A Stochastic Model for the High-Temperature Plasticity of Metals

E.A. Steck

Technische Universität Braunschweig, Institut für Allgemeine Mechanik u. Festigkeitslehre, Gauss-Str. 14, D-3300 Braunschweig, Germany

Abstract

High temperature plasticity of metals at temperatures ≥ 0.5 melting temperature is, at least for stress ranges of technical interest, explained by thermally activated dislocation movements, where the "structure" of the material, i.e. distribution and strength of the internal barriers, which act against these movements, are of strong influence on these processes.

The characterization of this structure by transition probabilities of a discrete Markov-chain results in a stochastic model which is able to represent essential and typical features which are characteristic for high temperature plasticity.

1. Introduction

The term "high-temperature plasticity" characterizes the behaviour of crystalline solids (metals, rock, mineral-salt) at temperatures above about half their melting temperature. At these high temperatures the relation between stresses and deformations is markedly time dependent. It is widely accepted, that the mechanisms which are responsible for the time dependent deformations at high temperatures are essentially the same as those, which are responsible for the spontaneous plastic behaviour. They are slip processes in the crystals which are supported by dislocations. This theory is supported by the observation, that volume changes connected with creep processes are negligible, and that for multiaxial loading the invariants of the deviatoric stress (mainly the second invariant) play the same governing role in characterizing the stress state, as for spontaneous plasticity.

Especially in the fourties, work was done which aimed on a description of creep processes from the properties of thermally activated dislocation movements. The flow units (dislocations or dislocation packages) are situated in the crystal lattice in front of obstacles, which are characterized by a potential barrier of hight U^* . The externally acting stresses reduce the obstacle hight in direction of their action by the amount $\Delta V \sigma$ (ΔV is the so called activation volume), and increase it in the opposite direction by the same amount. The assumption, that the energy distribution of the flow units follows a Boltzmann distribution, results in probabilities for overcoming the barriers in direction of the acting stress of

$$p_1 = A \exp(-\frac{U^* - \Delta V \sigma}{k_B T}) \quad (1)$$

(k_B is Boltzmanns konstant, T is the absolute temperature). In the opposite direction, the probability to overcome the barrier is given by

$$p = A \exp(-\frac{U^* + \Delta V \sigma}{k_B T}) \quad (2)$$

Connected with the movements of the flow units in the crystals is a macroscopic inelastic strain rate, which is assumed to be proportional to the difference $p_1 - p_2$. This model results in the following expression for the inelastic strain rate:

$$\dot{\varepsilon}_{ie} \sim A \exp(-\frac{U^*}{k_B T}) \sinh(\frac{\Delta V \sigma}{k_B T}) \quad (3)$$

The temperature dependency, which is given by the factor $\exp(-U^*/k_B T))$, is for creep processes in good agreement with experimental results.

The restriction of the model to one single barrier hight resulted in the fact, that the description could only be used for stationary processes. A description of the change of the structure of the material was not possible.
Taeubert /1/ proposed an extension of these models, which also considers the changes of the material structure due to hardening- and recovery processes.

2. The stochastic model with hardening and recovery

The model can be extended by assuming that there exists not only one barrier hight for the transitions of the flow mechanisms, which is connected with the activation energy for self diffusion, but there is a phase space defined for these barriers over which the flow units (whose number is assumed to be constant) are distributed according to the past history of the material. Additionaly a recovery process is defined, for which it is assumed, that the rate of recovery increases with increased hardening.

During the slip processes which are responsible for the inelastic deformations, the flow units have to overcome obstacles which can be represented by internal stresses of different magnitude. Slip steps which contribute to the macroscopic deformation result in hardening. This is considered in the model by the assumption, that the flow unit has to overcome in their next step a barrier whose hight has increased by $\Delta\sigma^{(i)}$. The thermal activation of this process is taken in account in the classical manner, by defining that there exists a temperature- and stress dependent transition probability from situation $\sigma^{(i)}$ to $\sigma^{(i)} + \Delta\sigma^{(i)}$ in the phase space of the system.

