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THEORETICAL CONSIDERATION OF THE INFLUENCE OF REFORMING
PROCESSES ON THE FRACTURE STRENGTH OF SOLIDS

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Theoretical Consideration of the Influence of Reforming
Processes on the Fracture Strength of Solids*

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The macroscopic strength of an oriented medium is investigated under the assumption that processes of breaking and reforming of microscopic components in the medium may occur. The differential equation governing the time dependent variation of the number of load carrying components is considered. Emphasis is placed on the study of the effect of the reformation processes on the stress time-to-fracture behavior. It is suggested that under small loads these processes may be responsible for the frequently observed phenomena of the deviation from linearity of the strength and logarithm of time-to-fracture relationship. An attempt is also made to compare theoretical results with some reported experimental data.

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Recently the mechanical properties of oriented solids have been carefully analyzed. The mathematical model used is a system of oriented linear elements embedded in an arbitrary domain. The time-dependent strength properties were also studied with good success¹⁻⁶. However, a complete understanding of fracture behavior under either large or small simple tensile stress is not yet obtained. The present paper is an attempt toward this end. Emphasis is placed upon the interpretation of the influence of molecular reformation processes on strength.

For simplicity we consider a perfectly oriented solid composed of a system of linear microscopic molecular elements. Let f be the relative number of unbroken elements. Stress concentration in any area shall be neglected. In general f will be affected by processes of reformation and breakage of molecular forces representing the kinetic nature of the system and thus leading to the following equation:

$$\frac{df}{dt} = (1 - f)K_r - fK_b \quad (1)$$

where K_r and K_b are the rates of reformation and breakage respectively. According to the reaction rate theory the rate of breakage may be expressed in the following manner:

$$K_b = \omega_b \exp[-(U_b - \beta_b F)/kT] \quad (2)$$

where ω_b is the frequency of molecular motion, U_b and β_b are material constants, F is the force applied on each element, and k and T are Boltzmann's constant and absolute temperature respectively. Similarly, the rate of reformation is given by

$$K_r = \omega_r \exp[-(U_r + \gamma_r F)/kT] \quad (3)$$

If the system is subjected to a constant axial tension σ_0

then F is proportional to σ_o/f . Let $\sigma_o/f = \psi(t)$ where $\psi(t)$ may be interpreted as the average stress on the unbroken elements. Using $\psi(t)$ and equations (1) - (3) one can obtain the following expression:

$$\frac{d\psi}{dt} = \psi \left[\Omega_b \exp(\beta\psi) - \left(\frac{\psi}{\sigma_o} - 1\right) \Omega_r \exp(-\gamma\psi) \right] \quad (4)$$

where Ω_b and Ω_r are associated respectively with ω_b and ω_r as well as other quantities independent of stress. Here β and γ are positive constants. Upon integration we obtain the time-dependent strength behavior for any given constant stress σ_o :

$$\int_{\psi_o}^{\psi_b} \frac{\exp(-\beta\psi) d\psi}{\psi \left\{ 1 - \left(\frac{\psi}{\sigma_o} - 1\right) \frac{\Omega_r}{\Omega_b} \exp[-(\beta + \gamma)\psi] \right\}} = \int_0^{t_b} \Omega_b dt \quad (5)$$

where ψ_o is the molecular stress at time $t = 0$. ψ_o is equal to σ_o if we assume that all the elements are unbroken initially. ψ_b is the molecular stress at time of breakage. It is conceivable that fracture will occur for any system if ψ_b reaches a certain limiting value ψ_m . For an elastic system this is also equivalent to fracture at some limiting value of strain. Other criteria can be based on maximum energy (mechanical) either for an individual element or for the entire system. Reluctance to assume any of these or similar criteria will leave us no choice but to use the condition $f = 0$ or $\psi_m = \infty$ at fracture which seems to be the most natural one to assume.

