Spontaneous thermal runaway as an ultimate failure mechanism of materials

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The first theoretical estimate of the shear strength of a perfect crystal was given by Frenkel [Z. Phys. 37, 572 (1926)]. He assumed that as slip occurred, two rigid atomic rows in the crystal would move over each other along a slip plane. Based on this simple model, Frenkel derived the ultimate shear strength to be about one tenth of the shear modulus. Here we present a theoretical study showing that catastrophic material failure may occur below Frenkel’s ultimate limit as a result of thermal runaway. We demonstrate that the condition for thermal runaway to occur is controlled by only two dimensionless variables and, based on the thermal runaway failure mechanism, we calculate the maximum shear strength $\sigma_c$ of viscoelastic materials. Moreover, during the thermal runaway process, the magnitude of strain and temperature progressively localize in space producing a narrow region of highly deformed material, i.e. a shear band. We then demonstrate the relevance of this new concept for material failure known to occur at scales ranging from nanometers to kilometers.

It is well known that the shear strength of real crystals is typically several orders of magnitude smaller than Frenkel’s ultimate shear strength limit. This discrepancy is explained by the fact that real crystals contain defects such as dislocations which lower the shear strength dramatically. Nevertheless, some materials, like rocks in the Earth’s interior and metallic glasses, apparently have strengths approaching Frenkel’s theoretical limit. For these materials it is reasoned that the mobility of the defects is in one way or another reduced. For instance, the closure of cracks at high confining pressures, non-planar crystal structure of minerals and disorder of mineral grain orientations are all factors contributing to the high strength of rocks in the Earth’s interior. The high strength of metallic glasses is attributed to the high degree of structural disorder causing dislocations to experience a large number of obstacles, reducing their mobility and inhibiting plastic flow.

However, even if dislocation mobility is greatly reduced, materials subjected to increasing loads do not necessarily fail according to Frenkel’s model. When subjected to a high shear stress which approaches, but is reproducibly lower than Frenkel’s limit, these materials may fail by deformation localized on a single or a few regions (shear bands) having thicknesses that are orders of magnitude larger than interatomic spacing, but which are still very narrow compared to the deforming sample size. Moreover, this extreme localization of shear is often accompanied by extensive melting and resolidification of the material. This mode of failure is manifested as viscoelastic, i.e. the rheology contains both viscous and elastic components. Since the phenomena of creep and relaxation are thermally activated processes, the viscosity is strongly temperature dependent (e.g. Arrhenius) and it is, in general, a non-linear function of the shear stress $\tau$. The strong temperature dependence of...
the viscosity has important implications as it leads to thermal softening of the material. Indeed, as first noted by Griggs and Baker \[7\], such a physical system is inherently unstable: an increase in strain rate in a weaker zone causes a local temperature rise due to viscous dissipation and weakens the zone even further. At high stresses, viscous dissipation becomes substantial, and if heat is generated faster than it is conducted away, the local increase in temperature and strain rate is strongly amplified. Under those conditions a positive feedback between temperature rise and viscous dissipation is established and a thermal runaway develops. To determine whether the thermal runaway mechanism can explain the aforementioned material failure, we approach the problem by considering a simple viscoelastic model which accounts for the non-elastic behavior below the ultimate yield point (Frenkel’s limit). The temperature \( T \) in the model is determined by the equation for energy conservation which is coupled, through temperature dependent viscosity, to the rheology equation.

Our one-dimensional model (see fig. 1) consists of a viscoelastic slab of width \( L \) at initial temperature \( T_{bg} \) except in the small central region having width \( h \) and slightly elevated temperature \( T_0 \). The boundaries are maintained at the temperature \( T_{bg} \). Our objective is to search for spontaneous modes of internal failure not aided or triggered by the effect of additional far-field deformation. Hence, for time \( t \geq 0 \) we impose zero velocity \( v \) at the boundaries and assume that, without addressing

the loading history \( (t < 0) \), the slab initially \( (t = 0) \) is subjected to a shear stress \( \sigma_0 \). The shear stress \( \sigma \) in the slab satisfies the equation for conservation of momentum

\[
\frac{\partial \sigma}{\partial x} = 0,
\]

which shows that \( \sigma \) is independent of \( x \) and hence only a function of the time \( t \). The viscoelastic rheology is represented by the Maxwell model \[13\], and is given by the equation

\[
\frac{\partial v}{\partial x} = \frac{1}{\mu(T,\sigma)} \sigma + \frac{1}{G} \frac{\partial \sigma}{\partial t},
\]

