

THERMOFLUCTUATIONAL KINETIC MODEL OF SPALL FRACTURE

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1. Fundamentals

The thermofluctuational mechanism of generating micropores due to tensile stresses is taken as a model basis. Initially, equations describing the material damage can be written in the following form:

$$\omega(t) = \int_0^t \frac{dN(\tau)}{dt} V_n(\tau, t - \tau) d\tau \quad (1)$$

Here, damage ω is the ratio between the specific volume of pores and the specific volume of damaged material; $V_n(\tau, t - \tau)$ is the volume of an evolving spherical pore, which evolution began at time τ . To avoid confusion, note that $V_n(t, 0)$ is the initial volume of a cavity emerged at time t , while $V_n(0, t)$ is the volume of a cavity emerged at time $t = 0$ and continued developing in the time interval from $t = 0$ to t .

Quantity $\frac{dN(t)}{dt}$ in equation (1) is the number of thermofluctuational micro-cavities emerged per unit volume per unit time, which is described by expression

$$\frac{dN(t)}{dt} = \frac{n(t)}{\tau_0} \exp \frac{-W_{\phi_n} A}{R_s T}, \quad (2)$$

where $n(t) = \rho(t)/m_a$ is the volumetric density of material atoms, m_a is an atom mass, $\rho(t)$ is the current density of a *damaged* material, R_s is gas constant, A is atomic (molecular) weight of material, T is temperature. Parameter τ_0 is the period of natural oscillations of an atom.

The probability of small fluctuations in a macroscopic system is measured by the work (W_{β}) to be done to change over to another state of the system. On the other hand, Gibbs thermodynamic potential [1] is the measure of work in the isothermal-and-isobaric process. Thus,

$$W_{\beta} = F_0 + E(V_s, S_s) + PV_s - TS_s = F_0 + F(P, T) + PV_s,$$

where E is the specific internal energy, P is the pressure in a damaged material, V_s is the specific volume of the *solid component* of a given material, S_s is entropy of the material's *solid component*, F is free energy of the system, and F_0 is the force imposed to break interatomic bonds under zero pressure and zero temperature conditions. Quantity F_0 is an empirical parameter of model. Thus, potential W_{β} is calculated for the *solid component* of material, however, with the current value of P in *damaged* material.

The effect of damage developing in a material on its thermodynamic properties is accounted in the following way [2]:

$$P(\rho, E, \omega) = (1 - \omega)P_s(\rho_s, E_s) = (1 - \omega)P_s\left(\frac{\rho}{1 - \omega}, E\right), \quad (3)$$

where $P_s(\rho_s, E_s)$ is the solid material EOS, $\rho_s = \frac{\rho}{(1 - \omega)}$ and $E_s = E$ is assumed. Entropy is

$$\begin{aligned} S(V, T, \omega) &= S_s((1 - \omega)V, T) \approx \\ &\approx \frac{R}{A} \ln \left[1 + \frac{3\pi^4 T^3 V^{3\Gamma} (1 - \omega)^{3\Gamma}}{5T_D^3 V_D^{3\Gamma}} \right], \end{aligned}$$

where Γ is Grueneisen coefficient (in general, its depends on specific volume V),

T_D is Debye temperature (the material constant to be set),

V_D is the specific volume of undamaged material at Debye temperature.

2. Accounting of the micropore size limitation

In equation (1), the probability of the thermofluctuational micro-cavity generation for one thermal fluctuation, $\exp \frac{-W_{\phi_n}(t)A}{R_s T(t)}$ corresponds to breaking of *one interatomic bond*. One broken bond leads to

