A constitutive model for dynamic plasticity of FCC metals

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ABSTRACT

This paper proposes a new constitutive model to describe the dynamic plasticity of FCC metals using the thermal activation mechanism of dislocation motion. In the model development, the constitutive parameters were directly linked with the characteristics of microstructures of materials. As an example of its application, the model was used to describe the behavior of OFHC copper. To determine the globally optimized parameters of the constitutive model for OFHC copper, an improved multi-variable optimization method of constrained nonlinear programming was used based on the flow stress of the material measured experimentally. A comparison with some models and experimental data in the literature shows that the new model is simple to apply and is much better in terms of its prediction accuracy. It was shown that compared with the MTS model the new constitutive equation is explicit and can be easily embedded into a computational code of material dynamics; while compared with the Zerilli–Armstrong and Johnson–Cook models the new one reflects more precisely experimental observations. It was concluded that the new model is applicable to a wide range of problems with temperature variation from 77 K to 1096 K, strain rates ranging from $10^{-3}\,\mathrm{s}^{-1}$ to $10^4\,\mathrm{s}^{-1}$, and strain as high as 1.

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1. Introduction

A reliable constitutive model is necessary to describe properly the dynamic response of a material under a deformation with large temperature variation, high strain rate and large strain. Such constitutive models must have the ability to reflect the complicated relationships among the main mechanical state variables of a material. In general, the dynamic yield stress of a material can be described by a function of some state variables such as plastic strain, strain rate, temperature, and some structural parameters related to deformation history. Over the past decades, quite some empirical constitutive models have been proposed based on the conventional phenomenological theory, of which the Johnson–Cook model, or called the J–C equation, is the most widely used [1]. It has been reported that the J–C equation can successfully describe the experimental results of the well-known Taylor cylinder impact test, and is convenient to use because the essential parameters of a variety of materials required by this constitutive equation can be obtained relatively easily. However, it has also been reported that the J–C equation cannot describe or represent many experimental observations/measurements, particularly when a material is subjected to a high strain rate, such as under high speed machining [2]. This is because the dynamic behavior of a material at high strain rates

is closely related to the microstructural evolution of the material during deformation, which is not included in a conventional phenomenological constitutive equation. A physical constitutive model is therefore necessary.

Dislocation dynamics has been used in constitutive modelling since the 1960s. For example, Campbell and Harding [3] studied the dynamic response of low-carbon steels at high strain rates through a thermal activation analysis of dislocation motion. Frost and Ashby [4] deduced various rate-dependent constitutive equations for dislocation motions in the plastic deformation of materials. They then described the regimes of deformation mechanisms relative to various strain rates and temperature variations. Zerilli and Armstrong proposed a constitutive relation using a thermal activation analysis [5]. They found that the dislocation mechanisms in metals of different crystalline structures were different. For face-centered cubic (FCC) metals, dislocations must traverse the barriers of forest dislocations, and the thermal activation area decreases with plastic strain because of the increase in dislocation density. Nevertheless, for body-centered cubic (BCC) metals, dislocations must overcome Peierls–Nabarro barriers (i.e. Peierls internal stress), and thus the thermal activation area is not related with strain. Hence, the yield stress of FCC metals is determined mainly by strain hardening, but that of BCC metals is basically determined by strain rate hardening and temperature softening. Based on these considerations, Zerilli and Armstrong proposed different constitutive relations for FCC and BCC metals. It was claimed that the Zerilli–Armstrong model can describe the behavior of metals with a hexagonal close-packed (HCP) crystalline structure, because HCP has the partial structural

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Nomenclature

b	Burgers vector
c_3	$=k/(g_{s0}\mu b^3)$
c_4	$=k/(g_0\mu b^3)$
c_p	specific heat of materials
d	the diameter of grain
f	the influencing factor (<1) of strain rate and temperature effects
$F(X)$	denoting a function relationship, where $X = \hat{\sigma}_{th}/\hat{\sigma}_{th,s}$
g_0	normalized free energy
g_{s0}	saturated normalized free energy
G_0	reference free energy
k	Boltzmann constant
$\tilde{k}$	the microstructural stress modulus
m'	Schmidt factor
n	$=n_2/n_1$
p, q	a pair of parameters representing the shape of crystal potential barrier
T	temperature
T_0	initial temperature
v	dislocation velocity
v_0	reference limit dislocation velocity
$\hat{Y}$	$= \lambda\hat{\sigma}_{s0}$

