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Aspects of power law flow rules in crystal plasticity with glide-climb driven hardening and recovery

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ABSTRACT

In this work we will examine three power law type flow rules that are commonly used in crystal plasticity. Glide and climb driven combined hardening/recovery effect has been considered within their respective internal variables. With finite strain framework, a highly complex intermetallic material (single crystal like Al-rich TiAl lamellar binary alloy) has been analyzed at high homologous temperature. We have adopted a novel approach of estimating critical stresses and modified evolution equation for the combined hardening and recovery. From a variety of options in identifying modeling parameters, which set of flow rule dependent parameters are meaningful is discussed here. Different related numerical aspects including slip activities are also outlined. The investigation employs three sets of compressive strain rate controlled experimental data in two lamellar directions. It is revealed that, irrespective of the type of the flow rules, two internal variables based flow rules including slip-system-level kinematic hardening variable makes significant improvement in simulating high temperature medium stress viscoplasticity with estimating reasonable material parameter set, and a specific choice of the flow rule provides better prediction capability. It is also found that the most active slip system dictates the overall plastic deformation in reproducing experimental data.

1. Introduction

Flow rule is the starting point in analysis of plastic deformation phenomena. In a plastic flow rule, we generally deal with the relation of measurable variables (strain rate, temperature) and associated variable (stress) along with one or more internal variables. Phenomenological plasticity modeling is based on the incorporation of one or more internal state variables. Plastic deformation depends on the loading history and on the continuously changing internal states that are considered representable by one of more internal variables. Based on that, there are various types of flow rules available in the literature including power law, hyperbolic sine, exponential, and mixed type etc. All flow rules can be roughly associated with different stress levels.

- Firstly, moderate stress level.
  Engineering applications dominate this regime where power law usually works fine. For example, power law creep has been used in Cui et al. [1] and Alfredsson et al. [2] for steel, in Vose et al. [3] and Yang et al. [4] for Cu, in Naumenko and Gariboldi [5] for Al, and in Staroselsky and Cassenti [6] for a single crystal superalloy, etc. Because of smaller effort in identification of material constants and simplicity in the structural analysis power laws are popular [7]. To accommodate power law with primary and tertiary creep often additional internal state variables along with damage variable are included [8].
- Secondly, low and moderate stress.
  At low stress, generally a transition to diffusion type creep occurs (Harper-Dorn Creep) where power exponent decreases and power law becomes linear [7]. Many engineering structural analyses belong to these regimes. Sometimes a sum of linear (diffusion type) and power law functions is applied to accommodate deformations with both low and moderate stress levels [7,8]. When the power law is extrapolated from moderate to low stress regime, a significant underestimation of the creep rate for the low stress values may result [1,7]. That is why sometimes hyperbolic sine function without power exponent is used [9]. Similar laws can also be found in [10,11].
- Third and finally, moderate and high stress.
  Generally breakdown of power law is observed at high stress. As a consequence, flow rule with hyperbolic sine is preferred when there is a breakdown of power law or a transition from power law to power law breakdown regime [12] i.e. medium to high stress regimes. Hyperbolic sine flow rule can be either Garofalo type [13] where the

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power exponent is outside the hyperbolic sine function, or Miller Type [14] i.e. the two power exponents in both inside and outside of the hyperbolic sine function. With two power exponents of inside and outside of hyperbolic sine function, Miller [14] considered it as a generalized flow rule for monotonic, cyclic and creep deformation. Flow rule with power of hyperbolic sine function has also been used in Becker [15] for texture evolution in channel die compression, in Chen and Feng [16] for cyclic viscoplasticity, in Zhang [17] for hot deformation of Ni alloy GH4698, in Längler et al. [18] for thermo-mechanical loading dependent deformation etc. Chen and Feng [16] also reported that the hyperbolic sine function can capture additional non-linearity in the relationship between the viscous-stress and the inelastic strain rate. Farnoush et al. [19] and Cowan and Khandelwal [20] considered the power law with hyperbolic sine function as a possible general case, which reduced to a power relation at lower stresses and to an exponential relation at high stress levels. Barrett et al. [21] claimed that the hyperbolic sine flow rule facilitates the identification of strain rate independent material parameters at high temperature. Sometimes it is considered that hyperbolic sine function is the best one to describe the strain rate and rupture behavior, while according to Dyson and McLean [9] it is advantageous in damage evaluation as well. Furthermore, apart from hyperbolic sine, sometimes flow rule with power exponent inside an exponential function can also be found e.g. in [22] for two phase single crystal deformation.