appearance of a micro-cavity, which size is so small that it immediately collapses due to surface tension. As it will be shown below, the micro-cavity radius should exceed the minimal radius, $R_{min}(t) = 2\sigma_{nos}/P(t)$. Note that for a single micro-cavity $P(t)$ means the pressure in solid material. However, in order to take into account the mutual interaction of pores in the model of interest we need to assume that $P(t)$ is the pressure in damaged material. With small tensile pressures $P(t)$ and/or large surface tensions, the minimum size of radius, $R_{min}(t)$ may be large enough in the sense that it must correspond to a sufficiently large number (q) of broken interatomic bonds. Then, the probability of the thermofluctuational generation of a micro-cavity per unit time should be written as $\frac{1}{\tau_0} \exp \frac{-q(t)W_{\phi n}A}{R_s T}$ and the minimum number of broken bonds is $q_{min}(t) = 4\pi R_{min}^2(t)n_s^{2/3}(t)/2$. For example, for aluminum we have $q_{min}(0) > 20$. Since the minimum number of broken interatomic bonds is $\gg 1$, we think it is possible to use the hydrodynamic approximation (see Section 4) for the evaluation of the development of emerged thermofluctuational micro-cavities.

Thus, in equation (2) instead of $\frac{1}{\tau_0} \exp \frac{-W_{\phi n}A}{R_s T}$ we should take the probability of breaking a minimum permissible number of bonds,

$$\frac{1}{\tau_0} \exp \frac{-q_{min}(\tau)W_{\phi n}A}{R_s T} = \frac{1}{\tau_0} \exp \frac{-8\pi\sigma_{nos}^2 n_s^{2/3}(\tau)W_{\phi n}A}{P^2(\tau)R_s T} \quad (4)$$

It includes the following ratio of the damaged material parameters, which is, in general, depends on the damage accumulation level:

$$\frac{n_s^{2/3}(\tau)}{P^2(\tau)} = \frac{n_s^{2/3}(\tau)}{[1-\omega(\tau)]^2 P_s^2(\tau)} = \frac{n_s^{2/3}(\tau)}{[1-\omega(\tau)]^{2/3} P^2(\tau)}. \quad (5)$$

The ratio of parameters in the solid component of damaged material, $\frac{n_s^{2/3}(\tau)}{P_s^2(\tau)}$ is quasi-steady [3] against

the background of rapid variations of damage ω . And with regard to the fact [4] that damage varies within a limited range of values, $0 \leq \omega \leq \omega_{kp} \leq 0.3$, in (5) we have $1 \leq \frac{1}{[1-\omega(\tau)]^2} \leq \frac{1}{(1-\omega_{kp})^2} \leq 2$. On the other hand,

if we neglect the presence of factor $[1-\omega(\tau)]^{2/3}$ in denominator when we calculate ratio (5) using of the current values of density and pressure in damaged material, this may lead to an erroneous result (by a factor of 1.27) in exponent index (4) and with large values of the index itself it may lead to a large error in the current value of $\omega(\tau)$ from integral equation (1). In this connection, we emphasize that equation (1) should be considered an integral equation for finding the current values of damage, but not an integral for damage accumulation with some simplifying assumptions for sub-integral functions.

3. Accounting of the full range of emerging micropore sizes

In reality, the full range of sizes of micropores with $R_0 \geq R_{min}(t)$ corresponding to the number of broken bonds $q(t) = 4\pi R_0^2 n_s^{2/3}(t)/2$ is possible. Only with sufficiently large values of exponent index $W_{\phi n}A/R_s T > 1$ it is really possible to restrict ourselves to the first member of this range with $R_0 = R_{min}(t)$.

In general, instead of equation (1) we should write equation

$$\omega(t) = \int_0^t \sum_{q=q_0(\tau)}^{\infty} \frac{dN_q(\tau)}{dt} V_q(\tau, t-\tau) d\tau = \frac{1}{\tau_0} \int_0^t n(\tau) \sum_{q=q_0(\tau)}^{\infty} V_q(\tau, t-\tau) \exp \frac{-qW_{\phi n}A}{R_s T} d\tau, \quad (6)$$

where $\omega_q(\tau, t-\tau) \equiv n(t-\tau)V_q(\tau, t-\tau)$ and

$$V_q(\tau, t-\tau) = \frac{4}{3} \pi [R_{0q}(\tau) + \int_{\tau}^t v_q(\tau, t') dt']^3, \quad (7)$$

with $v_q(\tau, t')$ being the micro-cavity expansion rate and the initial radius of this cavity at the time of its origination being determined by $q(\tau) = 4\pi R_{0q}^2(\tau)n_s^{2/3}(\tau)/2$, from which we obtain

$$R_{0q}(\tau) = \frac{1}{n_s^{1/3}(\tau)} \sqrt{\frac{q}{2\pi}}. \quad (8)$$

Summation in (6) is done over all possible numbers of broken bonds, from q to q_0 up to ∞ , where $q_0(\tau) \equiv \max\{1, q_{\min}(\tau)\}$.

