

ON THE APPLICATION OF DEFORMATION KINETICS
TO NONLINEAR CONSTITUTIVE RELATIONS
AT HIGHER TEMPERATURES

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ABSTRACT

A single phenomenological constitutive equation is derived theoretically from first principles and applied to aluminum, tin and lead. The theory is based on deformation kinetics of steady creep in which the fundamental mechanism is atomic transport over potential barriers whose conformation is distorted by the application of a stress field.

The form of the functional dependence of barrier distortion and stress over the entire temperature range is found to be a sigmoidal curve which tends to straight lines of a unit slope in the small and high stress regions. With this form of barrier distortion, the constitutive equation can predict very well the steady creep behavior of aluminum, tin and lead over a wide range of temperature and stress.

1. Introduction

Experimental results on high temperature creep of pure metals and solid solution alloys during past decades, [1,2,3] fall into two main categories: those establishing a relationship between steady-state creep rate and stress under constant temperature on one hand and a relationship between constant creep rate and temperature under constant stress, on the other. The functional dependence of the constant creep rate $\dot{\epsilon}_s$ on the stress σ under constant absolute temperature T may be divided basically into three regions whose boundaries depend on the material itself. In the low stress region, $\dot{\epsilon}_s$ is almost linearly proportional to σ . Hence it is called a newtonian-like viscous flow region. In the intermediate stress region, $\dot{\epsilon}_s$ appears to be proportional to σ^n , where n is a temperature dependent material parameter. The value of n lies predominately between 4 and 7 for pure metals and between 3 and 5 for solid solution alloys. In the high stress region, $\dot{\epsilon}_s$ is proportional to the exponential function of $\beta\sigma$, here β is a temperature dependent material parameter. The functional

dependence of $\dot{\epsilon}_s$ on T under constant σ is assumed to be governed by a type of Arrhenius relation. As a result the activation energy of creep can be found by a temperature cycling technique or the slope of the line in the Arrhenius plot of $\log_{10} \dot{\epsilon}_s$ vs T^{-1} . The values of activation energy thus found are very close to those of self diffusion in pure metals or the diffusion of one of the predominant elements in solid solution alloys. However, the slope of the Arrhenius plot is, in general, a function of stress and temperature. In addition the activation energy calculated from temperature cycling technique is, in general, a function of stress and strain.

Various theories of creep have been proposed in recent times. These fall basically into two broad categories: phenomenological and micromechanical, the final aim being, of course, a macroscopic constitutive equation. The first category includes theories that are strictly empirical [2-4], others that are mathematical [5], and others still which are "quasi" physical such as the internal state variable theories, a typical example being reference 6. In the second category fall theories in which the underlying micromechanisms are vacancy diffusion, dislocation climb and microcreep [7]. In the latter category belong also the absolute reaction rate theory by Eyring [8] and the very recent deformation kinetics theory of creep by the authors [9].

Micromechanical theories, where vacancies or dislocation are the building blocks, need more than one mechanism to describe the experimental phenomena over a wide range of temperature and stress. While for practical purposes this is not a disadvantage, one wonders if a single appropriate atomic mechanism cannot be found which describes steady creep phenomena over the entire range of stress and temperature.

In reference 9, we found reason to believe that this might be possible. One single constitutive equation was shown to predict very well the steady creep behavior

of AISI 316 stainless steel, pure polycrystalline aluminum and copper over a wide range of temperature and stress, above about 100 kg/cm^2 . The vehicle for this specific constitutive equation is deformation kinetics. The fundamental mechanism is the transport (diffusion) of atoms over potential barriers whose conformation is distorted by the application of a stress field.

In the case of one-dimensional flow, of interest here, the central element of the theory is the relation between the barrier distortion ω and the free energy gradient $-\frac{\partial \Psi}{\partial q}$ where q (an internal variable) is the statistical average of the displacement of atoms in motion facing a specific barrier. In the application of the theory [9] to uniaxial stress fields where the stress was above circa 100 kg/cm^2 a linear relation between ω and $-\frac{\partial \Psi}{\partial q}$ sufficed but proved inappropriate for lower stress levels. Evidently the task at hand is to find an appropriate relation that applies to all stress levels but the form of the relation does not negate the fact that we are dealing with a single mechanism of atomic diffusion over energy barriers. This is done in Section 3.

