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A constitutive description of the strain rate and temperature effects on the mechanical behavior of materials

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ABSTRACT

The Zerilli and Armstrong (Z–A) model and the mechanical threshold stress (MTS) model have been widely employed to study the strain rate-dependent behavior of materials, but their predictions may sometimes deviate from the experimental results. In this paper, the two well-known models are first reviewed and compared. Their essential relevance is discussed, and the temperature dependences of the parameters in the MTS model are clarified. By using the thermal activation theory, we propose a novel constitutive relation to describe the mechanical behavior of materials in a wide range of strain rate and temperature. Our model combines the advantages of Z–A and MTS models. It can appropriately predict the dependence of the flow stress on the strain rate and temperature, as well as the variation of the activation volume with the thermally activated stress and temperature. We demonstrate the rationality and efficacy of the present model by comparing our theoretical predictions with relevant experimental results in the literature.

1. Introduction

Understanding of the strain rate-dependent behavior of materials is of great interest for many engineering fields. In a wide range of strain rate, plastic deformation, associated with dislocation slipping, is closely related to the thermal activation mechanism. On one hand, the thermal activation mechanism is sensitive to temperature and, on the other hand, plastic deformation under a high strain rate loading can lead to a pronounced rise of temperature. Therefore, the effects of strain rate and temperature are usually coupled and should be considered simultaneously in studying the strain rate-dependent behavior of materials.

In the past three decades, a number of constitutive models have been proposed to describe the strain rate and temperature-dependent behavior of materials (see, e.g., Johnson and Cook, 1983; Zerilli and Armstrong, 1987; Follansbee and Kocks, 1988; Nemat-Nasser et al., 1998b; Khan and Liang, 1999; Preston et al., 2003; Voyiadjis and Abed, 2005; Armstrong and Walley, 2008). Among them, the Zerilli and Armstrong (Z–A) model and the mechanical threshold stress (MTS) model developed by Follansbee and Kocks (1988) are two typical mechanism-based models, which have been widely used and further elaborated by subsequent researchers (see, e.g., Cheng et al., 2001; Nemat-Nasser et al., 1998b).

Generally, increasing the strain rate and decreasing the temperature can both enhance the resistance of plastic deformation and cause a rise of the flow stress. Consequently, Zener and Hollomon (1944) suggested using the parameter $Z = \dot{\varepsilon}\exp(Q/kT)$ to account for the coupling effects of the strain rate $\dot{\varepsilon}$ and temperature T on the flow stress $\sigma(Z)$, where Q is the activation energy and k is the Boltzmann constant. However, Zener and Hollomon's parameter works only in a limited range of strain rate and temperature, and fails to describe the complex effects of temperature on the flow stress (Zerilli, 2004; Armstrong and Walley, 2008). In order to give a more reasonable relation between the flow stress and temperature, the Z–A and

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MTS models introduced additional temperature modifications in the activation energy of dislocation slipping by accounting for two different factors. In the Z–A model, the temperature modification is made by introducing a temperature-dependent average activation volume, whereas in the MTS model, the expression of the activation energy is modified by considering the variation of the shear modulus with temperature. In addition, Nemat-Nasser and Li (1998) and Cheng et al. (2001) made their modifications by considering the influence of temperature on the mean free path of dislocation slipping.

The present paper aims to establish the essential relevance between the Z–A model and MTS model and to develop the constitutive relationship of the mechanical behavior of materials over a wide range of strain rate and temperature. A novel expression is given to describe the energy profiles of thermal barriers for dislocation slipping, and further to predict more appropriately the dependence of the activation volume on the thermally activated stress. Combining this new expression with the thermal activation theory, the strain rate and temperature-dependent mechanical behavior of materials can be reasonably described. The flow stresses for FCC oxygen free high conductivity (OFHC) copper and for BCC tantalum (Ta) predicted by this model show good agreements with relevant experimental results in the literature.

2. Review and comparison between the Z–A model and MTS model

Many mechanism-based constitutive relations accounting for strain rate effects are based on the Orowan (1940) equation:

$$\dot{\varepsilon} = \rho_m b v, \tag{1}$$

where ρ_m is the mobile dislocation density, b is the length of the Burgers vector, and v, which is a function of the applied stress σ and temperature T, denotes the average speed of dislocation slipping. Johnston and Gilman (1959) proposed the following equation for v:

$$v = A\sigma^m \exp(-Q/kT), \tag{2}$$

where A, m and Q are material parameters. Combining Eqs. (1) and (2) gives $\sigma = (Ab\rho_m)^{-1/m} Z^{1/m}$. This expression is consistent with Zener and Hollomon's formula and gives a power-law relation of $\sigma \propto \dot{\varepsilon}^{1/m}$.