Instead of summation over q in equation (6) take integral and use the saddle-point method for approximately calculating the sum over q :

$$\begin{aligned} \sum_{q=q_0(\tau)}^{\infty} \frac{dN_q(\tau)}{dt} V_q(\tau, t-\tau) &= \frac{n(\tau)}{\tau_0} \cdot \sum_{q=q_0(\tau)}^{\infty} V_q(\tau, t-\tau) \exp \frac{-qW_{\phi n}A}{R_z T(\tau)} \Rightarrow \\ &\Rightarrow \frac{n(\tau)}{\tau_0} \cdot \int_{q_0(\tau)}^{\infty} V_q(\tau, t-\tau) \exp \frac{-qW_{\phi n}A}{R_z T(\tau)} dq = \frac{n(\tau)}{\tau_0} \cdot \int_{q_0(\tau)}^{\infty} \exp[\ln V_q(\tau, t-\tau) - \frac{qW_{\phi n}A}{R_z T(\tau)}] dq \end{aligned}$$

The first derivative of exponent index at the extremum point gives us

$$\frac{dV_{q_m}}{dq} = V_{q_m} \cdot \frac{W_{\phi n}A}{R_z T} \quad (9)$$

from which we obtain the value of $q_m(\tau)$ at the extremum point. The second derivative at the extremum point equals

$$\frac{d^2V_{q_m}}{dq^2} / V_{q_m} - \left(\frac{W_{\phi n}A}{R_z T}\right)^2.$$

Note that at the maximum point it must be below zero. Then,

$$\begin{aligned} \int_{q_0(\tau)}^{\infty} \exp[\ln V_q(\tau, t-\tau) - \frac{qW_{\phi n}A}{R_z T(\tau)}] dq &\approx \\ &\approx V_{q_m}(\tau, t-\tau) \exp \frac{-q_m W_{\phi n}A}{R_z T(\tau)} \cdot \int_{q_0(\tau)}^{\infty} \exp \left\{ -\left[\left(\frac{W_{\phi n}A}{R_z T}\right)^2 - \frac{d^2V_{q_m}}{dq^2} \right] \cdot \frac{(q-q_m)^2}{2} \right\} dq \approx \\ &\approx V_{q_m}(\tau, t-\tau) \exp \frac{-q_m W_{\phi n}A}{R_z T(\tau)} \cdot \frac{1}{\sqrt{\left(\frac{W_{\phi n}A}{R_z T}\right)^2 - \frac{d^2V_{q_m}}{dq^2}}} \cdot \int_{\sigma_0(\tau)}^{\infty} \exp \left\{ -\frac{\sigma^2}{2} \right\} d\sigma \end{aligned}$$

where

$$\begin{aligned} \sigma(\tau) &\equiv \sqrt{z_m(\tau)}[q - q_m(\tau)] \\ \sigma_0(\tau) &\equiv \sqrt{z_m(\tau)}[q_0(\tau) - q_m(\tau)] \\ z_m(\tau) &\equiv \left[\left(\frac{W_{\phi n}A}{R_z T}\right)^2 - \frac{d^2V_{q_m}}{dq^2} \right] \end{aligned} \quad (10)$$

Thus,

$$\sum_{q=q_0(\tau)}^{\infty} \frac{dN_q(\tau)}{dt} V_q(\tau, t-\tau) \approx \frac{n(\tau)}{\tau_0} V_{q_m}(\tau, t-\tau) \exp\left(\frac{-q_m W_{\phi n}A}{R_z T}\right) \cdot \sqrt{\frac{\pi}{2z_m}} [1 + \operatorname{erf}\left(\frac{\sigma_0(\tau)}{\sqrt{2}}\right)]$$

where $\operatorname{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-x^2} dx$ is the error function integral.