2. Brief Review of the Theory

Particle Equations

Let N be the number of particles whose motion is impeded by a barrier of height ϵ_0 and ω the distortion of the barrier due to the application of the stress field. See reference 9 for details. Then the number of particles N' partaking in the net motion is given by equation (2.1)

$$N' = 2N \exp(-\epsilon_0/kT) \sinh(\omega/kT) \quad (2.1)$$

where k is the Boltzmann constant and T the absolute temperature. Assuming a "square sinusoidal" barrier shape the average time $\bar{\tau}$ taken by the atoms to climb the barrier is given by equation (2.2)

$$\bar{\tau} = \frac{\sqrt{2} a}{\pi \sqrt{\epsilon_0}} F\left(2, \sin^{-1} k_0\right) \quad (2.2)$$

where a is the barrier width, F is the complete elliptic integral and

$$k_0 = \left(\frac{\epsilon_0 - \omega}{\epsilon_0}\right)^{1/2} \quad (2.3)$$

Rate (Evolution) Equation for q

The average velocity \dot{q} of the atoms crossing the barrier is given by equation (2.4)

$$\dot{q} = \frac{a N'}{\bar{\tau} N} \quad (2.4)$$

Use of equations (2.1), (2.2) and (2.4) gives the desired relation between the average velocity and the barrier distortion:

$$\dot{q} = \frac{\pi \sqrt{2\epsilon_0}}{F} \exp(-\epsilon_0/kT) \sinh(\omega/kT) \quad (2.5)$$

A convenient representation for F is the following

$$F = \frac{1}{2} \log(16\epsilon_0/\omega) \quad (2.6)$$

For $0 \leq \omega/\epsilon_0 \leq 0.35$ the maximum error is less than 5% [9]. If there exists n barriers to the motion, each of height ϵ_0^r with distortion ω_r , then equation (2.5) applies to each such barrier.

However in steady creep only the highest barriers come into play, the lowest ones having already been climbed by the atoms in the course of the deformation. Thus one internal variable suffices (approximately) to represent the effect of these barriers, if, indeed more than one is actual active. Otherwise the representation is exact.

Free Energy Representation

In general

$$\psi = \psi(\varepsilon, q, T) \quad (2.7)$$

where in the present work T is constant. The free energy is the potential energy stored by virtue of atoms being displaced within potential wells. The mean displacement generated as a result is directly related to the elastic strain. For instance in the case of a unidirectional equispaced atoms the elastic strain is exactly equal to the atomic displacement divided by the lattice spacing. Assuming parabolic wells, the potential energy is proportional to a quadratic function of the displacement, leading to the conclusion that the free energy is a quadratic function of the elastic strain [9].

To relate the above discussion to equation (2.7) we write ψ in the quadratic form

$$\psi = \frac{1}{2} A_{11} \varepsilon^2 + A_{12} \varepsilon q + \frac{1}{2} A_{22} q^2 \quad (2.8)$$

and insist that it is a perfect square, so that the squared linear term can then be identified with the elastic strain. This is possible if $A_{12}^2 = A_{11} A_{22}$. The principle of thermodynamic stability requires that ψ be positive definite. This implies $A_{11} > 0$, $A_{22} > 0$, $A_{12}^2 - A_{22}A_{11} < 0$. However, the last inequality can be relaxed and set into equality for the purpose of steady state creep in which the metal exhibits a fluid equilibrium configuration [9]. As a result, equation (2.8) becomes

$$\psi = \frac{1}{2} A (\varepsilon - Bq)^2 \quad (2.9)$$

where $A = A_{11}$ and $B = -A_{12}/A$. Thus since equation (2.9) is the mathematization of the statement at the end of the last paragraph $\varepsilon - Bq$ must be identified as an elastic strain. Note that A and B may be and are, in general, functions of temperature.