For further consideration let us use the following abbreviation:

$$\left(\frac{\psi}{\sigma_o} - 1\right) \frac{\Omega_r}{\Omega_b} \exp[-(\gamma + \beta)\psi] = \phi(\psi) \quad (6)$$

The function $\phi(\psi)$ has a maximum at ψ_g given by

$$\psi_g = \sigma_o + \frac{1}{\beta + \gamma} \quad (7)$$

The corresponding maximum value ϕ_g is:

$$\phi_g = [1/(\beta + \gamma)\sigma_o](\Omega_r/\Omega_b)\exp[-(\beta + \gamma)\sigma_o - 1] \quad (8)$$

For values of $\phi_g \ll 1$ a fairly good approximation towards the solution of (5) can be obtained. In this case the corresponding high and moderate applied stresses are considered. The effect of reformation is seen to be very small. The smallness of ϕ in this region can be asserted by (8) since $\beta\sigma_o$ is an appropriate large value. Then to a first approximation $(1 - \phi)^{-1} \cong 1 + \phi$. This region can be defined by $\phi_g < \phi_c$ where ϕ_c can be chosen according to the required accuracy. For $\phi_c = 0.1$, say, the accuracy of the approximation will be better than $\pm 1\%$. Therefore, using this approximation fairly good results can be obtained in evaluating (5):

$$\int_{\psi_o}^{\psi_b} \left\{ \frac{\exp(-\beta\psi)}{\psi} + \left(\frac{1}{\sigma_o} - \frac{1}{\psi} \right) \frac{\Omega_r}{\Omega_b} \exp[-(2\beta + \gamma)\psi] \right\} d\psi = \int_0^{t_b} \Omega_b dt \quad (9)$$

Integration of (9) gives:

$$\begin{aligned} \Omega_b t_b = & \text{Ei}(-\beta\psi_b) - \text{Ei}(-\beta\sigma_o) + \frac{\Omega_r}{\Omega_b} \left\{ - \frac{\exp[-(2\beta + \gamma)\psi_b]}{(2\beta + \gamma)\sigma_o} \right. \\ & \left. + \frac{\exp[-(2\beta + \gamma)\sigma_o]}{(2\beta + \gamma)\sigma_o} - \text{Ei}[-(2\beta + \gamma)\psi_b] + \text{Ei}[-(2\beta + \gamma)\sigma_o] \right\} \end{aligned} \quad (10)$$

Further approximation using the following properties of $\text{Ei}(-z)$ for large values of z that

$$-\text{Ei}(-z) \cong \frac{e^{-z}}{z} \left(1 - \frac{1}{z} \right) \quad (11)$$

and omitting higher order but small terms containing $2\beta\psi_b$ reduces equation (10) to:

$$\Omega_b t_b = \text{Ei}(-\beta\psi_b) - \text{Ei}(-\beta\sigma_o) + \frac{\Omega_r}{\Omega_b} \left\{ \frac{\exp[-(2\beta + \gamma)\sigma_o]}{(2\beta + \gamma)^2 \sigma_o^2} \right\} \quad (12)$$

which is a solution of equation (5) for high and moderate applied stresses. However, if σ_o approaches ψ_b then $\ln \Omega_b t_b$ goes to minus infinity and (12) can be developed into the following form:

$$\Omega_b t_b = \frac{\exp(-\beta\sigma_o)}{\sigma_o} [\psi_b - \sigma_o - (\frac{1}{\sigma_o} + \beta)(\psi_b - \sigma_o)^2 + \dots] \quad (13)$$

When the applied stresses are small, the corresponding condition is that $\phi(\psi) > \phi_c$, then it is found necessary to evaluate (5) by numerical methods. In the case that if a ψ_a is chosen so that $\phi(\psi > \psi_a) < \phi_c$ is satisfied, then (5) can be separated into two integrals:

$$\int_{\psi_o}^{\psi_b} = \int_{\psi_o}^{\psi_a} + \int_{\psi_a}^{\psi_b}$$

The first integral on the right hand side can be integrated numerically giving $\Omega_b t_a$, and the second one may be evaluated using (12) giving $\Omega_b (t_b - t_a)$.

Thus the complete time-dependent fracture behavior under simple tension may be roughly divided into three portions. The lower portion is for the case when σ_o is comparable to ψ_b . In this case the time-to-break t_b is extremely short and the curve is nearly vertical as it should be in view of the assumptions made. The middle portion is the major part of the curve which corresponds to moderate and relatively high applied stresses. Within this region the logarithm of lifetime is almost linearly related to the applied stress. This can be verified by differentiating equation (12) with respect to $\beta\sigma_o$ as follows:

$$\frac{d(\ln \Omega_b t_b)}{d(\beta\sigma_o)} = \frac{\exp(-\beta\sigma_o)}{\beta\sigma_o \text{Ei}(-\beta\sigma_o)} \approx -1 - \frac{1}{\beta\sigma_o} \quad (14)$$

Since $1/\beta\sigma_0$ is small in this region and varies only slowly the slope of the curve is almost constant.