It means the integral equation (6) for $\omega(t)$ is rewritten in the approximate form:

$$\omega(t) \approx \frac{1}{\tau_0} \int_0^t n(\tau) V_{q_m}(\tau, t-\tau) \exp\left(\frac{-q_m W_{\phi n}A}{R_z T(\tau)}\right) \cdot \sqrt{\frac{\pi}{2z_m(\tau)}} [1 + \operatorname{erf}\left(\frac{\sigma_0}{\sqrt{2}}\right)] d\tau, \quad (11)$$

where $q_m(\tau)$ is taken from (9) and $\sigma_0(\tau)$ is taken from (10).

The resultant approximate integral equation (11) is applicable both with $q_m(\tau) > q_0(\tau)$ and with $q_m(\tau) < q_0(\tau)$ as long as

$$\frac{dV_{q_m}}{V_{q_m} dq} - \frac{W_{\phi n} A}{R_z T} < \left[\frac{d^2 V_{q_0}}{V_{q_0} dq^2} - \left(\frac{W_{\phi n} A}{R_z T} \right)^2 \right] [q_0(\tau) - q_m(\tau)] + \frac{W_{\phi n} A}{R_z T} \frac{q_0}{q_0 - q_m},$$

i.e. with a sufficiently small relative difference between $q_m(\tau)$ and $q_0(\tau)$. With an opposite sign of this inequality and

$$\begin{aligned} q_m(\tau) < q_0(\tau) \text{ the sum over } q \text{ can be written in its approximate form:} \\ \sum_{q=q_0(\tau)}^{\infty} \frac{dN_q(\tau)}{dt} V_q(\tau, t-\tau) &\Rightarrow \frac{n(\tau)}{\tau_0} \cdot \int_{q_0(\tau)}^{\infty} \exp\left[\ln V_q(\tau, t-\tau) - \frac{q W_{\phi n} A}{R_z T(\tau)}\right] dq \approx \\ &\approx \frac{n(\tau)}{\tau_0} \cdot V_{q_0}(\tau, t-\tau) \exp\left[-\frac{q_0 W_{\phi n} A}{R_z T(\tau)}\right] \cdot \int_{q_0(\tau)}^{\infty} \exp\left[-\left(\frac{W_{\phi n} A}{R_z T} - \frac{dV_{q_0}}{V_{q_0} dq}\right)(q - q_0)\right] dq \approx \\ &\approx \frac{n(\tau)}{\tau_0} \cdot V_{q_0}(\tau, t-\tau) \exp\left[-\frac{q_0 W_{\phi n} A}{R_z T(\tau)}\right] \cdot \frac{1}{\frac{W_{\phi n} A}{R_z T} - \frac{dV_{q_0}}{V_{q_0} dq}} \cdot \int_0^{\infty} e^{-x} dx = \frac{n(\tau)}{\tau_0} \cdot \frac{V_{q_0}^2(\tau, t-\tau)}{\frac{W_{\phi n} A}{R_z T} - \frac{dV_{q_0}}{V_{q_0} dq}} \exp\left[-\frac{q_0 W_{\phi n} A}{R_z T(\tau)}\right] \end{aligned}$$

4. The volume of an evolving micropore

The approximate integral equation (11) includes the volume of an evolving micropore, which is described by (7) and depends on the micro-cavity expansion rate, $v_q(\tau, t)$ and original radius (8). Consider the equation of spherical pore development in a viscous continuous medium with surface tension [5]:

$$R\ddot{R} + \frac{3}{2}\dot{R}^2 + \frac{4\eta}{\rho_s R} \dot{R} + \frac{2\sigma_{nos}}{\rho_s R} = \frac{P}{\rho_s} = [1 - \omega(t)] \frac{P_s}{\rho_s} = [1 - \omega(t)] \frac{P}{\rho}. \quad (12)$$

Here, R – is a micro-cavity radius, $\dot{R} \equiv \frac{dR}{dt} \equiv v(t)$ is the cavity expansion rate, η is the material viscosity factor, ρ is the current density of *damaged* material, ρ_s is the *solid component* density of damaged material, σ_{dam} is the surface tension coefficient, P is the current tensile pressure modulus in *damaged* material, P_s is the tensile pressure modulus obtained from the EOS of solid material according to (3). Note that even with regard to the quasi-steady state of quantities P_s and ρ_s in a tensile material [3], equation (12) has a *rapidly changing* function in its right-hand part!