To obtain the desired analytical expression for creep we appeal to a

fundamental relation of irreversible thermodynamics according to which the stress is the gradient of free energy with respect to the strain i.e., $\sigma = \partial\psi/\partial\epsilon$. Thus $\sigma = A(\epsilon - Bq)$. Furthermore, as a result of equation (2.9), $\partial\psi/\partial q = -B\sigma$. Since during creep the stress is constant, it follows that $\dot{\epsilon} = B \dot{q}$. The strain rate can then be obtained from equations (2.5) and (2.6), i.e.,

$$\dot{\epsilon} = 2\sqrt{2\epsilon_0} \pi B e^{-\epsilon_0/kT} \frac{\sinh(\omega/kT)}{\log(16\epsilon_0/\omega)} \quad (2.10)$$

where ω is now a function of σ and T .

In the next section we will use equation (2.10) to predict the steady creep of aluminum, tin and lead, particularly under very high temperature and low stress. However before this can be done the relation between the internal force - $\partial\psi/\partial q$ and ω must be established. As noted above - $\partial\psi/\partial q = B\sigma$. The problem is therefore reduced to finding the relation between σ and ω , in this particular case.

3. Application of the Theory to Aluminum

Let the relation $\sigma(\omega)$ between σ and ω or conversely, $\omega(\sigma)$ be known. Specifically let

$$\sigma = \Sigma(\omega); \quad \omega = \Omega(\sigma) \quad (3.1a,b)$$

Substitution of equation (3.1b) in equation (2.10) gives a constitutive relation

$$\dot{\epsilon} = e^{-\epsilon_0/kT} \mathcal{F}(\sigma, T) \quad (3.2)$$

In an inverse fashion, given the experimental relation between σ and $\dot{\epsilon}$ at constant T , one may then use equation (2.10) to deduce the relation between σ and ω , i.e., the function $\Sigma(\omega)$.

The function of $\Sigma(\omega)$ in the case of aluminum can be found from figures 1 and 2. It may be seen that for higher values of stress the relation of σ and $\log_{10} \dot{\epsilon}_s$ is

linear. Thus, in this range, the linear relation implies that

$$\omega = kTK_2 \sigma \left(1 - \frac{\sigma'_0}{|\sigma|}\right) \quad (3.3)$$

where σ'_0 is a threshold stress below which equation (3.3) is not applicable, and K_2 is the slope of the straight portion of the curve. Equation (3.3) was the basis of the study in reference 9, where it was shown that the linear relation persists over a wide range of temperature with the proviso that K_2 and σ'_0 are temperature dependent. In this case $\mathcal{F}(\sigma, T)$ has the form

$$\mathcal{F}(\sigma, T) = \frac{K_1^0 \sinh K_2(\sigma - \sigma'_0)}{\log \left[\frac{16\epsilon_0}{kT} / K_2(\sigma - \sigma'_0) \right]} \quad (3.4)$$

where $K_1^0 = 2\sqrt{2}\epsilon_0 \pi B$. The determination of the constants K_1^0 , K_2 and σ'_0 was discussed at length in reference 9. Note that equation (3.3) implies that the distortion is linearly related to the internal force, i.e.,

$$\omega = kTC (Q - Q^0) \quad (3.5)$$

where Q is defined as $-\partial\psi/\partial q$ and thus equal to $B\sigma$, $Q^0 = B\sigma'_0$ and $C (=K_2/B)$ is the coefficient of proportionality.

As shown in figures 1 and 2, equations (3.2) and (3.4) predict quite well the experimental data in references 10 and 11, except the temperature at 920°k. The corresponding values of K_1^0 , K_2 , C and σ'_0 are shown in figures 3 and 4; $\epsilon_0 = 34$ KCal/mole which is the value of activation energy of self diffusion. It is seen that serious deviations begin to arise below a stress level of about σ'_0 . Of course this is to be expected in view of equation (3.3). Below σ'_0 , equation (3.3) no longer holds.

