Kinetic Equations of “Diffusion” Cracks and Delaminations in Adhesive Joints

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Abstract. In the cracks contained in such materials as metals under the action of corrosive media, degrading polymers and ceramics (for example, HTSC-ceramics), gas-saturated rocks, etc., gas can be accumulated. It is important to be able to predict the behavior of cracks under such conditions. In metals, hydrogen is usually dissolved in the proton form. When reaching crack surfaces, protons recombine with electrons to form molecular hydrogen inside the cavity. Then the crack can propagate only under the excessive pressure of gas hydrogen accumulated inside the crack even with no external loading. An important example of diffusion-controlled fracture growth is given by hydrogen induced delamination of pipe-line coating. In this work, for a penny-shaped crack in an unbounded elastic medium and for a thin penny-shaped delamination under the surface of a half-space, as well as for similar cracks-strips, in a uniform way – on the basis of the energy approach and with the use of Clapeyron theorem – kinetic equations are derived describing the growth of specified defects under gas diffusion into them. The analysis of the reasons leading to identity of the equations named, allows (under some conditions) to extend the results obtained for these problems to a number of other important cases: cracks on the interface of an adhesive joint of two pliable half-spaces with different mechanical and diffusion properties (with the interface being permeable as well as impermeable), the account of anisotropy, etc. It is shown, that exactly the same reasons (and under the same restrictions) make it possible to extend to the same cases the results obtained earlier for growth laws of a penny-shaped crack in an unbounded elastic medium versus laws of gas inflow into it as well.

Introduction

One of the models of crack growth as a gas is accumulated in the crack according to the diffusion mechanism (in what follows, a “diffusion” crack), which, for example, is typical of the process of structural steel hydrogenizing, was formulated and justified in [1] (different approaches are represented, for example, in [2, 3, 4, 5]). Later, in [6, 7, 8, 9, 10], this model was developed and generalized in different directions. In what follows, we analyze the derivation of the kinetic equations for this model, which allows for better understanding of the role and the action mechanism of its principal factors and also for showing the directions of extrapolation of the earlier results to different cases.

Derivation of kinetic equations

Let obtain kinetic equations for a penny-shaped crack in an infinite elastic space and for a circular crack, which is a delamination from the boundary of the half-space under gas diffusion into them (Фиг. 1) in a uniform way.

First we derive expressions for the case of a gas influx into the crack. Since the problem on a penny-shaped crack in infinite space is symmetric about the crack plane $z = 0$ ([6], p. 828), it suffices to consider the problem in the half-space $z \le 0$. We assume that the process is quasistationary ([1]; [9], p. 120) and take the axial symmetry of the problem into account. Then, for the unknown gas concentration $c(\rho, z, t)$, where ρ is the radial coordinate in the cylindrical system of coordinates, in the half-space $z \le 0$, we obtain the mixed problem from the theory of harmonic functions:

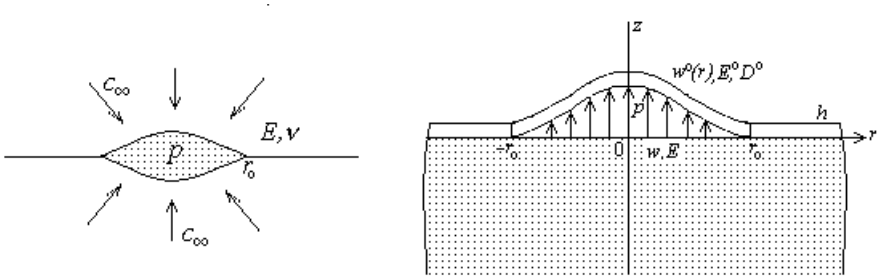

Fig.1.