According to the form of Equation (3), this transition probability is given by

$$\mathcal{P}(\sigma^{(i)} \to \sigma^{(i)} + \Delta\sigma^{(i)}) = V_{i,i+1} = C_1 \Delta t (\exp(-\frac{U^* - \Delta V(\sigma - \sigma^{(i)})}{k_B T}) + \exp(-\frac{U^* + \Delta V(\sigma + \sigma^{(i)})}{k_B T})) \quad (4)$$

U^* is the activation energy for self-diffusion in the considered material. The connected barrier-hight is decreased by the stress in the direction of its action by the amount $\Delta V \sigma$, and is increased by the internal backstress, connected with hardening, by the amount $\Delta V \sigma^{(i)}$.

Additionally it is assumed, that with the transition from $\sigma^{(i)}$ to $\sigma^{(i)} + \Delta\sigma^{(i)}$ there occurs a macroscopic, inelastic deformation in stress direction, which is given by

$$\dot{\varepsilon}_{ie} = C_1 \lambda \sum_{i=1}^{\infty} z_i \exp(-\frac{U^* - \Delta V(\sigma - \sigma^{(i)})}{k_B T}) \quad (5)$$

Hardening is opposed by a recovery process, for which it is also assumed that

it is thermally activated, where the driving force, which moves the flow units back to lower obstacles, is given by the internal stresses which are connected with the lattice deformations due to hardening. This process also occurs during the time interval Δt with a transition probability which is assumed in the form

$$P(\tau^{(i)} \rightarrow \tau^{(i)} - \Delta\tau^{(i)}) = E_{i,i-1} = C_2 \Delta t \exp\left(-\frac{Q^* - \Delta W \tau^{(i)}}{k_B T}\right) \qquad (6)$$

Q^* is the activation energy which determines this process. ΔW is the connected activation volume.

The parameters Q^*, ΔV, ΔW, C_1, C_2 and λ have to be determined by comparison with experimental results (Steck /5/). For U^* we use in the following, in agreement with experimental results, always the activation energy for self-diffusion.

A given distribution of the flow units changes their position in the phase space with transition probabilities (4) to higher internal stresses and with transition probabilities (6) to lower values. The probability for staying in the present position is therefore given by

$$B_{i,i} = 1 - V_{i,i+1} - E_{i,i-1} \qquad (7)$$

With these probabilities the change of the probable number of flow units at a certain point of the state-axis with time can be expressed by

$$\underline{z}(t+\Delta t) = \underline{\underline{SM}}\ \underline{z}(t) \qquad (8)$$

In this expression

$$\underline{z}(t) = Z\ \underline{p}(\tau^{(i)}, t) \qquad (9)$$

is the vector which describes the distribution of the number of active glide mechanisms over the magnitude of $\tau^{(i)}$. The vector $\underline{p}(\tau^{(i)}, t)$ gives the distribution of the probabilities, Z is the total number of flow units.

$\underline{\underline{SM}}$ contains the transition probabilities, calculated from equations (4), (6) and (7) in the form

$$SM = \begin{bmatrix} E_{i-1,i-2} & 0 & 0 \\ B_{i-1,i-1} & E_{i,i-1} & 0 \\ V_{i-1,i} & B_{i,i} & E_{i+1,i} \\ 0 & V_{i,i+1} & B_{i+1,i+1} \\ 0 & 0 & V_{i+1,i+2} \end{bmatrix} \qquad (10)$$

$\underline{\underline{SM}}$ is a matrix with a constant column-sum of value 1. It is therefore a stochastic matrix, and the evolution of the states of the system, given by eq. (8), is a Marcov-chain.

3. Mathematical properties of the Marcov-chain

With the transition probabilities defined by Eqs.(4) and (6) one obtains a stochastic matrix which is tridiagonal and not decomposable. It can always be transformed in diagonal form, due to the fact, that the coefficients outside the diagonal are all positive and never zero. Therefore the matrix posesses exclusively real eigenvalues. The spectral radius of stochastic matrices is one, therefore SM has a maximal eigenvalue $\lambda_1 = 1$. For all other eigenvalues $|\lambda_i| < 1$ is valid.

