

Kinetics of interfacial crack bridged zone degradation

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Abstract. A kinetic model of bonds destruction, interfacial adhesion strength and durability of interface junction is developed. It is assumed that a zone of weakened bonds exists at materials interface at an initial time instant. This weakened zone is considered as a crack-like defect filled with distributed spring-like bonds. Bonds mechanical properties are time-dependent under external loads. Bonds properties kinetics analysis is performed on the basis of Zhurkov's thermofluctuational approach of bonds destruction. The computational results those obtained on the basis of the developed numerical algorithm are presented.

1. Introduction

The model of a crack with bonds in the bridged zone allows one to determine the crack resistance and the adhesive strength of joints between different materials on the basis of micromechanical properties of the bonds [1–3]. The development of this model with consideration of time-variation in the physical and mechanical properties in the crack bridged zone allows one to estimate the long-term strength and time characteristics of material crack resistance.

In the present paper, Zhurkov's kinetic model of thermal fluctuation fracture [4,5] together with the crack bridged zone model, is used for bonds destruction and interfacial adhesion strength modelling. It is assumed that at least one of the materials is a polymer and the crack part occupied by the bridges (the bridged zone) is not small compared with the crack length. The estimate of the bonds destruction in the crack bridged zone and kinetic characteristics of the interfacial junction are based on the following assumptions:

- at the initial time, on the interface there is a region of weakened bonds between materials (this may be a technological defect or a weakened region caused, for example, by the diffusion activity of the medium);
- the bond density in that region varies in time according to the thermal fluctuation mechanism;
- the bond rigidity is proportional to their density at each point of the crack bridged zone;
- the defect nucleation occurs near the center of the weakened bond region;
- the condition for the crack-defect formation is the decreasing in the average bond density to the critical value on the corresponding part of the weakened bond region.

2. Kinetics of bonds in the crack bridged zone

The durability of materials under the action of the tensile stress σ satisfies the following experimentally established formula [4,5]

$$\tau = \mu\tau_0 e^{\frac{U(\sigma)}{kT}} \quad (1)$$



where τ is the specimen fracture time, k is the Boltzmann constant, T is the absolute temperature, $\tau_0 \approx h/(kT)$ is a constant of the order of the atomic thermal vibration period ($10^{-13} - 10^{-12}$ s), h is the Planck constant, μ is a dimensionless coefficient depending on the type of the material (polymer, metal, or ceramics), and $U(\sigma)$ is the bond destruction energy (fracture activation energy).

For a sufficiently wide interval of external loads and temperature, the function $U(\sigma)$ is linear,

$$U(\sigma) = U_0 - qT - A(\sigma), \quad A(\sigma) = \gamma\sigma \quad (2)$$

where U_0 is the interatomic bond breakage activation energy and q and γ are structure-sensitive parameters characterizing the material thermal and strength properties.

It follows from expression in Eq. (2) that $A(\sigma)$ decreases the bond breakage energy barrier and can be treated as the work done by external stresses in the body fracture.

A formula similar to that in Eq. (1) also holds for the average life time (durability) τ_b of a loaded interatomic bond [4,5]. The work of external stresses in this case depends on the stress value in the bond. The inhomogeneity of the stress distribution in the bonds in an actual body results in local damage accumulation and formation of defects. The most intensive damage accumulation occurs in the weakened interatomic (intermolecular) bond regions in the material. The weakened bond region in the material (or on the material interface) will be treated as a crack filled with bonds (bridges) whose properties vary in time according to the thermal fluctuation mechanism.

It is assumed that the expression in Eq. (1) also holds for bonds in the crack bridged zone but the work $A(\sigma)$ contained in Eq. (2) is the bond deformation work, which is determined with the inhomogeneous stresses distribution over the bonds in the bridged zone taken into account.

The bond deformation work A and the bond durability τ_b in the bridged zone of a rectilinear crack on the material interface (Fig. 1) depend on the tension of bond in the bridged zone σ_b (for details, see Eqs. (12)-(13) below) and the coordinate x determining the bond location along this zone, $A = A(\sigma_b, x)$ and $\tau_b = \tau_b(\sigma_b, x)$.

Assume (following [6]) that the time variation in the bond density $n(x, t)$ in the crack bridged zone is described by the chemical destruction equation

$$\frac{dn(x, t)}{dt} = -\frac{n(x, t)}{\tau_b(\sigma_b, x)} \quad (3)$$

where $\tau_b = \tau_b(\sigma_b, x)$ is the time till the breakage of the molecular bond located in the crack bridged zone at the distance $\ell - x$ from its tip (the bond durability).