Another widely used expression for the average speed of dislocation slipping in Eq. (1) is of the Arrhenius form (Kocks and Mecking, 2003):

$$v = v_0 \exp[-G(\sigma_{th})/kT], \tag{3}$$

where $v_0 = \upsilon_0 l$ represents the peak value of the slipping speed v, with l being the mean free path of dislocation slipping and υ_0 the attempt frequency for dislocations overcoming the thermal barriers. $G(\sigma_{th})$ is the activation energy and a function of the thermally activated stress σ_{th}, with $\sigma_{th} = \sigma - \sigma_a$. The athermal stress σ_a corresponds to the crystal lattice resistance and the long-range resistances induced by the interactions between slip dislocation and grain boundary or forest dislocations, as well as some other mechanisms. Two widely used expressions of $G(\sigma_{th})$ were proposed by Zerilli and Armstrong (1987) and Kocks et al. (1975), respectively, and were used to develop the well-known Z–A model and MTS model.

Assuming that dislocations are gradually activated to overcome the thermal barriers, Zerilli and Armstrong (1987) obtained the following expression:

$$G(\sigma_{th}) = G_0 - \int_0^{\sigma_{th}} V^*(\sigma)\mathrm{d}\sigma = G_0 - V\sigma_{th}, \tag{4}$$

where $V^* \equiv -\partial G(\sigma_{th})/\partial \sigma_{th}$ denotes the activation volume and $V = (1/\sigma_{th})\int_0^{\sigma_{th}} V^*(\sigma)\mathrm{d}\sigma$ is the average activation volume. The reference activation energy $G_0 = \int_0^{\hat{\sigma}} V^*(\sigma)\mathrm{d}\sigma$ and the mechanical threshold stress $\hat{\sigma}$ represent the strength of the thermal barriers. The variation of the activation volume V^* with the thermally activated stress σ_{th} and temperature T have been widely addressed (see, e.g., Hoge and Mukherjee, 1977; Kataoka and Yamada, 1980; Lee and Chen, 2002, 2008; Klassen et al., 2004; Kazantzis et al., 2008).

Substituting Eqs. (3) and (4) into (1), taking the temperature-dependent average activation volume to be $V = V_0 \exp(\beta_0 T)$, and assuming $|(kT/G_0)\ln(\dot{\varepsilon}/\dot{\varepsilon}_0)| \ll 1$, Zerilli and Armstrong (1987) derived:

$$\sigma_{th} = \frac{G_0}{V_0}\exp(-\beta T), \quad \beta = \beta_0 - \frac{k}{G_0}\ln\frac{\dot{\varepsilon}}{\dot{\varepsilon}_0}, \tag{5}$$

where $\dot{\varepsilon}_0 = \rho_m b v_0$, and V_0 is the activation volume at 0 K. For FCC crystals, $V_0 \propto 1/\sqrt{\rho}$, and for BCC crystals, V_0 is independent of ρ, where ρ is the dislocation density and is approximately proportional to the plastic strain ε (Johnston and Gilman, 1959).

Eq. (5) can be rewritten as $\sigma_{th} = f(T)(\dot{\varepsilon}/\dot{\varepsilon}_0)^{kT/G_0}$, where $f(T) = (G_0/V_0)\exp(-\beta_0 T)$. It is seen that the Z–A model predicts a power-law relation between the thermally activated stress σ_{th} and the strain rate $\dot{\varepsilon}$ with a temperature-dependent exponent, kT/G_0. Since the Z–A model assumes $|(kT/G_0)\ln(\dot{\varepsilon}/\dot{\varepsilon}_0)| \ll 1$, Eq. (5) can also be written as $\sigma_{th} \approx f(T)[1 + (kT/G_0)\ln(\dot{\varepsilon}/\dot{\varepsilon}_0)]$, which provides an approximate linear relation between σ_{th} and $\ln\dot{\varepsilon}$.

Kocks et al. (1975) proposed another phenomenological expression of $G(\sigma_{th})$:

$$G(\sigma_{th}) = G_0[1 - (\sigma_{th}/\hat{\sigma})^p]^q, \tag{6}$$

where the exponent q has a value in the range of $1 \leqslant q \leqslant 2$ and p is smaller than 1. Based on Eq. (6), Follansbee and Kocks (1988) developed the MTS model. Eq. (6) have been widely adopted in subsequent models (e.g., Nemat-Nasser et al., 1998b; Kapoor and Nemat-Nasser, 2000; Meyers et al., 2002; Banerjee and Bhawalkar, 2008), where different combinations of p and q values have been used to describe the profile of activation energy function $G(\sigma_{th})$.

Substituting Eqs. (3) and (6) into (1), the thermally activated stress can be calculated as

$$\sigma_{th} = \hat{\sigma}\{1 - [-(kT/G_0)\ln(\dot{\varepsilon}/\dot{\varepsilon}_0)]^{1/q}\}^{1/p}. \tag{7}$$

Taking $p = 1$ and $q = 1$, Eq. (7) gives a linear relation between σ_{th} and $\ln\dot{\varepsilon}$, which has been widely used in the literature. When $-|(kT/G_0)\ln(\dot{\varepsilon}/\dot{\varepsilon}_0)| \ll 1$ and $q = 1$, Eq. (7) predicts a power-law relation $\sigma_{th} = \hat{\sigma}(\dot{\varepsilon}/\dot{\varepsilon}_0)^{kT/(pG_0)}$, which