$\Delta c = 0,\ z \le 0;$ $\qquad c|_{z=0} = 0,\ \rho \le r(t);$

$\partial c/\partial z|_{z=0} = 0,\ \rho > r(t);$ $\qquad c|_{z=\infty} = c_\infty$

where time t is a parameter. Subtracting the equilibrium state $c = c_\infty$, we obtain

$\Delta c = 0,\ z \le 0;$ $\qquad c|_{z=0} = -c_\infty,\ \rho \le r(t);$

$\partial c/\partial z|_{z=0} = 0,\ \rho > r(t);$ $\qquad c|_{z=\infty} = 0$ $\qquad (1)$

This mixed problem of potential theory is formally equivalent to the contact problem on the indentation of a rigid die, that is circular in cross-section and has a smooth bottom, in to an elastic isotropic half-space ([11], p. 385, formula (11.6.8) and later). Taking use of the solution of the latter contact problem we obtain for the density $q(\rho, t)$ of the gas diffusive flux into the crack

$$q(\rho,t) = -D\left.\frac{\partial c}{\partial z}\right|_{z=0,\,\rho<r} = \frac{2c_\infty D}{\pi\sqrt{r^2-\rho^2}}$$

The total flux through the surface $z = -0$, $\rho < r$ is

$$Q_- = \int_0^r 2\pi\rho q(\rho,t)d\rho = 4c_\infty D\int_0^r \frac{\rho d\rho}{\sqrt{r^2-\rho^2}} = 4c_\infty Dr \qquad (2)$$

For the delamination problem, the obtained quantity Q_- is simultaneously the total gas influx Q into the crack. But, for the case of a crack in infinite space gas influx goes through the lower and upper surfaces of the crack and is equal to

$$Q = Q_- + Q_+ = 2Q_- = 8c_\infty Dr \qquad (3)$$

Combining Eq. 2 and Eq. 3, we write

$$Q = N \cdot 4c_\infty Dr \tag{4}$$

where N is the number of "gas transmitting" surfaces of the crack.
Taking into account the expression $Q/k = dn(t)/dt$, where k is the coefficient of gas recombination in the crack (in the case of hydrogen, $k = 2$, because, on the crack surface, the protons melted in the metal recover to the atomic hydrogen which, flowing inside the crack, recombines into molecular hydrogen) and $n(t)$ is the number of gas moles in the crack, we can rewrite Eq. 4 in the form

$$dn(t) = 4Nc_\infty Dr\, dt/k \tag{5}$$

From the equation of state for the ideal gas (the Mendeleev–Clapeyron equation), we have

$$pV = RTn(t) \tag{6}$$

where p is the gas pressure inside the crack and V is the crack volume.
Expressing $n(t)$ from Eq. 6 and substituting into Eq. 5, after the replacement $dt = dr/u$, we obtain

$$d(pV) = (4Nc_\infty DRT)rdr/(ku) \tag{7}$$

The Clapeyron theorem for linear media ([11], p. 160) implies that

$$U = pV/2, \;\; pV = 2U \tag{8}$$

where U remains the elastic energy of the body.
We introduce G, which is the elastic energy release rate or the "crack-moving force" ([12], p. 71, formula (3.12) and further) or the "force of resistance to the crack propagation" ([11], p. 686) or the "energy flux towards the crack vertex", the "intensity of released elastic energy" ([3, pp. 28–30, p. 51), or the "strain energy release rate" ([13], p. 119). For a linearly elastic body, all these quantities, as well as the Γ-integral ([14], Chapter 1, Sec. 1), as well as the J-integral, coincide ([15], pp. 107–116). By definition ([12], pp. 73–74, formulas (3.21)–(3.23)), we write

$$G = \left.\frac{\partial U}{\partial S}\right|_p \tag{9}$$

where U is the elastic energy of the body and S is the crack area.
Under the axisymmetric extension of a penny-shaped crack, we have $dS = 2\pi r dr$, and

$$G = \left.\frac{\partial U}{\partial S}\right|_p = \left.\frac{1}{2\pi r}\frac{\partial U}{\partial r}\right|_p$$

If the dependence of U (or of V, which is the same in the linear case, as it follows from Eq. 8) on r is power-law, i.e.