It follows from Eq. (3) that

$$n(x, t) = n_0 \exp\left(-\frac{t}{\tau_b(\sigma_b, x)}\right) \quad (4)$$

where $n(x, 0) = n_0$ is the initial bond density.

The time variation in the bond density leads to a variation in the bond compliance in the crack bridged zone. Let $k_s(x)$ denote the rigidity of a single molecular bond. Then the effective rigidity of bonds per unit area of the crack bridged zone is

$$k(x, t, \sigma_b) = k_s(x) n(x, t) = k_b(x) \exp\left(-\frac{t}{\tau_b(\sigma_b, x)}\right) \quad (5)$$

where $k_b(x) = k_s(x) n_0$ is the initial bond rigidity per unit area of the crack bridged zone.

It follows from Eq. (5) that the bond compliance in the crack bridged zone can be represented as

$$c(x, t, \sigma_b) = c_b(x) \exp\left(\frac{t}{\tau_b(\sigma_b, x)}\right) \quad (6)$$

where $c_b(\cdot) = 1/k_b(\cdot)$ is a function determining the initial bond compliance in the crack bridged zone.

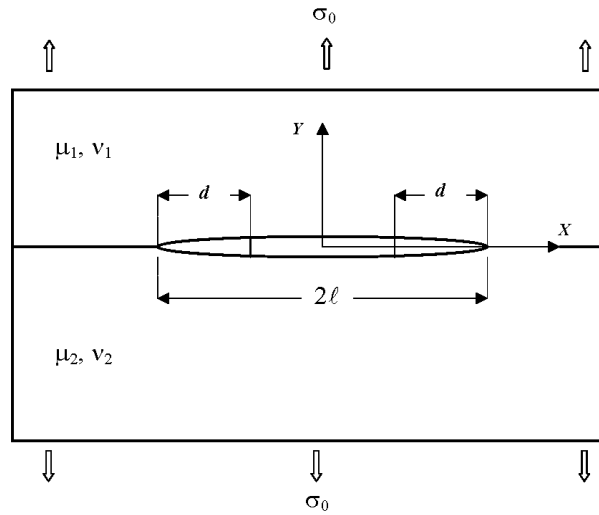


Figure 1. Bridged crack at the interface of different material

3. Bridged interface crack model

We use proposed in the previous papers [1-3] the bridged interface crack model with the assumption that the crack surfaces interact in some zones starting from the crack tips. Let us consider the planar elasticity problem on a crack ($|x| \leq \ell$) at the interface ($y = 0$) of two dissimilar joint half-planes, see Fig.1. Assume that the uniform load σ_0 normal to the interface is acted at infinity. The crack surface interaction is supposed to be existing in the bridged zones, $\ell - d \leq |x| \leq \ell$. The size of the interaction zone depends on time $d = d(t)$ due to the possibility the time changing of the bond properties. As a simple mathematical model of the crack surfaces interaction we will assume that the linearly elastic bonds act through the crack bridged zones.

Denote by $Q(x, t)$ the bond tractions occurring under the action of the external loads such that

$$Q(x, t) = q_y(x, t) - i q_x(x, t), \quad i^2 = -1 \quad (7)$$

where $q_y(x, t)$ and $q_x(x, t)$ are the normal and shear components of the traction, respectively.

By incorporating the superposition principle we'll consider the 2D-elasticity interface crack problem with the following boundary conditions at the crack surfaces ($y = 0$)

$$\sigma_{yy}(x,t) - i\sigma_{xy}(x,t) = -\sigma_o, \quad |x| \leq \ell - d(t) \quad (8)$$

$$\sigma_{yy}(x,t) - i\sigma_{xy}(x,t) = (-\sigma_o + q_y(x,t)) - iq_x(x,t), \quad \ell - d(t) \leq |x| \leq \ell \quad (9)$$

The opening of the interface crack, $u(x,t)$, can be written as follows

$$u(x,t) = u_y(x,t) - iu_x(x,t), \quad (10)$$

where $u_{x,y}$ are the projections of the crack opening on the coordinate axes x and y respectively.

