THE THERMAL FLUCTUATION THEORY

By: Aqeel M. Ali

University Of Basrah – Polymer Research Center

Department of Material Science

November/19/2018

Introduction

- Observed fracture strength is always lower than theoretical cohesive strength .
- The performance of the material in service is not same as it is expected from the material, hence, the design of a component frequently implores the engineer to minimize the possibility of failure.
- The level of performance of components in service depends on several factors such as inherent properties of materials, load or stress system, environment and maintenance.
- The reason for failure in engineering component can be attributed to design deficiencies, poor selection of materials, manufacturing defects, exceeding design limits and overloading, inadequate maintenance.

The general types of mechanical failure

- Failure by fracture due to static overload, the fracture being either brittle or ductile.
- Buckling in columns due to compressive overloading.
- Yield under static loading which then leads to misalignment or overloading on other components.
- Failure due to impact loading or thermal shock.
- Failure by fatigue fracture.
- Creep failure due to low strain rate at high temperature.
- Failure due to the combined effects of stress and corrosion.
- Failure due to excessive wear.

Brittle Fracture

- Brittle fracture is characterized by rapid crack propagation with low energy release and without significant plastic deformation.
- Brittle metals experience little or no plastic deformation prior to fracture. The fracture may have a bright granular appearance.
- The fractures are generally of the flat type and chevron patterns may be present.
- Materials imperfection, sharp corner or notches in the component, fatigue crack etc.

- Brittle fracture displays either cleavage (transgranular) or intergranular fracture.
- This depends upon whether the grain boundaries are stronger or weaker than the grains.
- This type of fracture is associated with nonmetals such as glass, concrete and thermosetting plastics.
- **In metals**, brittle fracture occurs mainly when BCC and HCP crystals are present.

In polymeric material

- Initially the crack grows by the growth of the voids along the midpoint of the trend which then coalesce to produce a crack followed by the growth of voids ahead of the advancing crack tip.
- This part of the fracture surface shows as the rougher region.
- Prior to the material yielding and necking formation, the material is quite likely to begin to show a cloudy appearance. This is due to small voids being produced within the material.

In Ceramics

- Typically fractured ceramic shows around the origin of the crack a mirror-like region bordered by a misty region containing numerous micro cracks.
- In some cases, the mirror-like region may extend over the entire surface.

An oil tanker that fractured in a brittle manner by crack propagation around its girth (Callister 1997, 4e) (This material is reproduced with permission of John Wiley & Sons, Inc.)

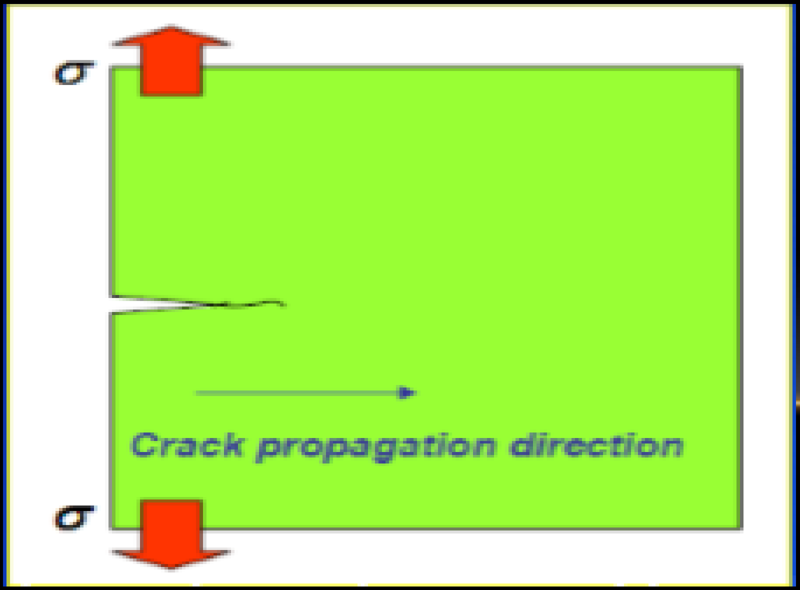
Griffith Crack Theory

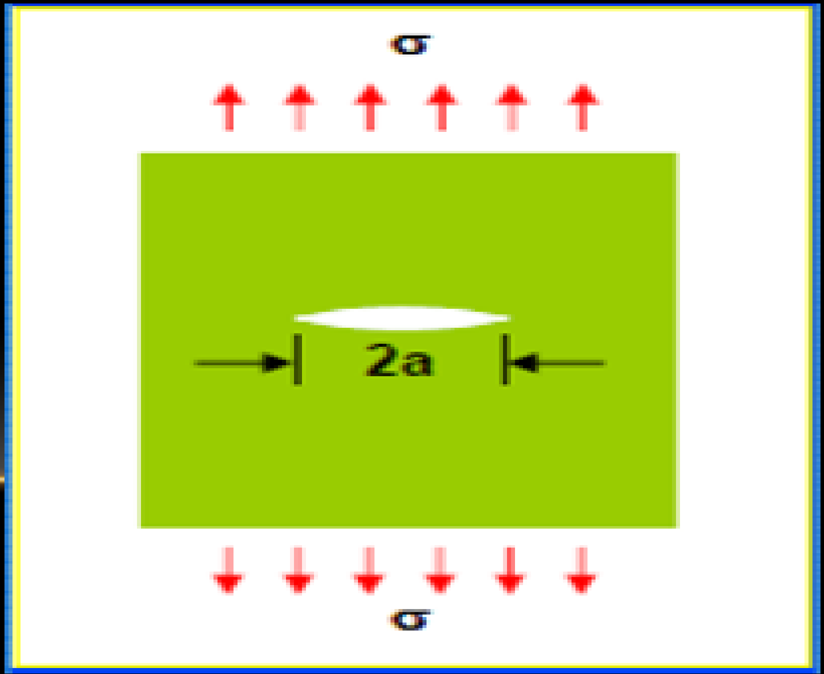
- **Griffith** explained that the discrepancy is due to the inherent defects in materials leading to stress concentration implies lower the fracture strength of the materials.
- In 1920, Griffith advanced the theory that all materials contain small cracks.
- A crack will not propagate until a particular stress is reached.
- The value of this stress depending on the length of the crack.
- Any defect (chemical, inhomogeneity, crack, dislocation, and residual stress) that exists is considered as Griffith crack.