Thus, the problem of evaluating the progress of accumulating damage $\omega(t)$ in a tensile material may be reduced to solving a system of two equations – integral equation (11) and differential equation (12). In equation (12) for radius of an expanding cavity $R(t)$ means radii from equation (11):

$$R_{q_m(\tau)}(\tau, t-\tau) = R_{0q_m(\tau)}(\tau) + \int_{\tau}^t v_{q_m(\tau)}(\tau, t') dt'.$$

Attempts to neglect the dependence on ω in the right-hand part of equation (11) are unacceptable, because the current damage values are included to exponential sub-integral terms in the right-hand part and, hence, this they may strongly influence the values of these terms. On the other hand, factor $(1-\omega)$ in the right-hand part of equation (12) varies within the limited range of values $0.7 \leq (1-\omega) \leq 1$, as we have mentioned above, and here we can neglect its variability for the sake of simplicity.

As it follows from equation (12), near the velocity minimum - at small values of dv/dt - we have

$$v(t) \approx -\frac{4\eta}{3\rho_s R(t)} + \sqrt{\left(\frac{4\eta}{3\rho_s R(t)}\right)^2 - \frac{4\sigma_{nos}}{3\rho_s R(t)} + \frac{2P}{3\rho_s}}.$$

With large viscosity factors, we have

$$v(t) \approx \frac{PR(t) - 2\sigma_{nos}}{4\eta}. \quad (13)$$

One can see that not only cavities of radii $R(t) > 2\sigma_{nos}/P(t)$ may expand.

With large radii values, if we neglect the $1-\omega(t)$ factor variability in equation (12), the cavity expansion

process approaches to that following the hydrodynamic law:

$$v \equiv v_{\infty} \approx \sqrt{\frac{2P}{3\rho_s}} \quad (14)$$

However, with regard to variability of $1-\omega(t)$, the cavity expansion process may stop, if the value of ω^* is such that

$$\frac{2\sigma_{nos}}{\rho_s R} = [1-\omega^*] \frac{P_s}{\rho_s} = [1-\omega^*] \frac{P}{\rho}$$

For an easier numerical implementation of the model, it is possible to restrict oneself to the consideration of the two limiting laws: "hydrodynamic" law (14) and "viscous" law describing the cavity expansion process near the velocity minimum - equation (13). The solution to approximate equation (13) is written in the form

$$\begin{aligned} R(t, t') &= \exp\left[\int_{t'}^t \frac{P(t'')}{4\eta(t'')} dt''\right] \cdot \left[R_0(t') - \int_{t'}^t \frac{\sigma_{nos}(t'')}{2\eta(t'')} \exp\left(-\int_{t'}^{t''} \frac{P(t''')}{4\eta} dt'''\right) dt''\right] = \\ &= R_0(t') \exp\left[\int_{t'}^t \frac{P(t'')}{4\eta(t'')} dt''\right] - \int_{t'}^t \frac{\sigma_{nos}(t'')}{2\eta(t'')} \exp\left(\int_{t'}^{t''} \frac{P(t''')}{4\eta} dt'''\right) dt'' \end{aligned}$$

Here, $P(t)$ is pressure in a damaged material. Viscosity and surface tension appear to be dependent on time owing to their dependence on the material temperature.

Conclusions

The work demonstrates a high level of complexity of the problem of mathematically describing the damage accumulation kinetics in a material and a high sensitivity of this kinetics to possible simplifications in the problem consideration. The naive expectation of researchers that the model of kinetics constructed in one, or another initially approximate form is able to describe "some things" in the problem of interest comes true, because usually such kinetic models have a sufficient number of "model parameters", which are adjustable parameters in reality. However, one should not expect that such models are wide-range.

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