The function $u(x,t)$ can be represented in the following form

$$u(x,t) = u_\infty(x) + u_Q(x,t), \quad u_\infty(x) = u_{\infty y}(x) - iu_{\infty x}(x), \quad u_Q(x,t) = u_{Qy}(x,t) - iu_{Qx}(x,t) \quad (11)$$

Where $u_\infty(x)$ is the crack opening caused by the loads, $-\sigma_o$, acting at the crack surfaces and $u_Q(x,t)$ is the crack opening caused by the bond induced tractions under the action of the external loads. The relation between the crack opening and bond tractions (the bond deformation law) will be written as follows

$$u(x,t) = c(x,t,\sigma_b)(q_y(x,t) - iq_x(x,t)), \quad (12)$$

where the function $c(x,t,\sigma_b)$ is determined by formula (6) and $\sigma_b = \sqrt{q_x^2 + q_y^2}$.

For dimensionality reasons one can represent function $c(x,t,\sigma_b)$ in the formula (6) in the following form [1]

$$c_b(x) = \frac{H}{E_B} \varphi(x,t,\sigma_b) = c_0 \frac{\ell}{E_B} \varphi(x,t,\sigma_b) \quad (13)$$

where H is a linear scale proportional to the bonding zone thickness, E_B is the effective Young modulus of the bonds and $\varphi(x,t,\sigma_b)$ is dimensionless function and

$$c_0 = \frac{H}{\ell}$$

is the relative bond compliance.

Let us write a system of the integral-differential equations for computation of the bond tractions $Q(x,t)$ in the crack bridged zone. From the first relation in expressions (11) we can obtain

$$\frac{\partial u(x,t)}{\partial x} = \frac{\partial u_\infty(x)}{\partial x} + \frac{\partial u_Q(x,t)}{\partial x} \quad (14)$$

The interface crack opening components caused by the external normal stresses, σ_o (or the stresses - σ_o at the crack surfaces), are equal to [7]

$$u_{\infty}(x) = \frac{\sigma_o \sqrt{\alpha}}{2(1+\alpha)} \left(\frac{k_1+1}{\mu_1} + \frac{k_2+1}{\mu_2} \right) \sqrt{\ell^2 - x^2} \left(\frac{\ell-x}{\ell+x} \right)^{-i\beta}, \quad \alpha = \frac{\mu_2 k_1 + \mu_1}{\mu_1 k_2 + \mu_2}, \quad \beta = \frac{\ell n \alpha}{2\pi} \quad (15)$$

where $k_{1,2} = 3 - 4\nu_{1,2}$ or $k_{1,2} = (3 - \nu_{1,2}) / (1 + \nu_{1,2})$ for the plane strain and plane stress, respectively; $\nu_{1,2}$ and $\mu_{1,2}$ are the Poisson ratios and shear moduli of the joint materials 1 ($Y > 0$) and 2 ($Y < 0$).

To obtain the expression of the derivative of the crack opening caused by the bond action $(\partial u_o(x, t) / \partial x)$ we had used the representations for the derivative of the displacements of the interface crack surfaces under the action of arbitrary loads given in [7], see details of transformations in [1].

Finally, by substituting the expressions for the derivatives (those obtained on the basis of Eqs. (12), (13) and (15)) into Eq. (14) we arrive to system of the integral-differential equations for unknown functions $p_{x,y}(x, t)$ (see details in [8])

$$\begin{aligned} \frac{\partial}{\partial s} \left[\varphi(s, t, \sigma_b) (q_y(s, t) - i q_x(s, t)) \right] - \frac{\pi \varepsilon (1 - \alpha)}{2(1 + \alpha)} (q_x(s, t) + i q_y(s, t)) + \\ \frac{\varepsilon}{\sqrt{1 - s^2}} \left(\frac{1 - s}{1 + s} \right)^{-i\beta} \int_{1-d/\ell}^1 R(s, \eta) [s p_y(s, t) - i \eta p_x(s, t)] d\eta = \frac{\pi \varepsilon \sqrt{\alpha} (2\beta i - s)}{(1 + \alpha) \sqrt{1 - s^2}} \left(\frac{1 - s}{1 + s} \right)^{-i\beta} \end{aligned} \quad (16)$$

where

$$\begin{aligned} q_y(s, t) - i q_x(s, t) = (p_y(s, t) - i p_x(s, t)) \left(\frac{1 - s}{1 + s} \right)^{-i\beta} \\ s = \frac{x}{\ell}, \quad t = \frac{\xi}{\ell}, \quad q_{y,x}(s, t) = \frac{q_{y,x}(x, t)}{\sigma_o}, \quad p_{y,x}(s, t) = \frac{p_{y,x}(x, t)}{\sigma_o} \end{aligned}$$

The singular kernel $R(s, \eta)$ and the parameter ε in Eqs. (16) are defined as

$$R(s, \eta) = \frac{\sqrt{1 - \eta^2}}{\eta^2 - s^2}, \quad \varepsilon = \frac{E_B \ell}{2\pi H} \left(\frac{k_1 + 1}{\mu_1} + \frac{k_2 + 1}{\mu_2} \right)$$

Parameter ε characterizes the ratio of the compliance of the joint part containing a crack without bonding to the bond compliance. Equations (16) represent the system of two singular integral-differential equations with the Cauchy type kernels. This system can be solved numerically.