Crack propagation criterion:

❖ Consider a through thickness crack of length 2a, subjected to a uniform tensile stress σ, at infinity.

❖ Crack propagation occurs when the released elastic strain energy is at least equal to the energy required to generate new crack surface.





- The stress required to create the new crack surface is given as follows :

γ_s : elastic work

$$\sigma = \left(\frac{2E\gamma_s}{\pi a} \right)^{1/2}$$

- In plane strain condition, the equation becomes :

$$\sigma = \left(\frac{2E\gamma_s}{(1-\upsilon^2)\pi a} \right)^{1/2}$$

Inglis introduce an elliptical cavity in a uniformly stressed plate

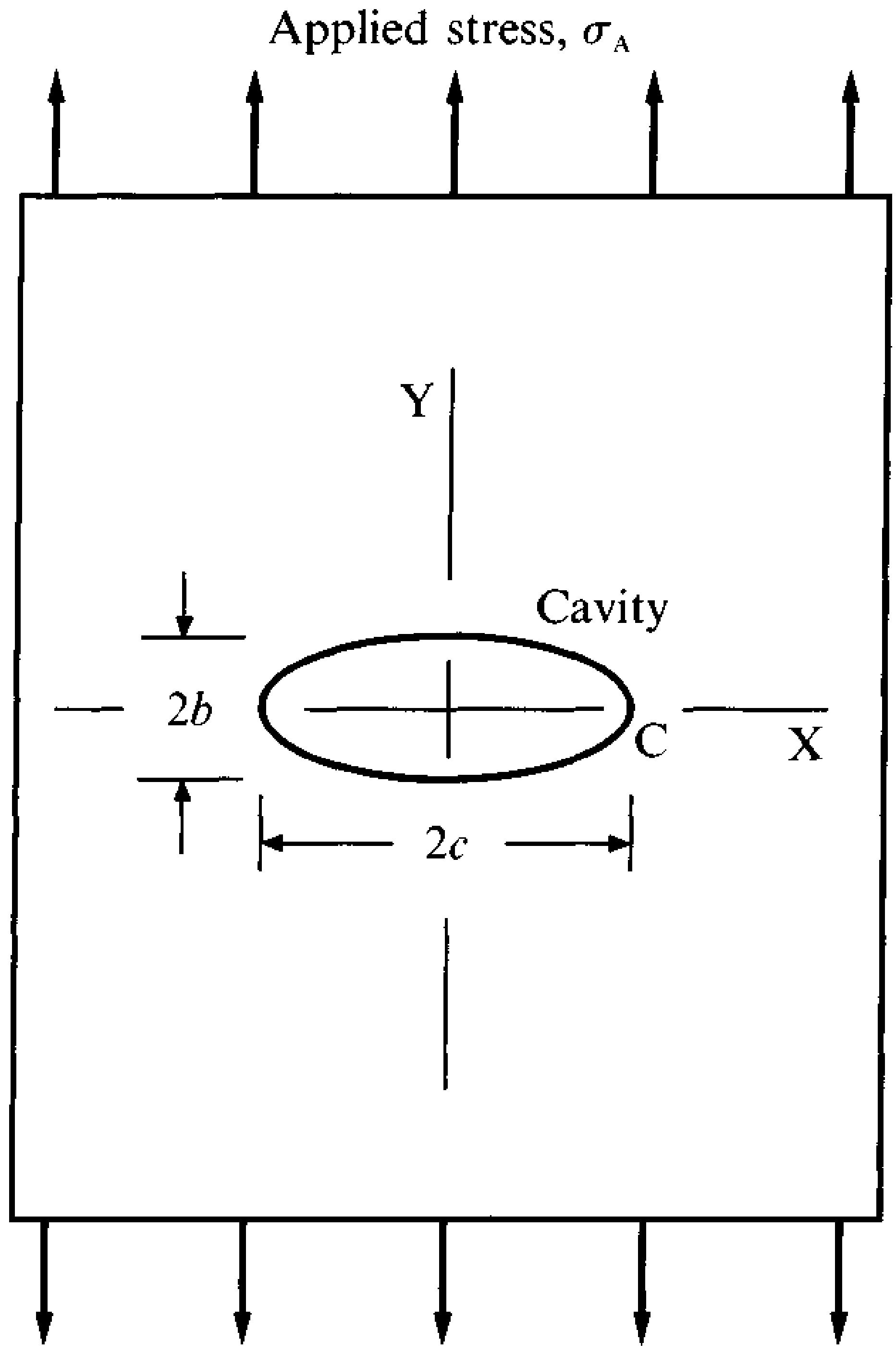
$$\rho = b^2/c, \quad (b < c)$$

$$\sigma_C = \sigma_A(1 + 2c/b) = \sigma_A[1 + 2(c/\rho)^{1/2}]$$

For the interesting case *b* << *c* this equation reduces to

$$\sigma_C/\sigma_A \simeq 2c/b = 2(c/\rho)^{1/2}$$

the stress concentration depends on the *shape* of the hole rather than the *size*