The upper portion reflects the importance of the reformation mechanism in the molecular motion. This part corresponds to the application of only small stresses. As a result the role of the molecular reformation processes becomes increasingly significant. It contributes to the increase in time required for rupturing all the elements, and thus the curve deviates from the linear relationship between $\ln t_b$ and σ_0 as verified by (14). In fact, for very small stresses applied, one may expect the time-to-break to be infinity. It can be seen by referring to (5), (6) and (8) that t_b goes to infinity as ϕ approaches 1. So the condition for infinite lifetime is $\phi_g \geq 1$. This condition can be satisfied by a range of small values of σ_0 . Corresponding to $\phi_g = 1$ there exists a stress σ_e which is the largest of these values obtainable from the following expression:

$$\frac{1}{(\beta + \gamma)\sigma_e} \frac{\Omega_r}{\Omega_b} \exp[-(\beta + \gamma)\sigma_e] = 1 \quad (15)$$

At the stress level of σ_e , the time-to-break t_b approaches infinity.

For the sake of illustrating qualitatively the complete time dependent strength behavior, Fig. 1 is plotted with assumed values of 2 for $\beta\sigma_e$ and of 30 for $\beta\sigma_m$. It must be pointed out, however, that the lifetime t_b at any stress $\beta\sigma_0 < 25$ will show no change if a larger maximum stress is assumed instead of $\beta\sigma_m = 30$. So the lifetime in the major stress region is not affected by the assumed values of the maximum stress. This relieves most of the difficulties that had been apparent in defining σ_m .

In order to show the validity of the concept and results, attempts were made to fit the theoretical curves with some available experimental data. In curve fitting the following experimental quantities have proved to be

useful:

- (1) The slope $b = -d(\log t_b)/d\sigma$ of the linear portion of the experimental curve.
- (2) The stress value σ_m where a deviation from linearity between $\log t_b$ and σ becomes significant.
- (3) The stress value σ_e where $\log t_b$ approaches infinity.

A relationship between these experimental values and the theoretical parameters γ , β and Ω_r/Ω_b can be established by the condition that at some stress σ_x the slope b of the experimental curve and the first derivative of the theoretical function are equal, i.e.

$$-(1 + \frac{1}{\beta\sigma_x}) = \frac{d(\ln\Omega_b t_b)}{d(\beta\sigma_0)} = \frac{1}{\beta} \frac{d(\ln t_b)}{d\sigma} = -\frac{\ln 10}{\beta} b \quad (16)$$

From which β is determined:

$$\beta = b \ln 10 - \frac{1}{\sigma_x} \quad (17)$$

If the experimental and theoretical curves correspond in their approach to infinite lifetime t_b at σ_e , equation (15) must be satisfied. This means that

$$-\ln(\beta + \gamma)\sigma_e + \ln\frac{\Omega_r}{\Omega_b} - (\gamma + \beta)\sigma_e = 0 \quad (18)$$

As for the stress value σ_n it is found to be convenient to assume that σ_n corresponds with $\phi_g = 0.08$ leading to a relation:

$$-\ln(\beta + \gamma)\sigma_n + \ln\frac{\Omega_r}{\Omega_b} - (\beta + \gamma)\sigma_e = -2.5 \quad (19)$$

Because the values for σ_n and σ_e cannot be clearly defined, the method of least squares was used for obtaining the best fit.

From (18) and (19) $\ln\frac{\Omega_r}{\Omega_b}$ and γ can be obtained as follows:

$$\ln \frac{\Omega_r}{\Omega_b} = 1 + \frac{2.5 - \ln(\sigma_n/\sigma_e)}{\sigma_n/\sigma_e - 1} + \ln \frac{2.5 - \ln(\sigma_n/\sigma_e)}{\sigma_n/\sigma_e - 1} \quad (20)$$

$$\gamma = \frac{2.5 - \ln(\sigma_n/\sigma_e)}{\sigma_n/\sigma_e} - \beta \quad (21)$$

As γ is considered positive, the value of σ_n/σ_e is restricted in (21). By (17), (20), and (21) the parameters β , γ and Ω_r/Ω_b can be calculated and thus the function for t_b determined on the basis of the known experimental information. Trial runs were carried out with a CDC 1604 computer. Fig. 2 shows the fitted curve together with the experimental data⁷ for organic glass. Since the model used is a fairly general one, efforts have also been made to fit a curve for aluminum tested at an elevated temperature.⁷

For organic glass at 70°C. as shown in Fig. 2 the following set of parameters was used to construct the best representation:

- (1) $\beta = 2.27 \times 10^{-2} \text{ cm}^2/\text{kp}$, $\gamma = 0.2 \times 10^{-2} \text{ cm}^2/\text{kp}$,
- (2) $\Omega_r/\Omega_b = 1718$, $\beta\sigma_n = 6.5$, $\beta\sigma_e = 4.5$, and (3) $\ln\Omega_b = \ln\omega_b - U/RT = -13.24$.