where \( v(x,t) \) is the velocity, \( G \) is the constant shear modulus and \( \mu(T,\sigma) \) is the viscosity. The dependence of \( \mu \) on \( T \) and \( \sigma \) may be written as

\[
\mu(T,\sigma) = A^{-1} n e^{E/RT} \sigma^{1-n},
\]

where \( A \) and \( n \) are constants, \( E \) is the activation energy and \( R = 8.3 \text{ JK}^{-1}\text{ mole}^{-1} \) is the universal gas constant. Since \( \sigma(t) \) is independent of \( x \), it follows from eq. (2) that the geometry of the strain rate \( (\partial v/\partial x) \) profile at any instant concurs with that of the temperature profile \( T(x,t) \). Utilizing the zero velocity boundary condition, equation (2) may be integrated to obtain the equation which governs the time-dependence of \( \sigma \):

\[
\frac{\partial \sigma}{\partial t} = -\frac{G A}{L} \sigma^n \int_{-\Delta}^{\Delta} e^{\frac{-x}{\tau_d}} dx.
\]

The temperature is determined by the equation for energy conservation

\[
\frac{\partial T}{\partial t} = \frac{\kappa}{\tau_d} \frac{\partial^2 T}{\partial x^2} + A \frac{C}{\sigma} \sigma^n e^{\frac{-x}{\tau_d}},
\]

where the last term accounts for viscous dissipation in the system. Equations (1) and (5) constitute a closed system of coupled ordinary and partial differential equations for two unknown functions \( \sigma(t) \) and \( T(x,t) \).

First, to determine the conditions necessary for thermal runaway to occur, a linear stability analysis was carried out. Equation (1) was approximated for the initial stages by substituting the initial conditions for \( \sigma \) and \( T \). This yields a characteristic time \( \tau_c = \mu_0/(2G\Delta\nu) \) for stress relaxation. Here \( \mu_0 \equiv \mu(T_0,\sigma_0) \) and \( \Delta\nu = h/L + e^{E/RT_0 - E/RT_{bg}} \) is a factor which characterizes the initial perturbation. Linearization of the temperature equation with account of stress relaxation yields that the growth of the perturbation in the initial stages is controlled by the two dimensionless variables \( \tau_c/\tau_d \) and \( \sigma_0/\sigma_c \), where the thermal diffusion time \( \tau_d = h^2/\kappa \) (\( \kappa \) is the thermal diffusivity) and the newly introduced stress

\[
\sigma_c = \sqrt{2\Delta\nu GCR \sigma_0 / E T_0}.
\]
Here \( C \) denotes the heat capacity per volume. The solution to the linearized temperature equation is found to be unstable if \( \sigma_0/\sigma_c > f(\tau_r/\tau_d) \). In the limit \( \tau_r/\tau_d << 1 \), which corresponds to near adiabatic conditions, the function \( f \) quickly approaches the lower bound \( f \approx 1 \) and the solution therefore becomes unstable if \( \sigma_0 > \sigma_c \). Thus \( \sigma_c \) is the critical stress above which a thermal runaway may occur and therefore provides an estimate of the maximum shear strength of viscoelastic materials. Initial stages of thermal runaway instability in a more general setup was recently investigated in ref. [14], including two-dimensional verification of the one-dimensional predictions. The results of our linear stability analysis are in agreement with these numerical estimates in the limit of vanishing boundary velocity.

Non-linear evolutions of the unstable runaway modes rapidly deviate from the exponential growth in time predicted by linear analysis. Since important information about the deformation process can be inferred from the increase in temperature, we choose the maximum temperature rise \( \Delta T_{\text{max}} = T_{\text{max}} - T_0 \) during the deformation process as our main physical quantity to study. This enables us to quantify even the later stages of the thermal runaway process not considered in the linear analysis. A simple estimate of \( \Delta T_{\text{max}} \) during thermal runaway may be obtained assuming adiabatic conditions. In this case all the elastic energy in the system is uniformly dissipated as heat in the perturbed zone and overall energy balance yields the adiabatic temperature rise

\[
\Delta T_{\text{max}}^a = \frac{L\sigma_c^2}{2hGC}.
\]  