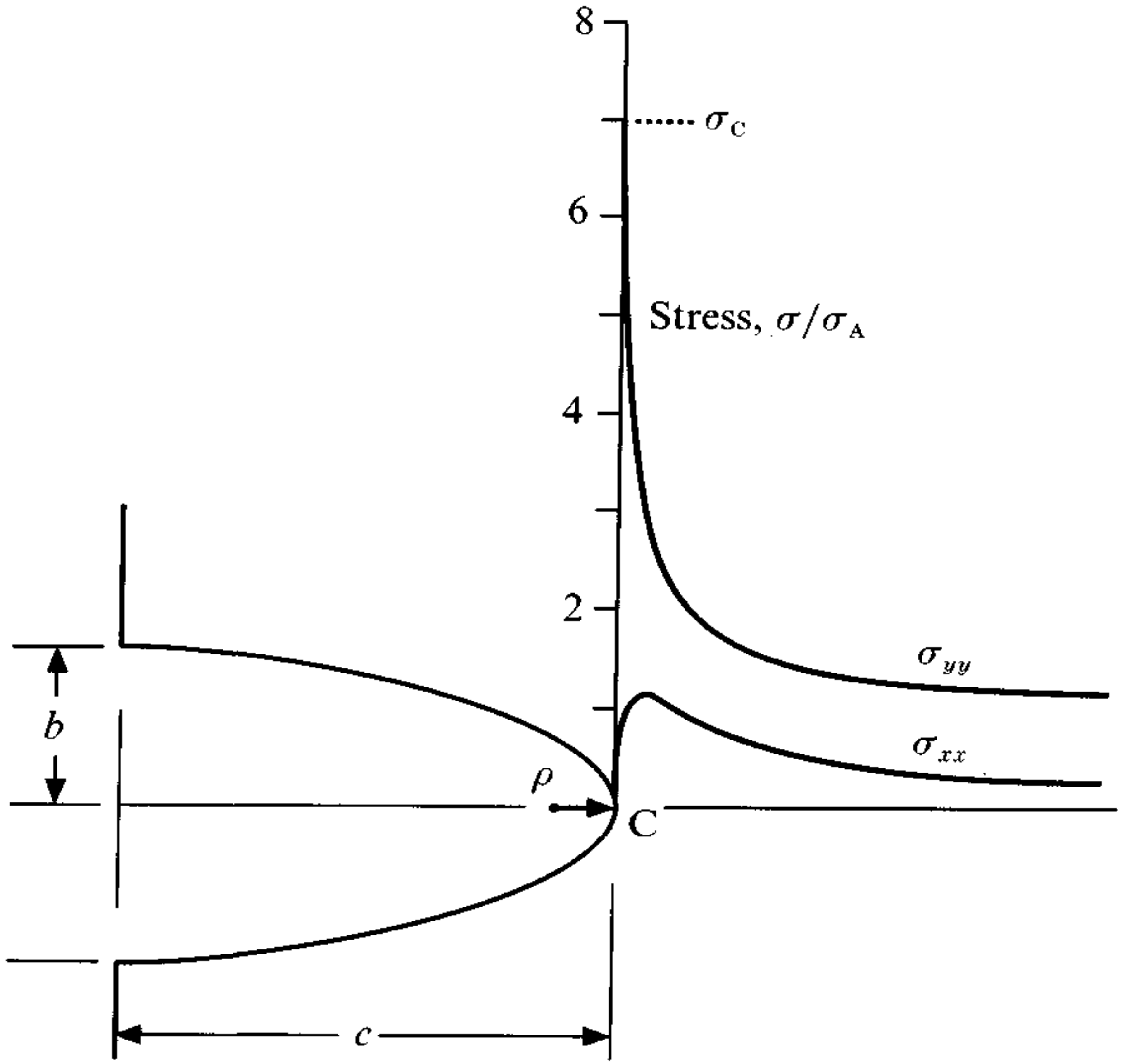


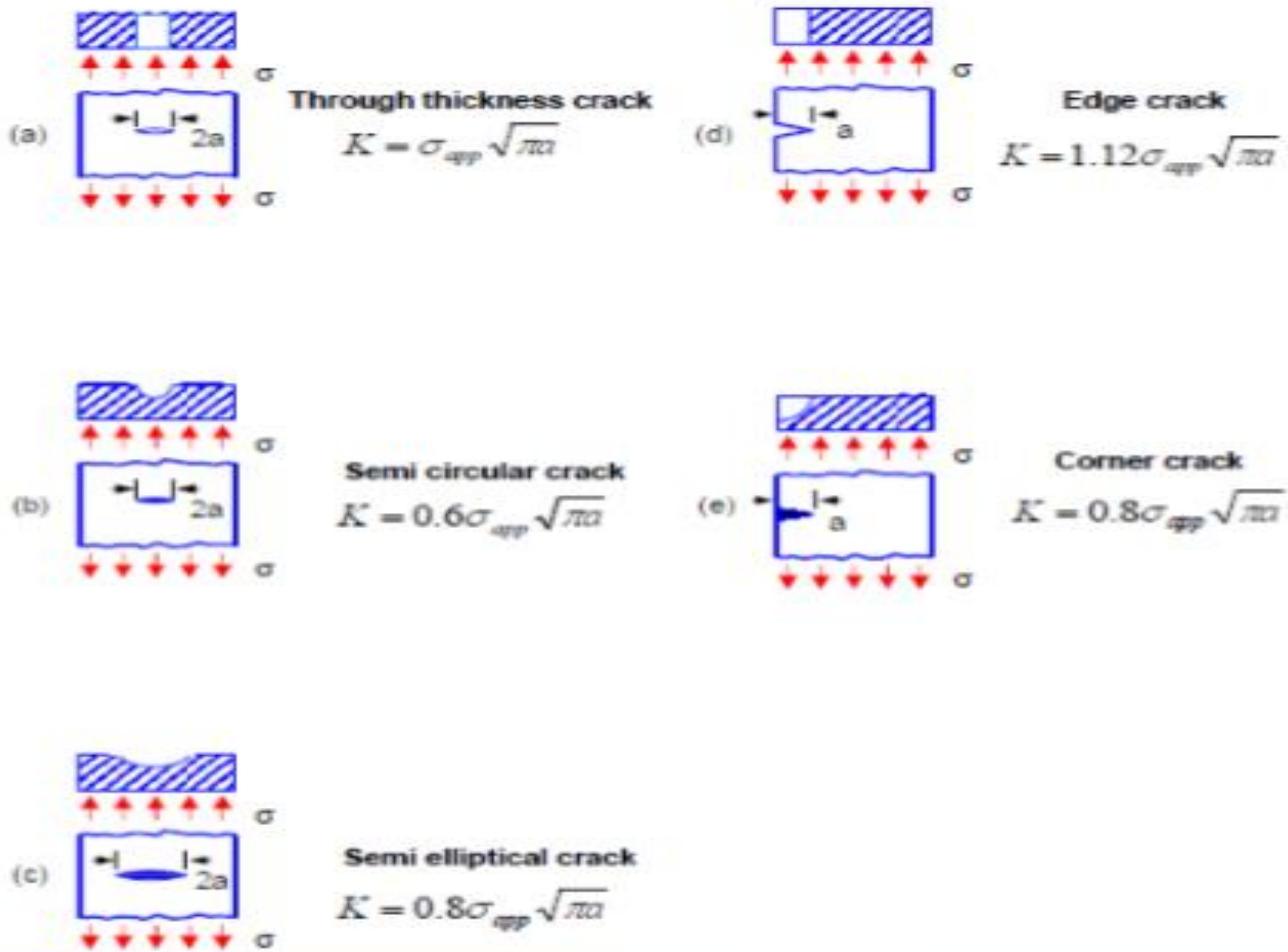
Fig. 1.2. Stress concentration at elliptical cavity, $c = 3b$. Note that concentrated stress field is localised within $\approx c$ from tip, highest gradients within $\approx \rho$.

- **Fracture toughness** can be defined as being a measure of the resistance of a material to fracture (a measure of the ability of a material to resist crack propagation).

- **Stress intensity factor (K_{IC})** is another way of considering the toughness of a material in terms of intensity factor at the tip of a crack that is required for it to propagate.

- **The parameter stress concentration factor** is the ratio of the maximum stress in the vicinity of a notch, crack or change in section to the remotely applied stress.

K_{IC} values of various crack geometries



The dynamic crack problem

- The manner in which the crack velocity varies as propagation proceeds.
- There is an upper limit to the crack velocity.
- The rate at which information concerning the local stress field can be communicated to the material immediately ahead of the crack tip is restricted by the velocity of elastic waves.
- Determine the kinetic energy in terms of *velocities.*

$$U_K = \tfrac{1}{2}(k'\rho c^2\sigma_A^2/E'^2)v^2$$

Terminal velocity

The crack velocity depends on the terminal velocity v_T

$$v(c) = v_T f(c/c_0, \alpha)$$

$$\alpha = 2\pi c_0^2/A$$

α the size of the crack relative to that of the specimen

where

$$v_T = (2\pi E'/k'\rho)^{1/2} = (2\pi/k)^{1/2} v_l$$

k dimensionless constant.

v_l the speed of longitudinal sound waves.

