frac{2\gamma}{B}. \quad (13)$$

The same value of critical pressure was established by Cottrell (1958).

3. Stress intensity factor of dislocation crack

Stress intensity factor is one of important parameter in fracture mechanics. Expressions for stress intensity factors are received using complex potentials $\Phi(z),\ \Omega(z)$.

$$\Phi(z) = \Omega(z) = \frac{p}{4}\left(\frac{2z-l}{\sqrt{z}\sqrt{z-l}}\right) + \frac{\mu B}{4\pi(1-\nu)}\frac{1}{\sqrt{z}\sqrt{z-l}} - \frac{p}{2}.$$

If in the right dislocation crack tip (Fig. 2) the transfer is done to the polar coordinate system according to the scheme $z = z_1 + l$, $z_1 = re^{i\beta}$, then when $z_1/l << 1$ potentials $\Phi_1(z_1) = \Phi(z_1 + l)$, $\Omega_1(z_1) = \Omega(z_1 + l)$ will be:

$$\Phi_1(z_1) = \Omega_1(z_1) = \frac{K_I^l}{2\sqrt{r}}e^{-i\frac{\beta}{2}} + O(r^0) = \frac{K_I^l}{2\sqrt{r}}\left(\cos\frac{\beta}{2} - i\sin\frac{\beta}{2}\right) + O(r^0). \quad (14)$$

where $O(r^0)$ – limited value, and the stress intensity factor in the right tip of the dislocation crack (Fig. 2) equals:

$$K_I^l = \frac{p\sqrt{l}}{2} + \frac{\mu B}{2\pi(1-\nu)\sqrt{l}}. \quad (15)$$

Analogous for the left crack tip (Fig. 2) $(z = z_1 = re^{i\beta})$

$$\Phi_1(z_1) = \Omega_1(z_1) = \frac{K_I^0}{2\sqrt{r}}e^{-i\frac{\beta}{2}} + O(r^0) = \frac{K_I^0}{2\sqrt{r}}e^{-i\frac{\beta}{2}}\left(\cos\frac{\beta}{2} - i\sin\frac{\beta}{2}\right) + O(r^0). \quad (16)$$

where

$$K_I^0 = \frac{p\sqrt{l}}{2} - \frac{\mu B}{2\pi(1-\nu)\sqrt{l}}. \quad (17)$$

Comparison of (15) and (17) shows that stress intensity factors for the dislocation crack without internal pressure are opposite in sign. In this particular case it is agreed with the results obtained by Stashchuk and Dorosh (2016).

From a physical point of view value $\sigma(x)$ in the point $x = 0$ should be limited, just as it was analyzed by Gupta and Erdogan (1974) and Savruk (1981). It also follows from (17). Function $\sigma(x)$ in the point $x = 0$ has the peculiarities of order lower then $1/\sqrt{r}$. So it is accepted that $K_I^0 = 0$. Under this condition

$$p = \frac{\mu B}{\pi(1-\nu)l}. \quad (18)$$

Using (13) the relation between B and the length of dislocation crack l is received, that is

$$B = \sqrt{\frac{2\pi(1-\nu)\gamma l}{\mu}}. \tag{19}$$

After entering $p_{cr} = 2\gamma/B$ into (15) it can be written that

$$K_I^l = \frac{\gamma\sqrt{l}}{B} + \frac{\mu B}{2\pi(1-\nu)\sqrt{l}}. \tag{20}$$

Since the right crack tip in fact is responsible for fracture substitution of (19) into (20) gives the formulae for definition through shear modulus, surface energy and Poisson's critical pressure coefficient:

$$K_I^l = \sqrt{\frac{2\mu\gamma}{\pi(1-\nu)}}. \tag{21}$$

4. Numerical results

Numerical calculations of full energy of a solid with a dislocation crack under pressure were carried out using (10) and (11). Dependences of full energy $F+U$ of a body with dislocation crack on the dislocation crack length l for p=0, $p<p_{cr}$, $p=p_{cr}$ and $p>p_{cr}$ are shown in Fig. 3. Calculations of $F+U$ energy correspond to that for cylindrical body of a unit thickness with R = 10^{-7} m. Such values were used for these calculations (Vladimirov (1984)): $E = 2\cdot10^{11}$ Pa; $\gamma = 0{,}01\cdot E_a = 0{,}6$ J/m^2; $\nu = 0{,}3$; lattice parameter $b = 3\cdot10^{-10}$ m; Burgers vector module $B = 3b$.