Guided by these analytical estimates, the complete time evolution of \( T \) and \( \sigma \) was subsequently investigated by numerical methods. We simplified the problem by dimensional analysis reducing it from one containing thirteen dimensional parameters to one containing six dimensionless parameters. The dimensionless form of the coupled set of equations [4] and [4] were solved numerically using a finite-difference method with non-uniform mesh and a tailored variable time-step in order to resolve the highly non-linear effect of localization. We have systematically varied all six dimensionless parameters and computed \( \Delta T_{\text{max}} \) for each temperature evolution. Remarkably, it is possible to present \( \Delta T_{\text{max}} \) normalized by the adiabatic temperature rise (eq. (7)) as a function of only two combinations of parameters, namely \( \sigma_0/\sigma_c \) and \( \tau_r/\tau_d \), as previously suggested by the linear stability analysis. A representative set of runs is shown in fig. [2a]. This “phase diagram” was computed by varying two of the dimensionless parameters and fixing the remaining four. The plot exhibits a low-temperature region corresponding to thermal runaway processes and a high-temperature region corresponding to thermal runaway processes. These regions are sharply distinguished by a critical boundary having a location that correlates well with stability-predictions of the linear analysis. The phase diagram is “representative” in that it is insensitive

\[\sigma_c \]

\[\tau_d \]

\[\tau_r \]

\[\sigma_0 \]

\[T_0 \]

\[L \]

\[h \]

\[G \]

\[C \]
to which two out of the six dimensionless parameters are varied, keeping the remaining four fixed.

In the neighborhood of the critical boundary in the high-temperature region, however, the temperatures are found to be much larger than the adiabatic temperature rise $\Delta T_{\text{m}}^\text{m}$. In this region we observe a continuous localization of the temperature and strain profiles during the deformation process, i.e. the runaway is spatially self-localizing. This localization effect is illustrated for the temperature profile in fig. 2b. The elastic energy is thus dissipated in a zone much narrower than the width of the initial perturbation resulting in much larger temperatures. The self-localization of the runaway process arises from the effects of thermal diffusion: by diffusion the temperature profile acquires a peak in the center where the effect of the positive feedback mechanism accordingly is maximized. The runaway therefore accelerates faster in the center than in the regions outside and the deformation process finally terminates in a highly localized shear band with a characteristic width much smaller than the characteristic width $h$ of the initial perturbation.

To evaluate the relevance of thermal runaway as a potential failure mechanism in nature, we now consider two case examples comparing critical stress for thermal runaway with Frenkel’s ultimate shear strength limit ($\sigma \sim G/10$). First, we estimate the condition necessary for thermal runaway to occur in olivine-dominated mantle rocks. For olivine (see ref. [12]) $G = 7 \times 10^{10}$ Pa, $C = 3 \times 10^6$ J m$^{-3}$ K$^{-1}$ and $E = 5.2 \times 10^5$ J mole$^{-1}$, while we assume $T_{bg} = 700$ K (corresponding to a depth of about 40 km), $T_0 = 701–720$ K and $h = 10$ m, $L = 10$ km. Substituting these values in equation (6) we predict that thermal runaway possibly occurs if the stress exceeds a critical value in the range $\sigma_c = 0.5–1.7$ GPa, i.e. $\sigma_c = G/140–G/40$. This estimate agrees rather well with the values observed in experimental studies of rock deformation under high confining pressure, where typical failure stresses are in the range 0.5–2 GPa $\sigma_c$. Second, for a metallic glass, typical values are $C = 2 \times 10^6$ J m$^{-3}$ K$^{-1}$ (ref. [4]), $G = 44$ GPa (ref. [16]) and $E = 100–400$ kJ mole$^{-1}$ (ref. [17] and [18]). Assuming $h = 1$ $\mu$m, $L = 1$ cm, $T_{bg} = 300$ K (room temperature) and $T_0 = 301$ K we obtain a critical stress in the range $\sigma_c = 0.4–1.1$ GPa, i.e. $\sigma_c = G/90–G/30$. For comparison, we note that the shear yield strength of the metallic glass Vitreloy 1 is about 0.8 GPa = $G/40$ $\sigma_c$, a value consistent with our estimate of the critical stress necessary for thermal runaway.

The magnitude of the critical stress in these two estimates is remarkably similar considering the very different types of materials discussed and the enormous difference in time and length scales. However, as is evident from eq. (6), the quantities which govern the kinetic processes in these systems (in particular the scale $h$ and the poorly constrained viscosity $\mu$) do not appear in the expression for $\sigma_c$. It is not surprising, therefore, that the stress required to initiate spontaneous thermal runaway is relatively well constrained to about 1 GPa.

These estimates and the concept of self-localizing thermal runaway demonstrate that our simple model is sufficient to explain failure below Frenkel’s ultimate shear strength limit and strain localization at scales much larger than the lattice spacing. The fact that initiation of thermal runaway depends so weakly on the kinetic quantities gives confidence in the application of such models even to the very large scales involved in continental deformation.

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