$$v_l = (E/\rho)^{1/2}$$

$$v_T \approx 0.38\, v_l$$

Thermofluctuational Theory

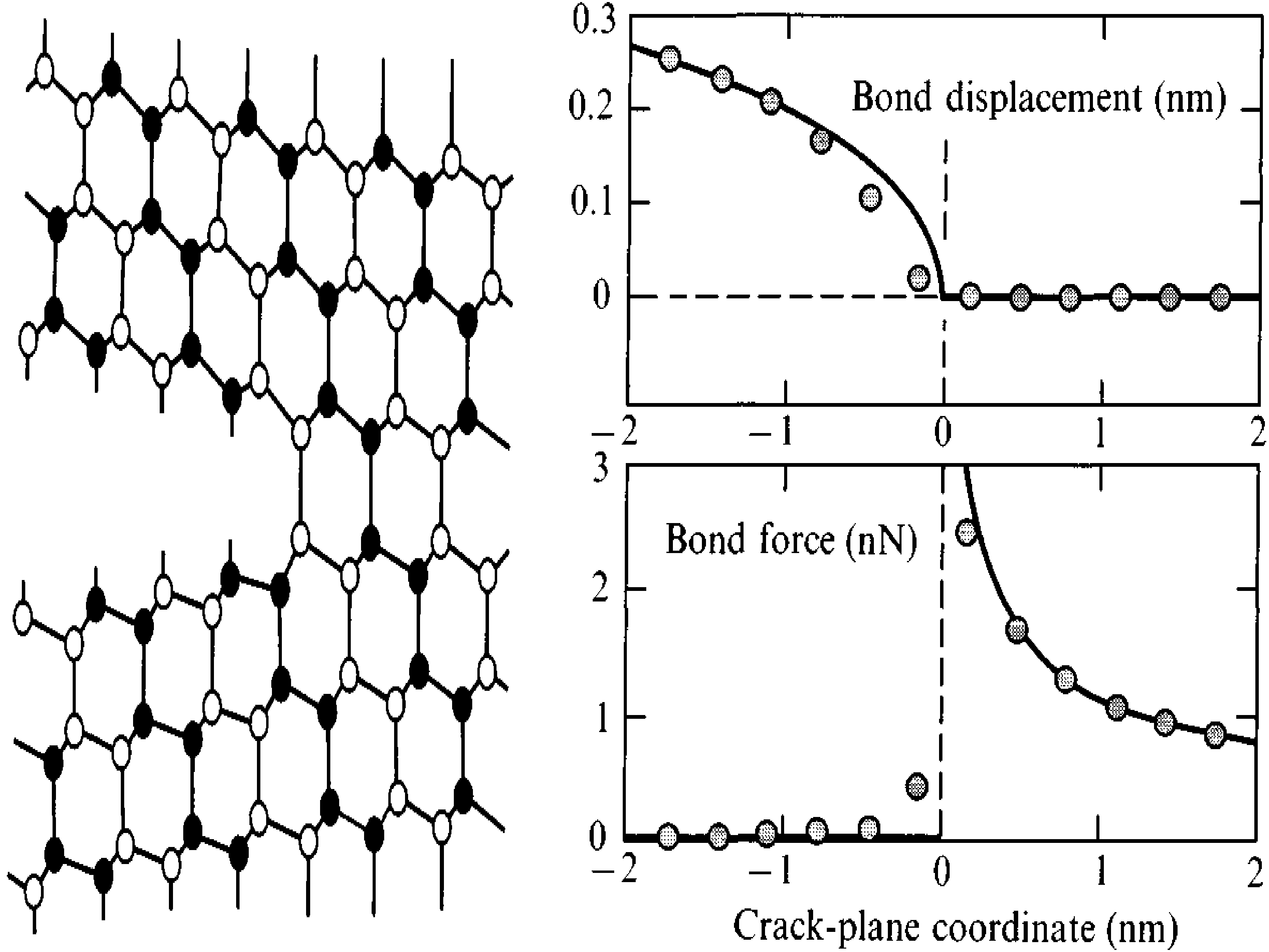
- Time-dependence in the physical and mechanical properties of bonds in the crack bridged zone allows one to estimate the long-term strength and time characteristics of material joint fracture toughness.

- Zhurkov's kinetic model of thermal fluctuation fracture is used for bonds destruction and interfacial adhesion strength modeling.

- It is assumed that at least one of the materials is a polymer and the part of crack occupied by the bridges (the bridged zone) is not small compared with the crack length.

Assumptions

1) 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).
2) Bonds density in that region varies in time according to the thermal fluctuation mechanism.
3) Bonds rigidity is proportional to their density at each point of the crack bridged zone.
4) The defect nucleation occurs near the center of the weakened bond region.
5) 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.



0.3
0.2
0.1
0
Bond displacement (nm)
−2
−1
0
1
2
3
2
1
0
Bond force (nN)
−2
−1
0
1
2
Crack-plane coordinate (nm)

The durability

The durability of materials under the action of the tensile stress σ

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

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:

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

U is the interatomic bond breakage activation energy, q and γ are structure-sensitive parameters

The Time Dependence of The Strength

- G. M. Bartenev developed the thermal fluctuation theory of brittle fracture in a surface active media medium or in vacuum.
- The medium, penetrating into the surface micro-defects, appreciably accelerates fracture, since the surface free energy at the solid body/surrounding medium interface is reduced, in comparison with its value in a vacuum.
- the pressure of molecules of the medium on the material in the apexes of the cracks leads to supplementary stretching stress at the apex, $\sigma_{\alpha}{*}= C\ (\alpha - \alpha')$ where α and α' are the free surface energies for the solid body in a vacuum and in the medium, respectively, und C is a constant.

In a vacuum, bond splitting corresponds to transfer of atoms, forming linkages from one transfer potential minimum to another across the barrier $U\text{-}\omega\sigma^*$; the restoration process is the transfer in the opposite direction across the barrier $U'+\omega\sigma^*$, where U and U' are potential barriers in the absence of stresses.

ω is the fluctuating volume, $\omega = \lambda\lambda_p\lambda_m$

where λ is an elementary path in the series of interparticle spacings, in which the fissure alex is displaced with each fluctuation which causes a bond fission λp is the elementary period of the fissure front, consisting of one or more bonds, simultaneously affected by fluctuations; λm is the separation between the maximum and minimum of the potential energy curve.