$$U \sim r^m \tag{10}$$

then

$$\frac{1}{r}\frac{\partial U}{\partial r} = m\frac{U}{r^2}, \quad G = \frac{mU}{2\pi r^2}, \quad U = \frac{2\pi r^2 G}{m} \tag{11}$$

Substituting Eq. 11 into Eq. 8 and then into Eq. 7, we obtain

$$d(r^2 G) = \frac{Nm}{2\pi k} c_\infty DRT \frac{d(r^2)}{u} \tag{12}$$

When a crack grows really, its propagation rate cannot be arbitrary, but, according to the kinetic diagram of static fracture strength at each time instant, is determined by the current value of the stress intensity factor on its contour or by the current energy release rate G. Thus, to derive the kinetic equation, we must assume in Eq. 12 that the the crack propagation rate u is the function of G determined by the kinetic diagram of static fracture strength, $u = u(G)$. This is that gives the desired kinetic equation, expressed in variables G и r, which, by the way, does not contain time t explicitly. But what is the real, actual character of the dependences $U(r)$, $V(r)$? For a penny-shaped crack under internal pressure in an infinite body, we have $V = V(r, p, E, \nu)$, and it follows from dimension considerations that $V \sim r^3 p/E$ (the exact formulas see in ([16], p. 548, formula (10.131)). In this case $m = 3$, $N = 2$, and Eq. 12 becomes

$$d(r^2 G) = \frac{3}{\pi} c_\infty DRT \frac{d(r^2)}{ku} \tag{13}$$

In the case of a thin parallel-to-the-boundary impenetrable delamination of thickness h from the half-space, the problem is reduced [9] to the problem of axisymmetric bending of a circular plate fixed on the boundary under the action of uniform pressure, $V = V(r, p, D_0)$, and it follows from dimension considerations that $V \sim r^6 p/D_0$ (the exact formula is ([9], Eq. 12). Thus, here we have $m = 6$ and $N = 1$ and Eq. 12 becomes

$$d(r^2 G) = \frac{6}{2\pi} c_\infty DRT \frac{d(r^2)}{ku} = \frac{3}{\pi} c_\infty DRT \frac{d(r^2)}{ku} \tag{14}$$

which coincides exactly with the similar Eq. 13.

Kinetic equation integral. Step-like kinetic diagram

Eq. 12 can be easily integrated

$$\ln\left(\frac{r}{r_0}\right) = \frac{1}{2}\int_{G_{SCC}}^{G} \frac{dG}{\frac{\alpha}{u(G)} - G}$$

$$\alpha = \frac{Nm}{2\pi k} c_\infty DRT$$

When $r \to \infty$, $\ln(r/r_o)^2 \to \infty \leftrightarrow [\alpha/u(G) - G] \to 0$

$G \to G_\infty$: $u(G_\infty) = \alpha/G_\infty$, $u \to u_\infty = u(G_\infty)$ (15)