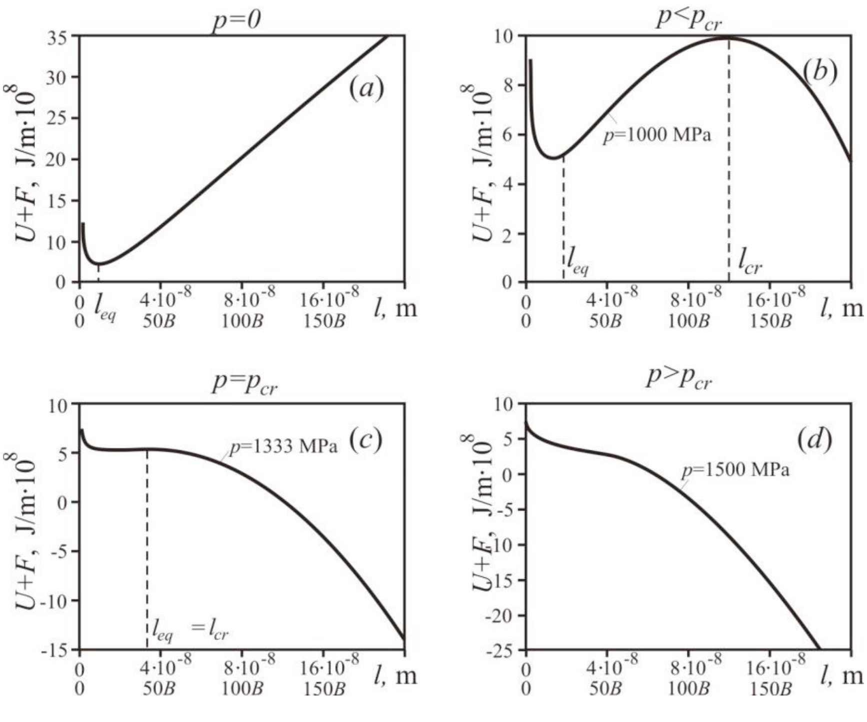

Fig. 3. Dependence of the solid energy $F+U$ on dislocation crack length when (a) p=0; (b) $p<p_{cr}$; (c) $p = p_{cr}$ and (d) $p>p_{cr}$.

Dislocation crack when $p<p_{cr}$ has both equilibrium and critical length (see Fig. 3). Curves of analogous character schematically given by Weertman (1986). It is seen from Fig. 3*a* that dislocation does not cause fracture when p=0. Setting of the internal pressure in the dislocation nucleus changes the form of the energy in the body with dislocation crack (Fig. 3*b*). Critical pressure p_{cr} causes such a form of energy in the cracked body that leads to its fracture (Fig. 3*c*). Curve in Fig. 3*d* corresponds to real spontaneous fracture of the body.

Calculations of critical pressure for different Burgers vector modules were carried using (13).

Calculations of l_{eq} and l_{cr} depending on the changes of internal pressure (Fig. 4) were performed using (11). Burgers vectors $B=3b$ and $5b$ were assumed.

Table 1 and Fig. 4 show that the increase of Burgers vector module values decreases the value of critical pressure. But the value of dislocation crack critical length is higher for larger values of Burgers vector.

Table 1. Numerical calculations of critical pressure depending on Burgers vector module

B, m	$b=3\cdot10^{-10}$	$2b=6\cdot10^{-10}$	$3b=9\cdot10^{-10}$	$5b=15\cdot10^{-10}$	$10b=30\cdot10^{-10}$
p_{cr} , MPa	4000	2000	1333	800	400
$l_{eq}=l_{cr}$, m	$0.26\cdot10^{-8}$	$1.05\cdot10^{-8}$	$2.36\cdot10^{-8}$	$6.56\cdot10^{-8}$	$26.23\cdot10^{-8}$

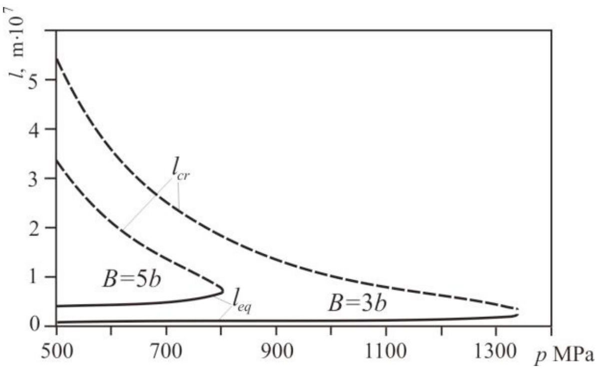

Fig. 4. Dependence of equilibrium and critical dislocation crack lengths l_{eq} and l_{cr} on internal pressure p.