In the presence of a molecule of surface-active medium, the specified barrier

$$U_1 = U - \omega\sigma^* - \omega\sigma_\alpha^* \qquad U_2 = U' + \omega\sigma^* + \omega\sigma_\alpha^*$$

where $\Delta U = \omega\sigma_\alpha^*$ is the change of potential barriers for splitting and restoration of bonds.

The difference *U_1- U_2* is the free surface energy of two new elementary micro-areas of free surface in active media

$$U_1 - U_2 = 2\lambda\lambda_p\alpha'$$

and $U - U' = 2\lambda\lambda_p\alpha$ in a vacuum

we have $\omega\sigma_\alpha^* = \lambda\lambda_p(\alpha - \alpha')$

and $\sigma_\alpha^* = 1/\lambda_m(\alpha - \alpha')$

At a safe stress σ_0^c, when the probabilities of bond cleavage and restoration are equal, which corresponds to a state of dynamic equilibrium between these processes i.e. (cracking not increasing) we have

$$U - \omega\sigma_0^{*c} - \omega\sigma_\alpha^{*} = U' + \omega\sigma_0^{*c} + \omega\sigma_\alpha^{*}$$

the thermofluctuational threshold for fracture in the medium

$$\sigma_0^{*c} = \alpha'/\lambda_m$$

The rate of *growth* of fissure fracture

$$V(l, \sigma^*, T) = 2\lambda\nu_0 \exp\left(-\frac{U - \omega\sigma_0^{*B}}{kT}\right) \sinh\left[\frac{\omega}{kT}(\sigma^* - \sigma_0^{*c})\right]$$

where $\sigma_0^{*B} = \alpha/\lambda_m$

With uniaxial stretching of a sample in the form of a thin plate, width L, the local stress σ* in a small vicinity of the apexes of surface fissures, of length l, equals

$$\sigma^* = \beta\sigma\sqrt{l/l_0},$$

where $\beta = 0{\cdot}79\sqrt{l_0/\lambda}$ is the coefficient of stress concentration in the apex of the crack, l_0 is the initial length of the crack and σ is the stress applied to the sample.

the durability

$$\tau = \tau_f + \tau_{cr} = \int_{l_0}^{l_{cr}} \frac{dl}{V(l, \sigma, T)} + \frac{L - l_{cr}}{v_{cr}}$$

The first item in relation reflects the contribution to durability of the thermofluctuation stage of fracture, the second is the athermal.

the durability

$$\tau = \frac{2l_0 \exp(-q/k)}{\lambda \nu_0 \tilde{\alpha} \sigma} \exp\left(\frac{U_0^* - \omega\beta\sigma}{kT}\right) + 2{\cdot}63 L \sqrt{\rho/E}\left(1 - \frac{l_{cr}}{L}\right)$$

$$U_0^* = U_0 - \lambda\lambda_p(\alpha - \alpha')$$

As an example, evaluate the magnitude of U_o^* for an organic glass, during its fracture in the vapour of vacuum oil.

We have $U_o = 134 \times 10^3$ J/mole

$$\lambda = 12 \times 10^{-10}\ m$$

$$\lambda_p = 8 \times 10^{-10}\ m$$

$$\alpha = 39 \times 10^{-3} J/m^2$$

$$\alpha' = 20 \times 10^{-3} J/m^2$$

we find $U_o^* = 117 \times 10^3$ J/mole, which corresponds to the experimental value of $U_o^* = 113 \times 10^3$ J/mole

For PVC (non-oriented) in the vacuum.