To determine $\Omega(\sigma)$ in this region we recall equation (2.10), which because of

the smallness of ω/kT we can write in the approximate form

$$\dot{\epsilon}_s = K_1^{\circ} e^{-\epsilon_0/kT} \frac{\omega/kT}{\log(16\epsilon_0/\omega)} \quad (3.6)$$

and note that insofar as this region is concerned the experimental data at 920°k indicate a linear relation between $\log_{10} \dot{\epsilon}_s$ and $\log_{10} (\sigma - \sigma_0^{\prime\prime})$, when the net stress $\sigma - \sigma_0^{\prime\prime}$, is very small [11,12]. As indicated in reference 11, $\sigma_0^{\prime\prime} = 3\text{psi}$, below which creep was not measurable. Since $\log \log (16\epsilon_0/\omega)$ is an insensitive function of ω in this small net stress region, the above observation suggests the following relation between ω and σ :

$$\log_{10} \beta\omega = \log_{10} A_0 + \log_{10} (\sigma - \sigma_0^{\prime\prime}) \quad (3.7)$$

where A_0 and $\sigma_0^{\prime\prime}$ are at most functions of temperature; $\beta = 1/kT$. These parameters were determined respectively from the intercept and the constraint of a unit slope of the curve. In the present case A_0 is a constant (4.6×10^{-5}) and $\sigma_0^{\prime\prime}$ is a decreasing function of temperature (see figure 4). Indications are that as the temperature approaches the melting point (T_m), $\sigma_0^{\prime\prime}$ goes to zero at which point the metal exhibits a truly newtonian behavior.

The form of the functional dependence of ω on σ over the entire temperature range is shown in figure 5. The relationship is sigmoidal tending to a linear form in the small and high stress regions (see equations (3.7) and (3.3)). The theoretical predictions based on figure 5 are shown in figure 2.

4. Application of the Theory to Tin and Lead

The procedure of Section 3 is repeated here without change. It has been shown by a three-dimensional argument [13] that the constitutive equation (2.10) applies to pure shear without change in form. A comparison between theory and experiment is shown in figures 6 and 7. A further treatment will be the subject of a more

extensive article to appear at a later date.

5. Conclusions

In this paper we apply the theory of deformation kinetics to aluminum, tin and lead and show that equation (2.10) suffices to predict accurately steady creep behavior over a wide range of stress and temperature. We may conclude that one micromechanism, that of atomic transport over potential barriers whose conformation is distorted by the application of a stress field, is sufficient to account for the steady creep process in the entire range of temperature and stress.

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PURE POLYCRYSTALLINE ALUMINUM