For aluminum at 400°C. as plotted in Fig. 3, the following set of parameters proved to be best:

- (1) $\beta = 7.0 \times 10^{-2} \text{ cm}^2/\text{kp}$, $\gamma = 0.2 \times 10^{-2} \text{ cm}^2/\text{kp}$,
- (2) $\Omega_r/\Omega_b = 16.5$, $\beta\sigma_n = 2.8$, $\beta\sigma_e = 1.398$, and (3) $\ln\Omega_b = -13.72$.

From these results the effect of reformation processes in the molecular motion is clearly brought out. It may be stated again that the deviation of the linearly related $\ln t_b$ and σ_o for small stresses may be attributed to this reformation mechanism.

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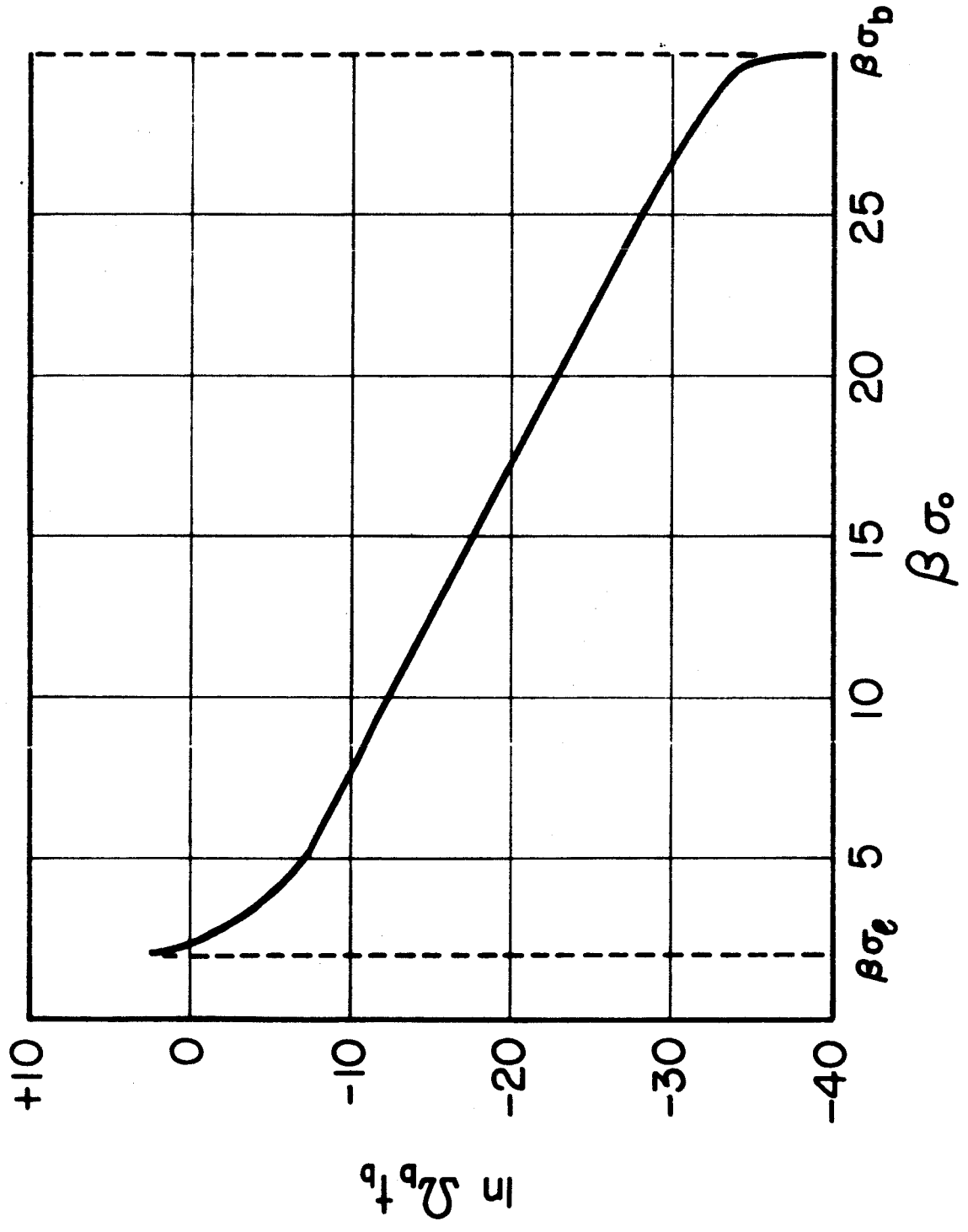