Greek letters

ΔG	free energy of thermal activation
λ_1, n_1	material constants
λ_2, n_2	material constants
λ	$=(\lambda_2/\lambda_1)^{1/n_1}$
σ	flow stress
σ_a	athermal stress
σ_{th}	thermal stress
$\hat{\sigma}$	mechanical threshold stress (MTS)
$\hat{\sigma}_a$	athermal component of MTS
$\hat{\sigma}_{th}$	thermal component of MTS
$\hat{\sigma}_s$	saturated threshold stress
$\hat{\sigma}_{s0}$	reference saturated threshold stress
$\hat{\sigma}_{th,s}$	thermal component of $\hat{\sigma}_s$
σ_G	the stress brought by initial defects
ε	plastic (true) strain
$\dot{\varepsilon}$	plastic strain rate
$\dot{\varepsilon}_0$	reference strain rate
$\dot{\varepsilon}_{s0}$	saturated reference strain rate
μ	shear modulus
ρ	material's density
ρ_m	moving dislocation density
θ	strain hardening rate
θ_0	hardening rate due to dislocation accumulation
θ_τ	dynamic recovery rate
η	the converting efficiency from plastic work to dissipated heat

characteristics of BCC and FCC. However, Voyiadjis and Abed [6] pointed out that the Zerilli–Armstrong model is not applicable to the deformation of metals under high temperature because of an approximation in its formulation and because the strain rate effect on thermal activation area has not been considered. Voyiadjis and Abed then proposed an improved model [7]. Nemat-Nasser and Li [8] introduced a variable reference strain rate, as a function of strain and temperature, and obtained a model applicable to both FCC and BCC metals [9,10].

Follansbee and Kocks developed a constitutive model for copper using the concept of mechanical threshold stress (MTS) [11–13]. They found in their experiment that the strain rate sensitivity of flow stress of pure copper dramatically increases when strain rate approaches $10^4\,s^{-1}$. They explained that this was due to the dependence of strain hardening rate on strain rate. A disadvantage of the Follansbee–Kocks model is that the MTS representing the structural evolution cannot be expressed as an explicit function of strain, leading to a complex equation which is not so straightforward for application. There are many similar works on the constitutive modelling of dynamic deformation involving physical mechanisms [14–17] and microstructural evolution [18,19], but their applicability was limited.

This paper will develop a new physical constitutive model for FCC metals. Section 2 of the paper will formulate our new constitutive model based on the theory of thermal activation mechanism of dislocation motion, where the physical meaning of each constitutive parameter will be shown by their relationships with microstructural characteristics. Section 3 of the paper will describe the method to determine the optimal constitutive parameters for oxygen-free high conductivity (OFHC) copper. Section 4 will compare the model with experimental data and some representative models in the literature. Finally, Section 5 will summarize the main advantages of the new model.

2. Physical constitutive formulation of FCC metals

The plastic deformation of metals can be explained as the process of dislocation motion and accumulation with the rate-controlled deformation mechanism. The physical constitutive models of metals have been developed based on the notion of thermally activated dislocation kinetics for moderate strain rates less than $10^4\,s^{-1}$, and on the notion of the dislocation-drag deformation mechanism for greater strain rates [8]. In the thermal activation analysis, plastic flow is mainly controlled by the motion of dislocations which is opposed by both short-range and long-range obstacles. The short-range barriers may be overcome by thermal activation, whereas the long-range barriers are essentially independent of the temperature (i.e. it is athermal). The short-range barriers may include forest dislocations (i.e., the intersection of dislocation forests, which is the principal mechanism in FCC metals [5]), Peierls stress (i.e., the overcoming of Peierls–Nabarro barriers, which is the principal mechanism in BCC metals), point defects (e.g., vacancies and self-interstitials), alloy elements, solute atoms (interstitials and substitutionals), impurities, deposits and so on. The long-range barriers may include grain boundaries, far-field dislocation forests, and other microstructural elements with far-field influence. Therefore, the flow stress of the materials, which is essentially defined by the material resistance to dislocation motion, can be correspondingly decomposed into

$$\sigma = \sigma_a + \sigma_{th} \tag{1}$$

where σ_a is the athermal component of the flow stress reflecting the long-range barriers and is independent of the thermal activation, while σ_{th} is the thermal component of the flow stress reflecting the short-range barriers but depends on the thermal activation. Similarly, the MTS (the flow stress at 0 K, denoted as $\hat{\sigma}$) can be decomposed as the sum of the athermal and thermal components, $\hat{\sigma} = \hat{\sigma}_a + \hat{\sigma}_{th}$. As there is no thermal activation energy at 0 K, the height of the short-range barriers is maximal. This height will fall when temperature increases due to the increase of the atom vibration amplitude activated by the thermal energy, which helps a dislocation to overcome barriers. Accordingly, the thermal stress will decrease while the athermal stress remains unchanged. If the MTS is regarded as a reference stress that characterizes the struc-