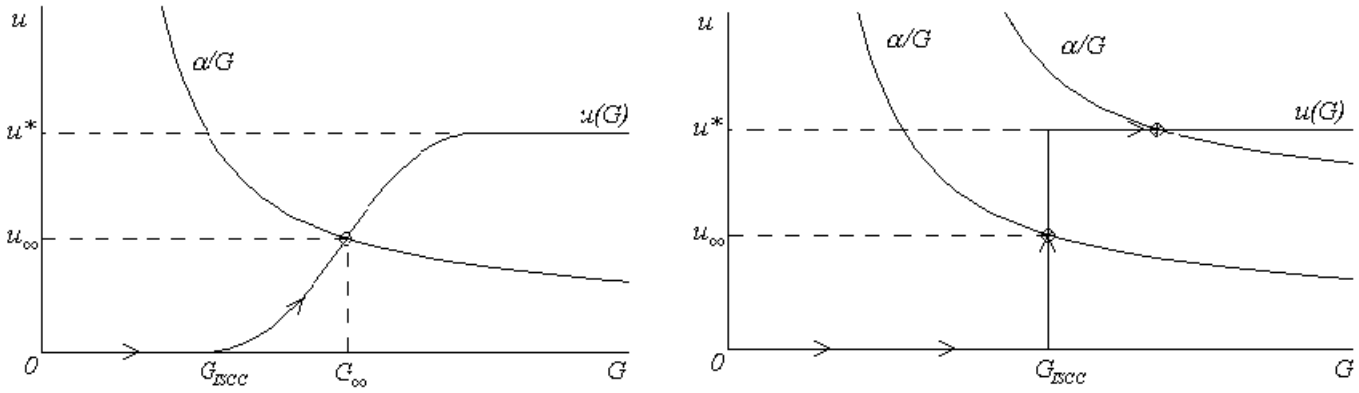

Fig. 2

For metals and rocks kinetic diagram $u(G)$ is nearly step-like (Fig. 2). In this case it follows from Eq. 15 that

if $\alpha/G_{SCC} < u^*$, then $G_\infty = G_{SCC}$, $u_\infty = \alpha/G_{SCC}$,
if $\alpha/G_{SCC} > u^* \rightarrow u_\infty = u^*$, $G_\infty = \alpha/u^*$

Example: life-time evaluation of a massive piece of structural steel with a penny-shaped crack under hydrogenation

We use these results to analyze the kinetics of a penny-shaped crack in a bulk sample of low-carbon low-alloy steel in hydrogenation. We simulate a sample as infinite elastic medium and assume that the material has the $u(G)$ diagram of threshold type (which is close to reality).

The process of crack development consists of two stages: incubation period, t_i (gas accumulation in the stationary crack), followed by a period of growth (movement) t_m.

During the period of incubation, $r = r_0 = \text{const}$. Corning back in (2.16) from dr^2 to rdr, dividing both sides by r, substituting $k = 2$, substituting dr/u on dt, and r on r_0 and integrating, we obtain

$$G = 3c_\infty DRTt/(\pi r_0) \qquad (16)$$

The incubation time is determined by the achievement of G its critical value G_{ISCC}, which gives

$$t_i = \pi r_0 G_{ISCC}/(3c_\infty DRT) \qquad (17)$$

In the literature they give the values not for G_{ISCC}, but for the corresponding SIF K_{ISCC}, which is related to G_{ISCC} by the Irwin formula $G_{ISCC} = (1 - \nu^2)K^2_{ISCC}/E$. For the concentration c_∞ of the hydrogen dissolved in the metal the literature values given are for the so-called "weight parts" (the ratio of the weight of hydrogen per unit volume to the weight of the metal containing it), we denote this quantity by c^∞, while c_∞ has the dimension of mol/volume and is numerically equal to $c^\infty g$, where g is the steel density. Therefore, passing in Eq. 17 from G_{ISCC} to K_{ISCC} and from the c^∞ to c_∞ we finally obtain

$$t_i = \pi(1 - \nu^2)K^2_{ISCC} r_0/(3c^\infty g\, DRTE) \qquad (18)$$

During the period of growth with the $u(G)$ diagram of threshold-type $G = const = G_{ISCC}$. Substituting this into (2.16), substituting $k = 2$, dividing both sides by dr^2 and replacing c^∞ through c_∞ and G_{ISCC} through K_{ISCC}, we obtain

$$u = 3c_\infty DRT/(2\pi G_{ISCC}) = 3c^\infty gDRTE/[2\pi(1-\nu^2)K^2_{ISCC}] = const \quad (19)$$