The matrix $\underline{\underline{SM}}$ can therefore be transformed on principal axes and obtains the form of the diagonal matrix:

$$\tilde{\underline{\underline{SM}}} = \underline{\underline{M}}^{-1}\,\underline{\underline{SM}}\,\underline{\underline{M}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & \lambda_2 & 0 & 0 & 0 \\ 0 & 0 & \lambda_3 & 0 & 0 \\ 0 & 0 & 0 & \lambda_4 & 0 \\ 0 & 0 & 0 & 0 & \lambda_i \end{bmatrix} \qquad (11)$$

The transformation matrices are the modal matrix $\underline{\underline{M}}$ (matrix of the columnwise arranged eigenvectors) and their inverse. If this transformation is applied to the Markov-chain (8) it results in the following expressions

$$\begin{aligned} \tilde{\underline{z}} &= \underline{\underline{M}}^{-1}\,\underline{z} \qquad\qquad \underline{z} = \underline{\underline{M}}\;\tilde{\underline{z}} \\ \underline{z}(t+\Delta t) &= \underline{\underline{SM}}\;\underline{z}(t) \\ \tilde{\underline{z}}(t+\Delta t) &= \underline{\underline{M}}^{-1}\,\underline{\underline{SM}}\;\underline{z}(t) \\ &= \underline{\underline{M}}^{-1}\,\underline{\underline{SM}}\,\underline{\underline{M}}\,\tilde{\underline{z}}(t) \\ \tilde{\underline{z}}(t+\Delta t) &= \tilde{\underline{\underline{SM}}}\;\tilde{\underline{z}} \end{aligned} \qquad (12)$$

for the description of the evolution of the distribution.

As long as stress and temperature are held constant, the coefficients of the stochastic matrix do not change. The process is homogeneous. For this case the transition probabilities after n time steps can be calculated by repeated multiplication of the matrix $\underline{\underline{SM}}$ with the recent state vector $\underline{z}$ as follows:

$$\begin{aligned} \underline{z}(t_0+\Delta t) &= \underline{\underline{SM}}\;\underline{z}(t_0) \\ \underline{z}(t_0+2\Delta t) &= \underline{\underline{SM}}\;\underline{z}(t_0+\Delta t) = \underline{\underline{SM}}^2\;\underline{z}(t_0) \\ \underline{z}(t_0+n\Delta t) &= \underline{\underline{SM}}^n\,\underline{z}(t_0) \end{aligned} \qquad (13)$$

One obtains obviously directly the transition from t_0 to $t_0 + n\Delta t$ by taking the n-th power of the matrix $\underline{\underline{SM}}$. The same is valid for the description of the process in the system of principal axes:

$$\tilde{\underline{z}}(t_0+n\Delta t) = \tilde{\underline{\underline{SM}}}^n\,\tilde{\underline{z}}(t_0) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \lambda_1^n & 0 \\ 0 & 0 & \lambda_i^n \end{bmatrix} \tilde{\underline{z}}(t_0) \qquad (14)$$

This equation shows directly that the homogeneous process develops towards a stationary distribution and therefore to a steady-state inelastic strain rate. The eigenvalues λ_i for $i \neq 1$ are all smaller than 1 and their influence decreases with increasing the number of time steps. The state vector assumes, independent of the initial distribution, a stationary value, which is determined by the actual stress and temperature. This stationary distribution corresponds to the eigenvector for the largest eigenvalue $\lambda_1 = 1$. The stationary distribution and the connected strain rate can therefore be calculated for given stress and temperature immediately.

For the calculation of transients it is most suitable to use eq. (14). As long as stress and temperature have not changed, with this equation the distribution for time $t_0 + n\Delta t$ can be obtained from the distribution at time t_0 directly. This allows an arbitrary choice of the time scale which is used for the calculations.

4. Transients

It can immediately be seen, that eq. (14) for the development of transients in the space of principal axes can be written in the form

$$\underline{\tilde{z}}(t+n\Delta t) = \lambda_1^n \begin{bmatrix} \tilde{z}_1 \\ 0 \\ . \\ . \\ 0 \end{bmatrix} + \dots \lambda_i^n \begin{bmatrix} 0 \\ . \\ 0 \\ \tilde{z}_i \\ 0 \end{bmatrix} + \lambda_k^n \begin{bmatrix} 0 \\ . \\ . \\ 0 \\ \tilde{z}_k \end{bmatrix} \tag{15}$$

With this representation, the back-transformation is done by the expression

$$\underline{z}(t+n\ t) = \underbrace{\lambda_1^n \underline{\underline{M}} \begin{bmatrix} \tilde{z}_1 \\ 0 \\ . \\ . \\ 0 \end{bmatrix}}_{\underline{r}_1} + \dots + \underbrace{\lambda_i^n \underline{\underline{M}} \begin{bmatrix} 0 \\ . \\ 0 \\ \tilde{z}_i \\ 0 \end{bmatrix}}_{\underline{r}_i} + \underbrace{\lambda_k^n \underline{\underline{M}} \begin{bmatrix} 0 \\ . \\ . \\ 0 \\ \tilde{z}_k \end{bmatrix}}_{\underline{r}_k} \tag{16}$$