We have $Uo = 134 \times 10^3$ J/mole

$\lambda = 12 \times 10^{-10}\ m$

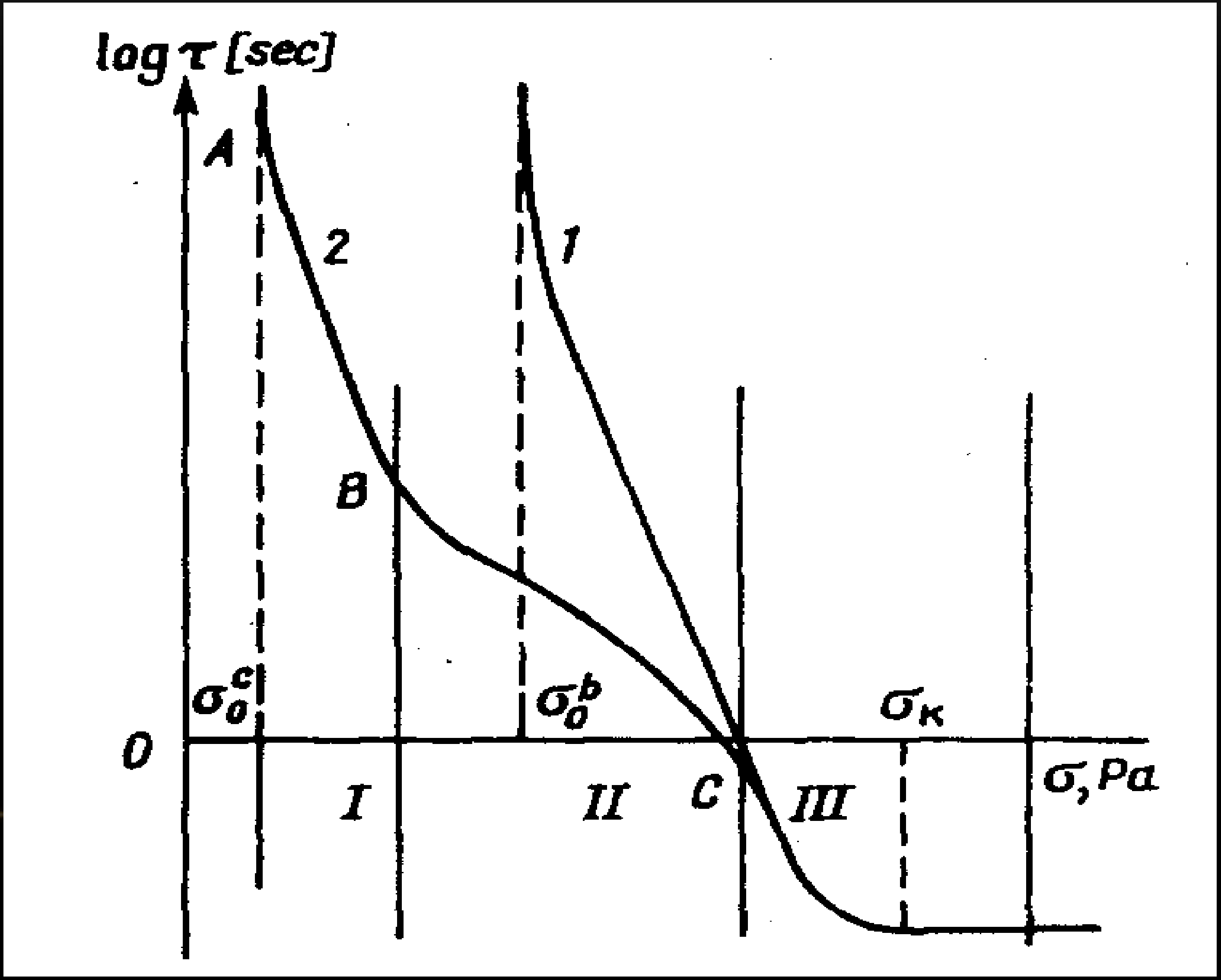
$\lambda p = 8 \times 10^{-10}\ m$

$\alpha = 39 \times 10^{-3} J/m^2$

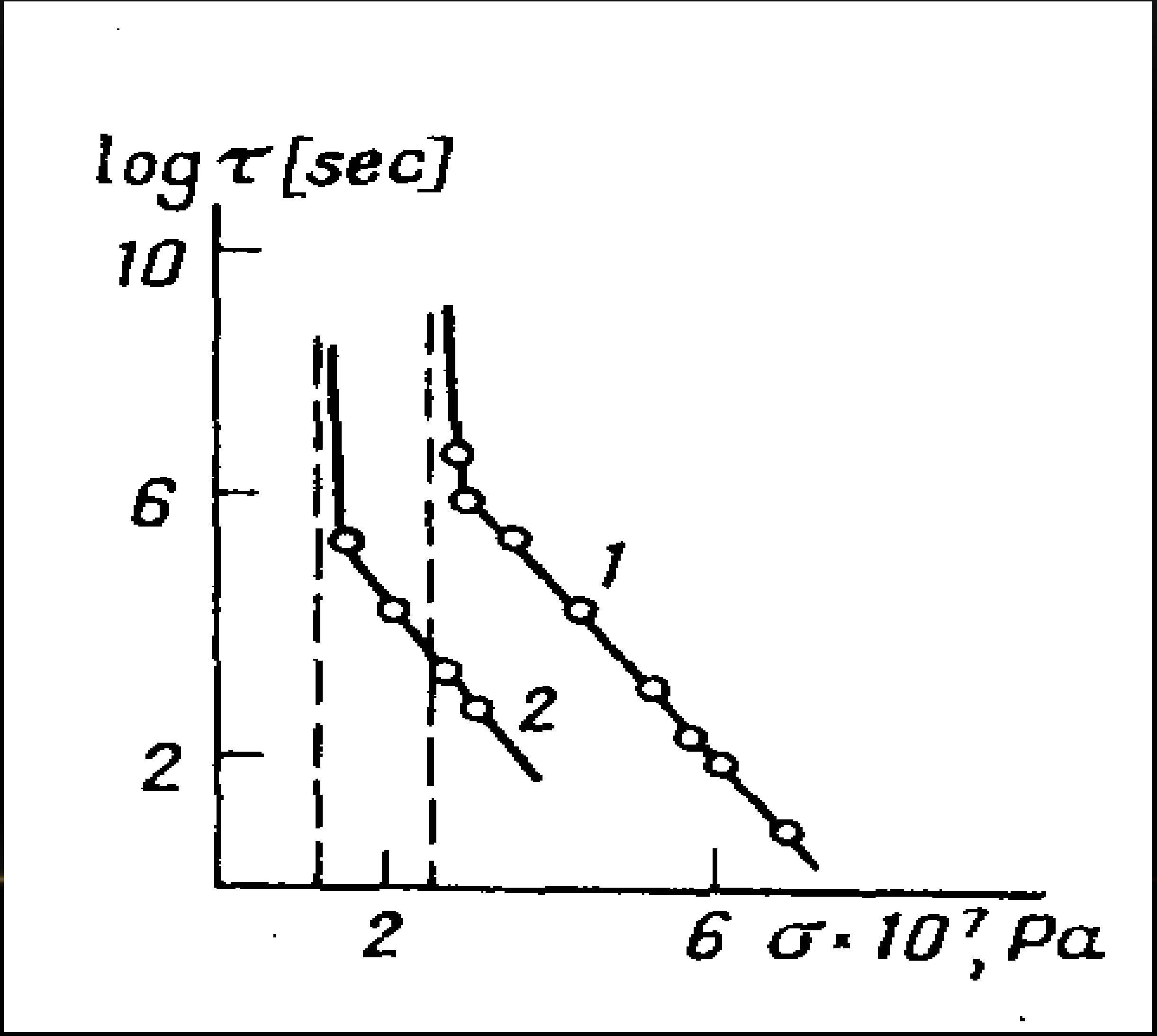
$\alpha' = 9 \times 10^{-3} J/m^2$

we find $Uo^* = 105 \times 10^3$ J/mole, which corresponds to the experimental value of $Uo^* = 97 \times 10^3$ J/mole

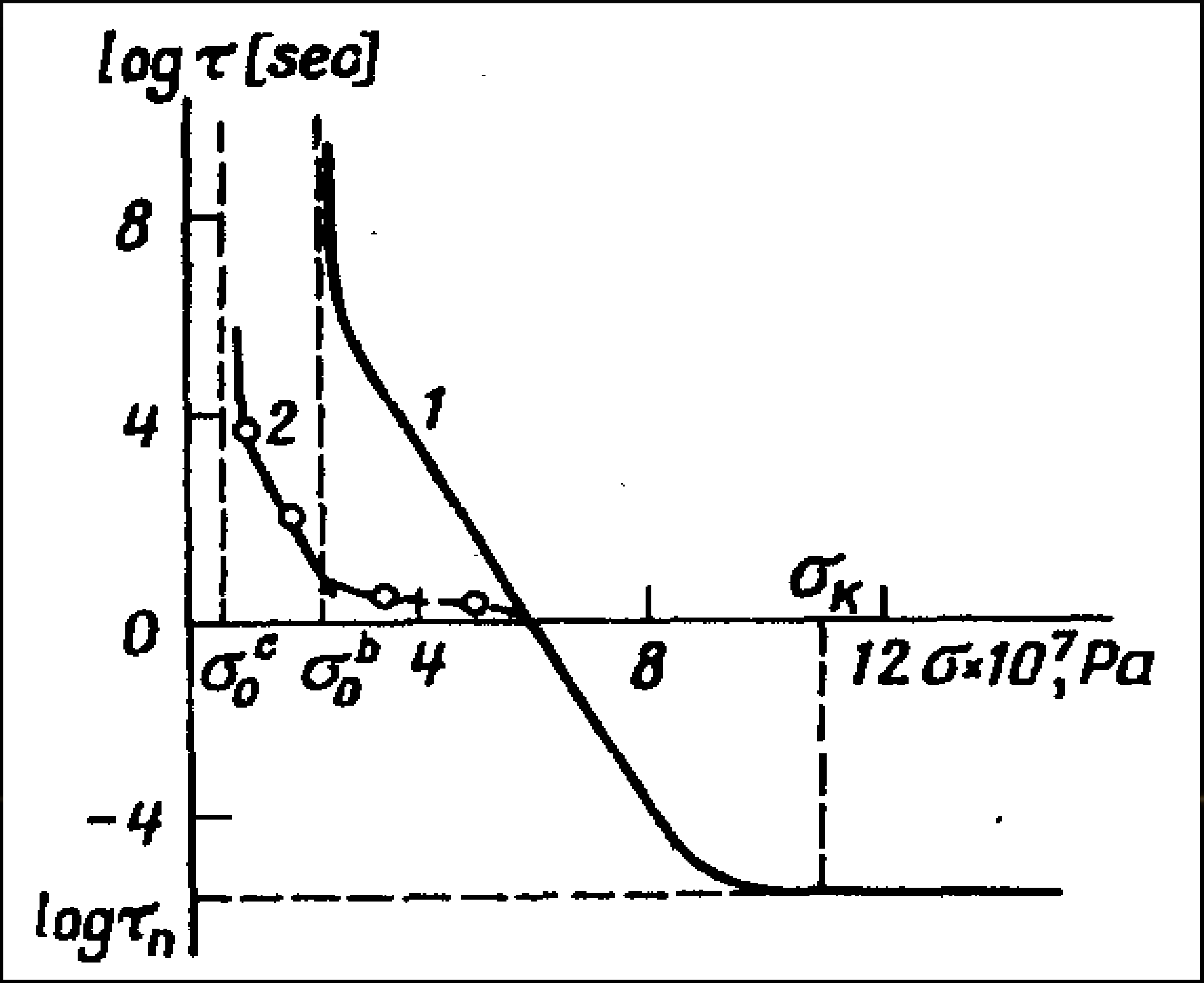
Temperature-time dependence of strength of polymer glasses (diagrammatic); 1-full durability isotherm in a vacuum, 2-the same in a surface-active medium



Time dependence of strength of an organic glass at 18°: 1-in vacuum, 2-in vacuum oil vapours; the continuous line is the theoretical one, the points represent the experimental data



Time dependence of *PVC* strength at 20°; 1-in a vacuum; the continuous line is the theoretical curve, the points represent experimental data (sloping section) and (horizontal section); 2-in water, the continuous line is the theoretical one, the points are the experimental data




Thank you