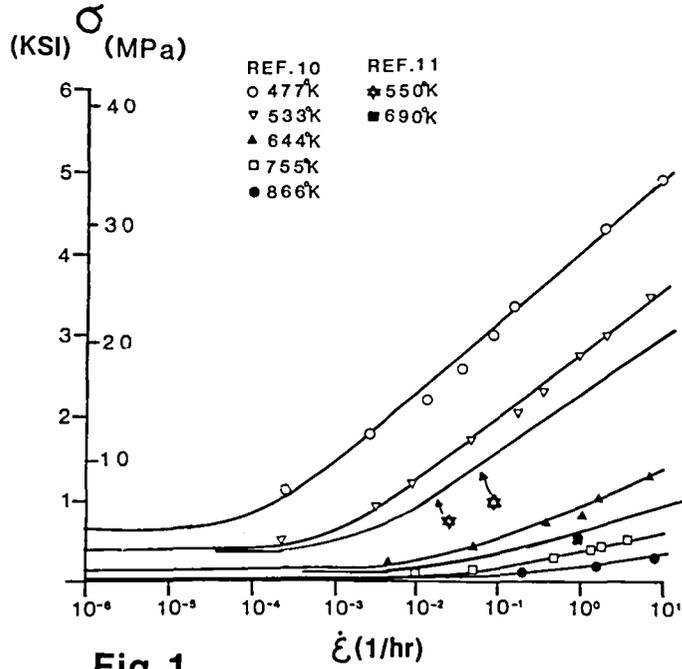


Fig. 1

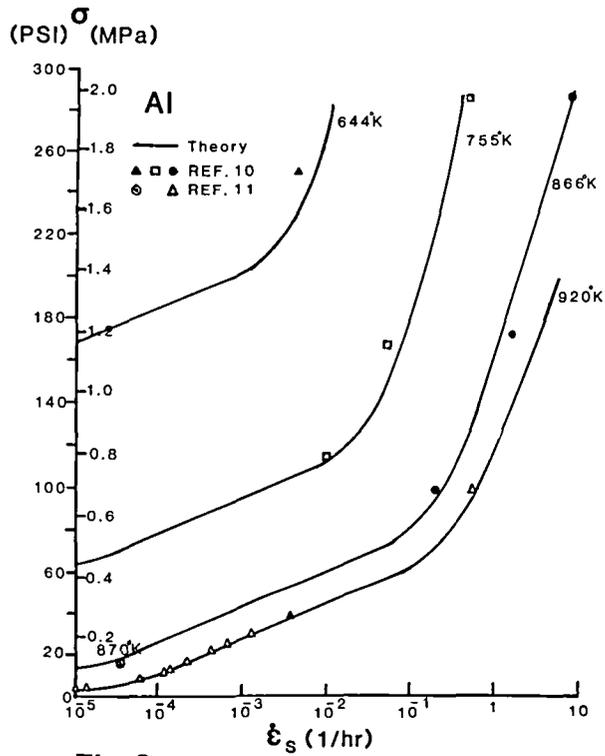


Fig. 2

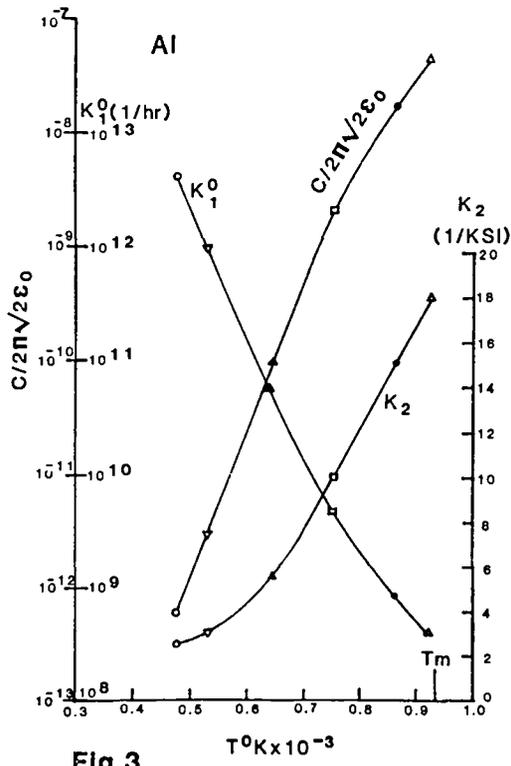


Fig. 3

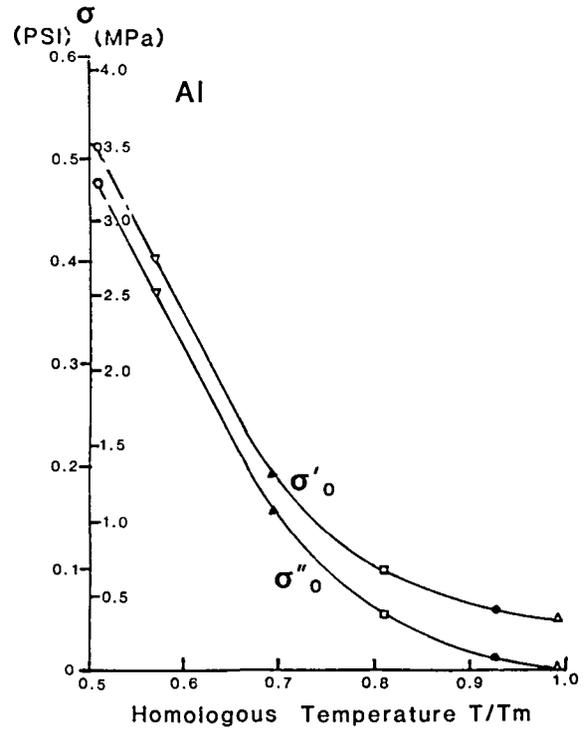