Therefore, the state vector at time t+n t assumes the form

$$\underline{z}(t+n\Delta t) = \lambda_1^n \underline{r}_1 + \dots + \lambda_i^n \underline{r}_i + \lambda_k^n \underline{r}_k = \begin{bmatrix} \sum_{j=1}^{k} \lambda_j^n r_{j1} \\ . \\ . \\ . \\ \sum_{j=1}^{k} \lambda_j^n r_{jk} \end{bmatrix} \tag{17}$$

With

$$z_i = \sum_{j=1}^{k} \lambda_j^n r_{ji} \tag{18}$$

one obtains from eq. (5) for the inelastic strain rate

$$\dot{\varepsilon}_{ie} = \bar{C} \sum_{j=1}^{k} \lambda_j^n \sum_{i=1}^{k} r_{ji}\ e^{-\frac{U^w - \Delta V(\sigma - \sigma^{(i)})}{k_B T}}$$

$$= \lambda_1^n \dot{\varepsilon}_1 + \dots + \dots + \lambda_k^n \dot{\varepsilon}_k \tag{19}$$

Due to

$$\lambda_i^n = e^{n\, i n \lambda_i} \quad ; \ n = t/\Delta t$$

equation (19) results in

$$\dot{\varepsilon}_{ie} = \dot{\varepsilon}_S + f_1 e^{-\alpha_1 t} + \dots + f_k e^{-\alpha_k t} \tag{20}$$

The functions f_i depend on the distribution at the beginning of the transient and on the elements of the stochastic matrix. They are, however, just as the eigenvalues λ_i not dependent on time and are for σ = const., T = const. also constants. Physically, equation (20) allows the interpretation, that creep transients are a summation of individual processes with different time constants.

Relations of this type are known from experimental work for some time (e.g. Blackburn /3/), they were, however, due to a lack of theoretical support, not widely examined. Our calculations with data for aluminum (Servi, Grant /2/) and copper (Meakin /4/) showed however (Steck /6/), that already the use of two terms in equation (20), besides the stationary term, gives an excellent representation of the experimental findings.

5. Conclusions

The treatment of plasticity and creep with Marcov-chains as mathematical models provides calculation methods, where with the transition probabilities in

the stochastic matrix and the distribution of flow units over the state-axis, which is identified with internal stresses, the structure of the system and its changes as functions of temperature and external stress are easy to survey. The model possesses inherently typical properties which are characteristic for creep processes (stationary states for homogeneous processes, typical time dependencies of transients after changes of stress or temperature). The calculation of stationary states, of the connected strain rates, and of the changes of the system after load changes is rigid, i.e. the information introduced in the system is preserved for arbitrarily long process times.

Investigations concerning the numerical determination of the parameters of the model showed that with a small number of parameters a description of experimental findings is possible, and that the relations, obtained by these methods, correspond to well known empirical creep laws.

/1/ Taeubert, P. Eine Kriechtheorie fuer Metalle unter Beruecksichtigung von Verfestigung und Erholung. Abhandlungen der Deutschen Akademie der Wissenschaften zu Berlin, Klasse Mathematik, Physik und Technik. Jahrgang 1958, Nr. 7, Berlin

/2/ Servi, I.S. N. J. Grant Creep and Stress Rupture Behavior of Aluminum as a Function of Purity. J. of Metals. Trans. AIME 191, p. 909.

/3/ Blackburn, L.D. Isochronous Stress-Strain Curves for Austenitic Steels. In A.O. Schaefer (Ed.): The Generation of Isochronous Stress-Strain Curves. New York, p. 15.

/4/ Meakin, J.D. The Creep of Face-Centered Cubic Metals with Special Reference to Copper. Ph.D. Thesis, Leeds. 1957

/5/ Steck, E. Entwicklung von Stoffgesetzen fuer die Hochtemperaturplastizitaet. in Fundamentals of Metal Forming Technique I, Symposium Stuttgart 1983. Springer Verlag 1983

/6/ Steck, E. A Stochastic Model for the High-Temperature Plasticity of Metals. International Symposium of Current Theories of Plasticity and Their Application. Norman, Oklahoma 1984