4. Bonds deformation work and stress intensity factors

The bond deformation work (per unit width of the body) on the crack bridged zone of size dx is given by the expression [1, 8]

$$dU(x) = \left[\int_0^{u_x(x)} q_x(u_x) du_x + \int_0^{u_y(x)} q_y(u_y) du_y \right] dx \quad (17)$$

where $u_{x,y}(x)$ are the opening components in the crack bridged zone at the point with coordinate x and $q_{x,y}(x)$ are the bonds tractions. The number of molecular bonds on the interval dx is

$$dn = n(x, t)dx$$

The work per one intermolecular bond is estimated under the assumption that the adhesion junction is formed by chains of polymer molecules of size of the monomer link a_m . It is assumed that the bond elongation (of the chain molecule) in deformation within the limits of linear elasticity is much less than its initial length and the crack opening in the bridged zone at the distance $\ell - x$ from the crack tip is approximately equal to the length of the loaded segment of the chain molecule bridging the crack surfaces. In this case, the number N_m of monomer links between the crack surfaces on an interval of length dx is

$$N_n = \omega dn, \quad \omega = \sqrt{u_x^2(x, t) + u_y^2(x, t)} / a_m \quad (18)$$

where ω is the number of monomer links of the polymer chain making a bond between the crack lips. The work per one intermolecular bond is equal to

$$A(\sigma_b, x) = \frac{dU(x)}{\omega dn} \quad (19)$$

Finally, expression (1) can be rewritten in the form convenient for computations,

$$\tau_b(\sigma_b, x) = \tau_0 \exp\left(\frac{U_M - A_M(\sigma_b, x)}{RT}\right) \quad (20)$$

where U_M is the energy of activation of one mole of intermolecular bonds, $U_M = U_0 N_A$, $A_M(\sigma_b, x) = A(\sigma_b, x) N_A$, $R = k N_A$ is the gas constant, and N_A is the Avogadro number.

Having the solution of system (16) one can calculate the stress intensity factors (SIF) K_I and K_{II} following to [9]

$$K_I + iK_{II} = \lim_{\delta \rightarrow 0} \sqrt{2\pi\delta} (\sigma_{yy}(\delta, t) + i\sigma_{xy}(\delta, t)) \delta^{-i\beta}, \quad (21)$$

where $\sigma_{yy}(\delta, t)$ and $\sigma_{xy}(\delta, t)$ are the stresses ahead the crack tip caused by the external loads and bond stresses, δ is the small distance to the crack tip. On the other hand, the SIF can be written as follows

$$K_I + iK_{II} = (K_I^{ext} + K_I^{int}) + i(K_{II}^{ext} + K_{II}^{int}), \quad (22)$$

where $K_{I,II}^{ext}$ and $K_{I,II}^{int}$ are the SIF caused by the external loads and bond stresses.

Taking into account relations (21) and (22) we can obtain (see details in [1])

$$K_I + iK_{II} = \frac{\sqrt{\pi\ell}}{(2\ell)^{i\beta}} \left[\sigma_o(1 + 2i\beta) - \frac{2 \cosh(\pi\beta)}{\pi} \int_{1-d/\ell}^1 \frac{q_y(s, t) + itq_x(s, t)}{\sqrt{1-s^2}} ds \right], \quad K = \sqrt{K_I^2 + K_{II}^2} \quad (23)$$

where K is modulus of the SIFs.

5. Numerical algorithm

The system of the integral-differential equations (16) is solved by a collocation scheme for each time-step. The crack bridged zone, $d(t)$, is divided into M quadratic finite elements. Unknown functions are represented by parametric quadratic polynomials on each element. This procedure enables us to obtain expressions for the unknown functions and their derivatives through the nodal values of these functions. Then the system of the integral-differential equations is reduced to a system of linear algebraic equations relative to the nodal values of the unknown functions [1].

For each time step bond compliances are assumed to be proportional to the density of unbroken bonds. The following condition is used as the criterion of full bonds destruction on a part of bridged zone of size $\Delta\ell$ at its trailing edge

$$\bar{N}(t_k) \leq N_{cr} \quad (24)$$

where $\bar{N}(t_k)$ is the average density of bonds at the time step t_k and N_{cr} is the limit value of the bond density.