Fig. 1 Qualitative Stress-dependent Lifetime

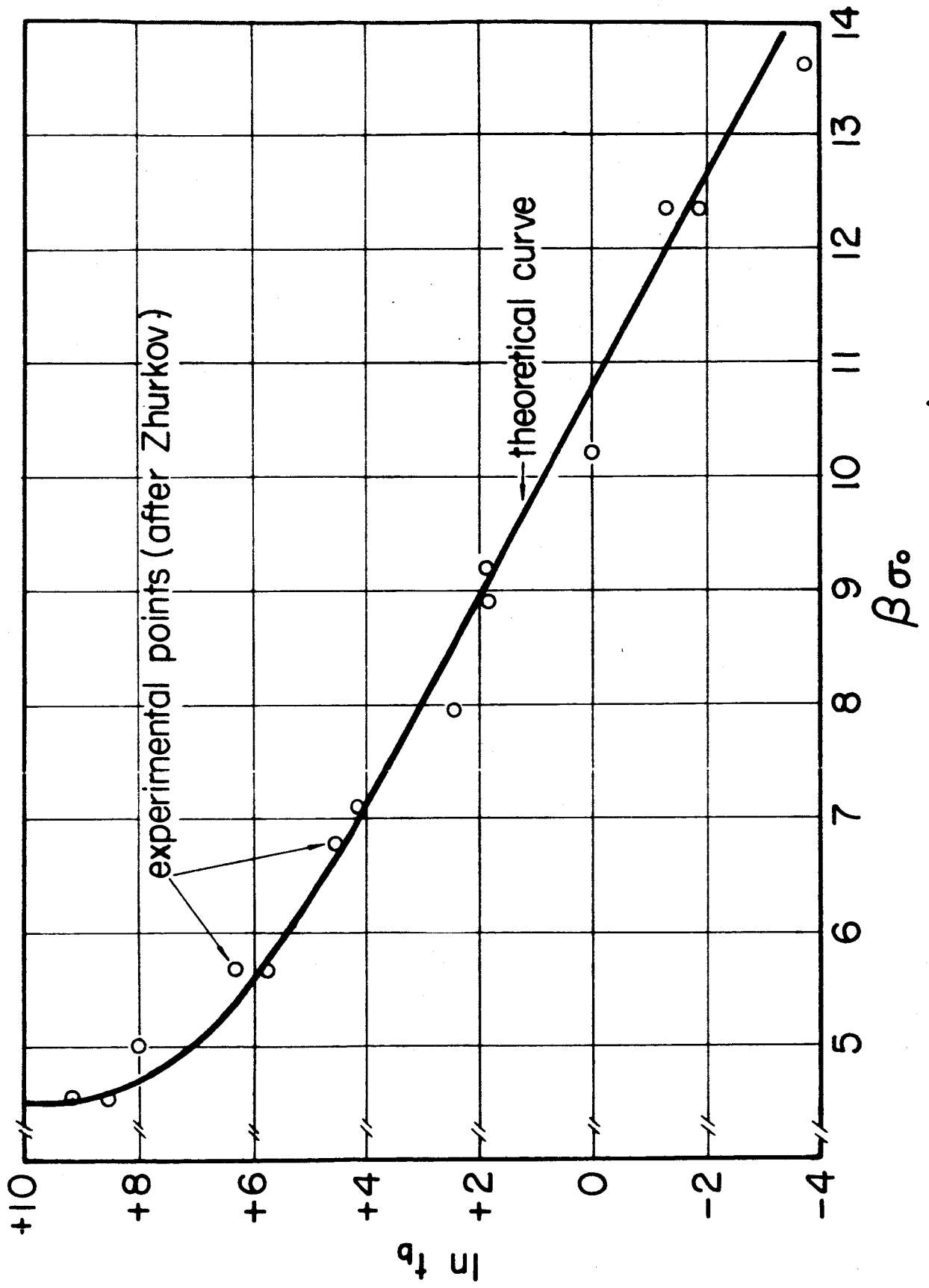


Fig. 2 Stress-Lifetime Behavior of Organic gears at 70°C.