Fig. 4

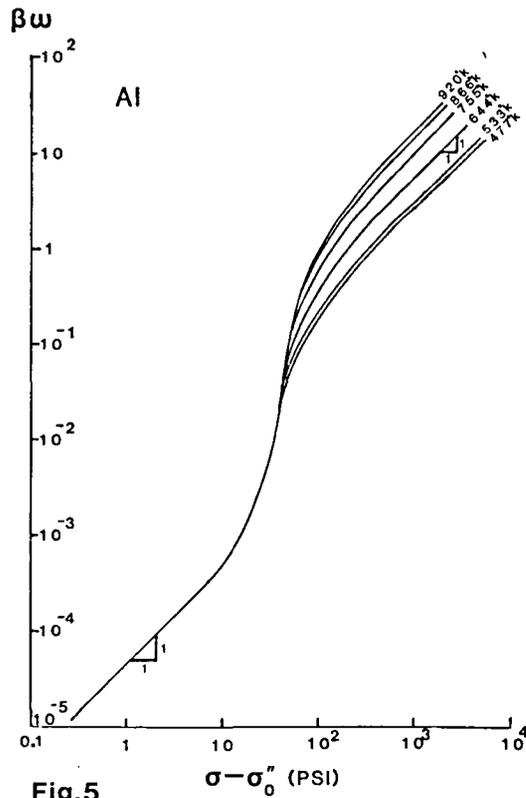


Fig. 5

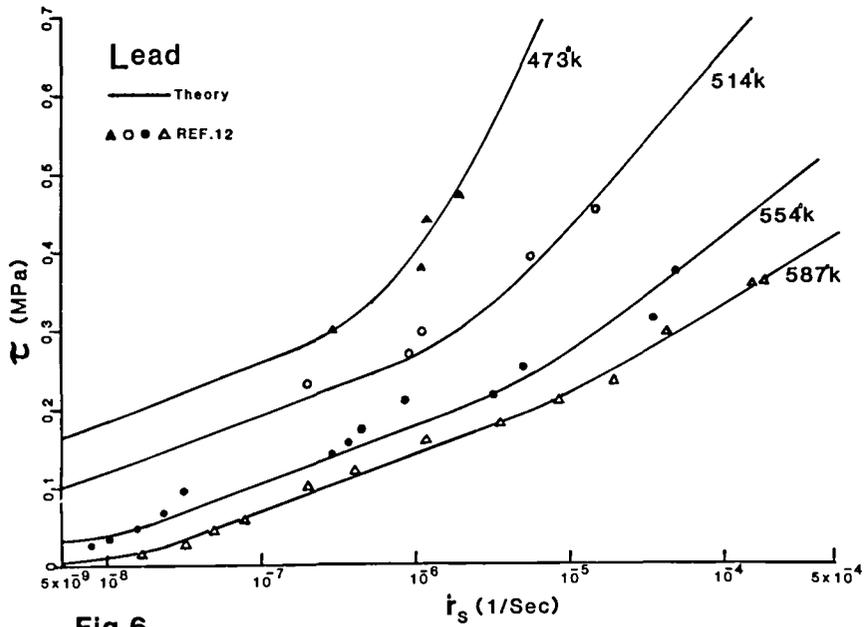


Fig.6

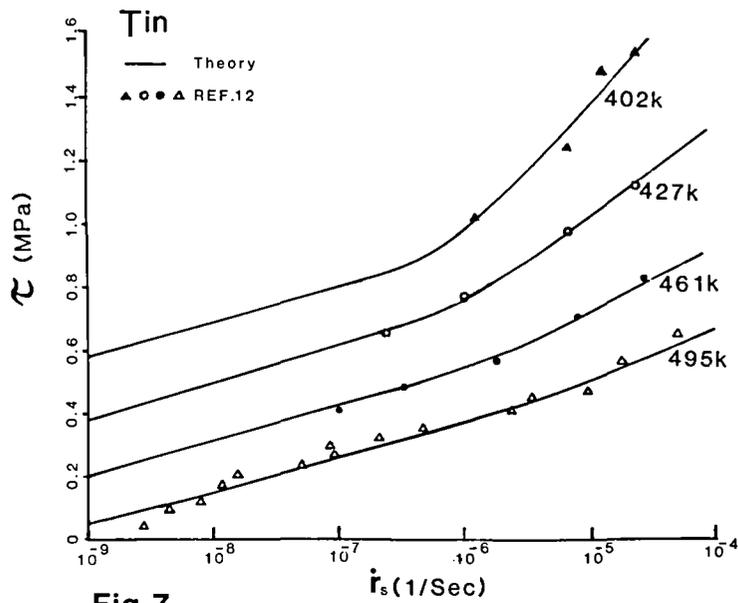


Fig.7