The plastic/creep deformation is usually divided into three stages where each regime can be fit (over a range of stress) by a power law [23]. A pure power relation of strain rate and stress is often used to characterize steady creep of metal and alloy at temperature above $0.3T_\mathrm{m}$ in the stress range of one or two digits, below a certain stress level. Experimental data show that the power law can be applied for one to two order of stress, four to eight order of strain rate [24]. Each power law flow rule generally takes a term of stress or dimensionless stress like quantity with a power exponent. In these flow rules, temperature dependency is often accommodated by a separate multiplicative Arheneius type function, even sometimes this function is considered with a power exponent, like temperature dependent drag variable in the power law [25] flow rule. Whatever the variety, the most important part of these flow rules is the ratio of plastic driving force to flow resistance, or dimensionless stress quantity, which directs the internal slip mechanisms and activities during inelastic deformation. Specific choice of the definition leads to a unique number of consequences. Some authors recently considered this ratio both in the temperature dependent term and in the remaining term with power exponent, such flow rules can be found in dislocation density based crystal plasticity modeling [26,27]. The foremost point is, how to define effective stress in the dimensionless quantity, which is to be considered as the driving force for the plastic deformation and how to define the drag or flow resistance along a slip system. In spite of various flow rules, power law is the most widely used one in engineering calculations both at low and high temperatures because of its effectiveness in simulating steady state creep. They have retained a pre-eminent position in both the metallurgical and mechanics literatures [9]. Irrespective of the scale whether it is micro or macro, whether the flow rule is phenomenological or mechanism based [28], the application of the power law type flow rule is abound in the literature especially at high homologous temperature and moderate to low stress conditions [29]. Specifically in crystal plasticity, power law remains as the central one, and hence, our focus is limited to the power law flow rules of crystal plasticity. Based on the driving force and flow resistance definitions there are three types of flow rules, mostly used for isothermal case, generally found in the literature for classical crystal plasticity, as shown in Eqs. (1)–(3). See for example [30,31], among others. These commonly used flow rules are purely phenomenological. In this work we will try to highlight different aspects based on the choice of the flow rule with the possibility of accommodating climb driven recovery at high temperature.

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{g^\alpha} \right|^n \operatorname{sgn}(\tau^\alpha) \tag{1}$$

$$\dot{\gamma}^\alpha = \left| \dot{\gamma}_0 \frac{\tau^\alpha - X^\alpha}{g^\alpha} \right|^n \operatorname{sgn}(\tau^\alpha - X^\alpha) \tag{2}$$

$$\dot{\gamma}^\alpha = \left\langle \frac{|\tau^\alpha - X^\alpha| - R^\alpha}{K} \right\rangle^n \operatorname{sgn}(\tau^\alpha - X^\alpha) \tag{3}$$

Here $\dot{\gamma}^\alpha$ indicates the slip rate of the slip system α, similarly τ^α is the shear stress, X^α is the backstress or the internal stress, and g^α and R^α both are the threshold stress, a component of friction that evolves with slip [32], of the same slip system. K is the temperature dependent drag while g in Eqs. (1)-(2), and X and R in Eqs. (2)-(3) are phenomenological internal variables. R and g can be considered for the critical resolved shear stress (CRSS) evolution. One important point is, the backstress variable allows us to distinguish a tensile and a compressive yield strength. K and n are two material coefficients characterizing the viscous effect of a hardened material. Macaulay brackets $< y >$ indicate the following:

$$< y > = \begin{cases} y, & y \geq 0 \\ 0, & y < 0 \end{cases} \tag{4}$$

Due to the microstructural and morphological complexity, the plastic behavior of a single crystal material is inherently anisotropic. More and more complex materials (e.g. intermetallic compounds) are currently of growing interest at high-temperature applications. So sophisticated microstructures nowadays are becoming heterogeneous and complex. Moreover, rate dependent and temperature dependent anisotropic phenomena are becoming more important. This study is also concerned with the prediction power of the most commonly used approaches in crystal plasticity at very high homologous temperature by analyzing a highly rate sensitive alloy with complex microstructure and morphology. Details of slip interactions are essential in understanding the overall hardening of single crystals. Secondary slips are not only the key to fundamental hardening behaviors, they are also the key to coarse slip band formation and, to a lesser extent, the details of macroscopic shear band formation [33]. That is why, this work also highlights model dependent behaviors particularly slip activities, secondary slip activation, and material parameters etc. The main body of the paper has been arranged in seven sections. Apart from introduction and concluding remarks, Section 2 describes the material, microstructure and deformation mechanisms, while Section 3 summaries the mathematical framework. Flow rules with different assumptions and corresponding simulation results with experimental data are presented in Section 4. Material and model parameters are discussed in Section 5 with many relevant cases from the literature. The last two sections of the main body, i.e. Sections 6 and 7, deal with the most dominant slip system and its role in characterizing CRSS.

2. Material, microstructure, deformation mechanisms and experimental procedures

Many versions of Ti-rich intermetallic alloys including Polysynthetically twinned (PST) crystals with γ-TiAl + α_2-Ti$_3$Al are highly successful till 900 °C [34] in various industrial applications like aerospace engine, gas turbine, petroleum, medical and defense industries due to their high strength, good oxidation and ignition resistance combined with good creep properties at high temperatures, fracture toughness, corrosive resistance, low density, high thermal capability, and biocompatibility, etc. For temperatures up to 1050 °C, phases from the Al-rich region of this alloy system are considered to be highly potential candidates for high temperature structural applications. Due to higher oxidation resistance, 20% lower density and higher (about 150 °C more) operating temperature application possibility of Al-rich TiAl alloys over