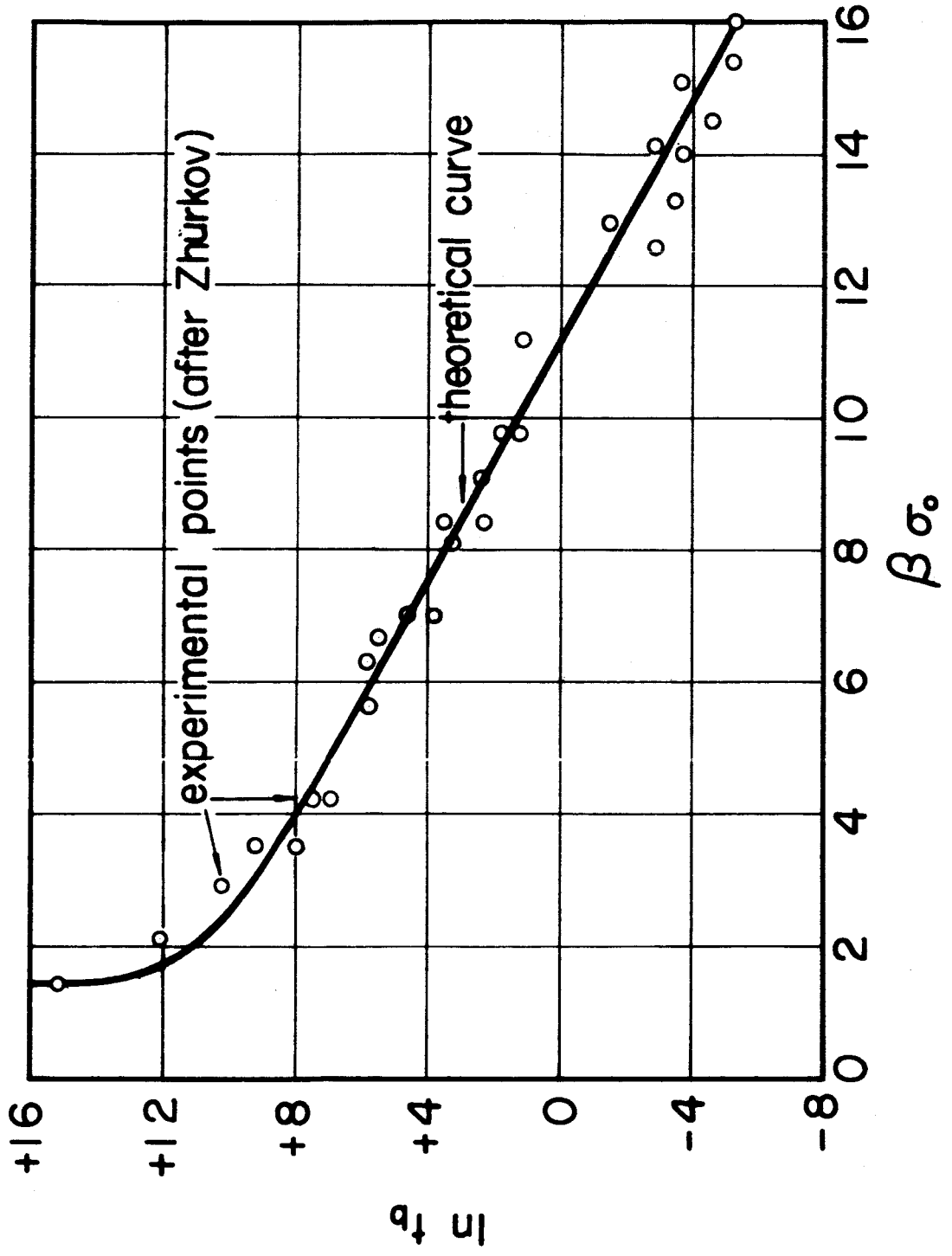


Fig. 3 Stress-Lifetime Behavior of Aluminum at 400°C.