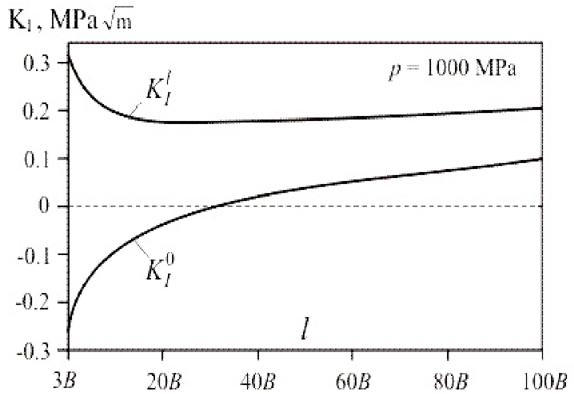

Fig. 5. Dependence of K_I^l and K_I^0 on dislocation crack length l.

Changes of K_I^l and K_I^0 according to (15) and (17) are presented in Fig. 5. Calculations were made using $B=3b$ Burgers vector and internal pressure p =1000 MPa.

5. Conclusions

Consideration of dislocation crack as an investigation object establishes the relations between the fracture mechanics and theory of dislocations. Evaluation of elastic energy in the body with dislocation crack was carried out on this base. As a result the value of critical pressure in a crack using Burgers vector and body surface energy was defined. Critical pressure of fracture in a body with dislocation crack using the criterion of equality of equilibrium value of crack length to critical value was calculated. Connection of Burgers vector B and material fracture toughness K_{IC} was established.

References

Chen, Y., 2004. Multiple Zener–Stroh crack problem in an infinite plate, Acta Mechanica 170, 11–23.
Cottrell, A., 1958. Theory of brittle fracture in steel and similar metals, Transactions of the Metallurgical Society of AIME 212, 192–203.
Cottrell, A., 1964. Theory of Crystal Dislocation, Blackie and Son LTD, London-Glasgow, pp. 94.
Eshelby, J., 1954. The Continuum Theory of Lattice Defects, in Solid State Physics 3. In: Seitz F., Turnbull D. (Ed). Academic Press, New York, 79–144.
Fan, H., Xiao, Z., 1997. A Zener–Stroh crack near an interface, International Journal of Solids and Structures 34(22): 2829–2842.
Fan, H., 1994. Interfacial Zener–Stroh crack, Journal of Applied Mechanics 61, 829–834.
Friedel, J., 1964. Dislocations, Pergamon Press, Oxford, pp. 491.
Griffith, A., 1920. The phenomenon of rupture and flow in solids, Philosophical Transactions of the Royal Society of London, A 221, 163–198.
Griffith, A., 1924. The theory of rupture, Proceeding of the First International Congress for Applied Mechanics, April 22–26, Delft, 55–63.
Gupta, G., Erdogan F., 1974. The problem of edge cracks in an infinite strip, Transactions of ASME, E41, 1001–1006.
Hirth, J., Lothe J., 1968. Theory of Dislocations, McGraw-Hill, New York, pp. 510.
Hoh, H., Xiao, Z., Luo, J., 2012. On the fracture behavior of a Zener–Stroh crack with plastic zone correction in three-phase cylindrical composite material, Mechanics of Materials 45, 1–9.
Muskhelishvili, N., 1977. Some basic problems of the mathematical theory of elasticity, Reprint of the 2nd English edition. Springer-Science + Business Media, Dordrecht.
Savruk, M., 1981. Two-dimensional Problems for Body with Crack, Naukova Dumka, Kyiv (in Russian).
Stashchuk, M., Dorosh M., 2015. Evaluation of the potential energy and geometric sizes of a dislocation crack, Materials Science, 51, 1, 88–95.
Stashchuk, M., Dorosh, M., 2016. Energy of deformation of an elastic body containing a microcrack under pressure, Materials Science, 52, 3, 339–348.
Timoshenko, S., Goodyear J., 1970. Theory of Elasticity, McGraw Hill Book Co, New York.
Vladimirov V., 1984. The physical nature of the destruction of metals, Metallurgy, Moscow (in Russian).
Weertman, J., 1986. Zener-Stroh crack, Zener-Hollomon parameter, and other topics. Journal of Applied Physics 60, 1877–1887.