$$t_i = r_0/(2u) \quad (20)$$

$$r = r_0 + (t - t_i)\cdot u = r_0 + t_m \cdot u \quad (21)$$

We assume room temperature $T = 273^0$K and use the default values for the universal gas constant $R = 8.31$ J/(mol·grad) = $8.32\cdot10^7$ erg /(mol·grad) ([17], p. 153 [18], p. 151) and typical values for density and elastic constants of low-alloy steel $g = 7.8$ g·cm^{-3} ([17], p. 40), $E = 2\cdot10^4$ kg·mm^{-2}, $\nu = 0.3$ ([17], p. 116). We also know that $D = 10^{-3}$ mm^{2}s^{-1} [19], $K_{ISCC} \cong 120$ kg·mm$^{-3/2}$ [20], and the values of c^∞ can reach 10^{-5} parts by weight [21]. In addition, we assume that the initial radius of the crack r_0 is equal to $r_0 = 10$ mm.

T^0 [K]	R [J/(mole·K)]	g [g·cm^{-3}]	E [kG·mm^{-2}]	ν	D [mm^{2}c^{-1}]	K_{ISCC} [kG·mm$^{-3/2}$]	c^∞	r_0 [mm]
273	8.31	7.8	$2\cdot10^4$	0.3	10^{-3}	120	10^{-5}	10

Substituting these values in Eq. 19, we obtain

$u \cong 10^{-5}$ mm/s

Thus, the crack front velocity turned out to be of the order of 10^{-5} mm/s and according to Eq. 20, incubation time

$t_i = r_0/(2u) = 10$ mm/($2\cdot10^{-5}$ mm/s) = $5\cdot10^5$ s $\cong 1.5\cdot10^2$ h = 150 h $\approx$ 6 days and nights.

If the front crack after the start begins to move at a speed of about 10^{-5} mm/s, then the radius equal, for example, $r = 50$ mm, will be according to Eq. 21 achieved through

$t_m = (r - r_0)/u =$ (50–10) mm/(10^{-5} mm·s^{-1}) = $40\cdot10^5$ s $\cong 1.1\cdot10^3$ h $\approx$ 46 days and nights.

As can be seen from Eqs. 19-21, the values of durability can vary by orders of magnitude depending on the concentration of the gas in the metal.
In the case of the $u(G)$ diagram of general form, as well as in the presence of tensile stresses and taking into account a number of additional physical and physical-chemical factors [5] the range of possible values of life can range from several hours up to many hundreds of years.

Main assumptions and the scope of the equation obtained above
To specify the scope of the kinetic Eq. 12 and the results obtained from this equation earlier in [1, 6, 7, 8, 9], we list the assumptions used above in its derivation:
1. The medium is homogeneous and diffusively linear, see Eq. 5.
2. The gas is thermodynamically ideal (obeys the Mendeleev–Clapeyron equation of state), see Eq. 6.
3. The medium is mechanically linear, see Eq. 8.
4. The dependence of V , and hence of U, on r is power-law, see Eqs. 10, 11.

As to the last assumption, it follows from dimension considerations that, in any case, the expression for the volume V of the crack must have the form

$$V = r^3 \frac{p}{E} f\left(\frac{r}{h_i}, \nu_i\right)$$

where h_i are the problem parameters of dimension of length (except for r), ν_i are the dimensionless parameters (except for r/h_i), $f(r/h_i, \nu_i)$ is a function determined by the geometry and physics of the problem.

Thus, condition 4 means that either the problem does not contain any geometric parameters other than the crack dimensions (as in the case of an infinite homogeneous body) or all the parameters of dimension of length in the formula for the volume V are combined into a single factor (as in the case of delamination from the half-space).

On the one hand, this implies that all the main results must remain valid if the complication of the problem is not related to the appearance of new parameters of dimension of length. For example, these are (under some conditions) the following cases: cracks on the adhesion boundary between two compliant half-spaces with different mechanical but equal (close) diffusive properties (in the case of an impenetrable boundary, the diffusive properties can also be different); the case of taking the anisotropy into account; delamination from the membrane half-space; etc.

Since the argument in [8] is also based on the same assumptions 2–4, the results in [8] can be generalized (under the same conditions) to all problems where the above assumptions remain valid.

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