The modeling further growth of the initial nucleated defect is performed by decreasing the bridged zone size according to condition (24). The time-step scheme of numerical solving the integral-differential equation for a crack-like region with the bridged zones is used at each step of the defect increasing [8].

The computations were carried out for a combination of materials typical of microelectronic devices [10]: one of the materials is metal (copper-based alloy) with elasticity modulus $E_1 = 130 \text{ GPa}$, and the other is an (epoxy-based) polymer with elasticity modulus $E_2 = 2 \text{ GPa}$, the Poisson ratios of the materials are $\nu_1 = 0.3$ and $\nu_2 = 0.35$, respectively, and the elasticity modulus of the bonds is $E_b = E_2$. The size of the weakened bond region located along the material interface is set to be equal to $2\ell = 10^{-5} \text{ m}$. It is assumed that the bonds are formed by chains of polymer molecules where the size of the molecule monomer chain is equal to $a_m = 10^{-9} \text{ m}$. The bond deformation law in the computation process was assumed to be linearly elastic with compliance constant along the weakened bond region at the initial time. (Estimates of mechanical parameters of bonds in the crack bridged region can be found in [1].) The kinetic dependences were calculated for the following parameter values [4,5]: $q \cdot N_A = 8.3 \text{ J / mole} \cdot \text{K}$, the energy of activation of the molecular bond breakage was $U_M = 150 \text{ kJ / mole}$, the initial bond density was $n_0 = 10^{18} \text{ m}^{-2}$, $\tau_0 = 10^{-12} \text{ s}$, and $\mu = 1$. The limit value of the bond density in the initial defect formation region was chosen as $N_{cr} = 0.1n_0$. The external load was assumed to be constant in time.

As an example of proposed model application in Fig. 2 is shown the time variation of the stress intensity factor module in the process of growth of the bond-free crack part for different values of temperatures. In the bond breakage process, their strengthening effect decreases, and the stress intensity factor increases. The largest increase in the stress intensity factor occurs at the last stages of the defect growth when the stress intensity factor tends to the corresponding value for the bond-free crack. Assuming (for the conservative estimate) that the ratios of the time intervals in which the stress intensity factor attains the largest value are proportional to the durability of the joint, one can see that the increase in the temperature (in the range under study) by $\Delta T = 25 \text{ K}$ decreases the joint durability by more than one order of magnitude. The values of the stress intensity factor modulus are normalized by the value K_0 , the stress intensity factor modulus due to the action of the external load for cracks without bonds.

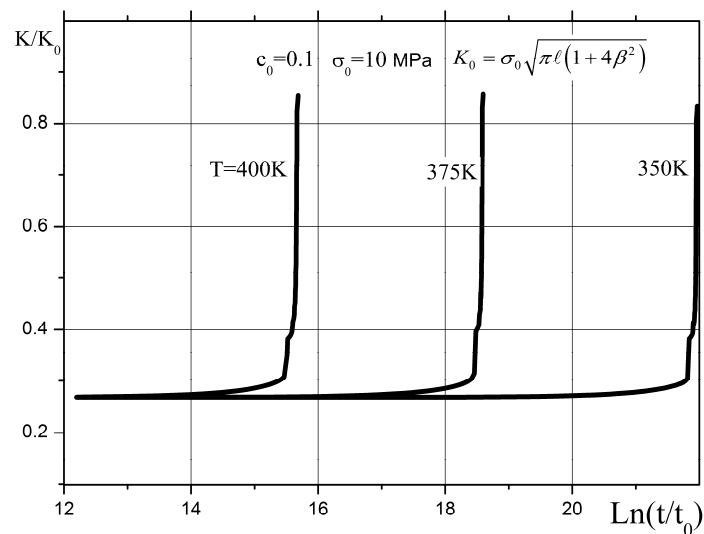


Figure 2. Variation of SIF module due to bonds destruction

6. Summary

The method of estimation of bonds degradation in the weakened region on the interface between materials is proposed. The theory of thermal fluctuation fracture and the interfacial crack bridged zone model are combined and numerical algorithm based on singular integral-differential equations is proposed. The results of computations allow to estimate the increasing the SIF module due to bonds degradation over time. These results might be helpful for durability analysis of adhesion joints. Since the computational parameters strongly depend on the initial data (which is caused by the exponential dependence of the durability in formula (1)), the comparative analysis of joints of different materials under appropriate loading conditions is of greatest practical interest in this method.

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