

DISLOCATION-MECHANICS-BASED CONSTITUTIVE DESCRIPTIONS OF CRYSTAL PLASTICITY OF METALS: AN OVERVIEW

Chongyang Gao*, Liangchi Zhang**

*Department of Engineering Mechanics, Zhejiang University, Hangzhou, 310027, China

**School of Mechanical and Manufacturing Engineering, The University of New South Wales, NSW 2052, Australia

Summary A reliable constitutive model is crucial to the robust description of the dynamic response of a material under large deformation at high strain rates. Recently, the authors have developed a class of dislocation-mechanics-based models to reflect the thermo-viscoplastic behaviors of fcc, bcc and hcp metals. Especially, a unified fcc model considering mobile dislocation density evolution was established across a wide strain rate range $10^{-4} - 10^6 \text{ s}^{-1}$, which can successfully describe the flow stress upturn phenomenon beyond 10^4 s^{-1} .

INTRODUCTION

In the engineering applications of plasticity and impact, a suitable thermo-viscoplastic constitutive model is crucial for an effective material dynamics analysis. Nevertheless, it is not easy to establish a model which is not only precise but also tractable to use especially under high strain rates. In the past decades, various empirical constitutive models for dynamic plasticity have been proposed. These models can be divided into two types: one is the high-pressure models, which considers the pressure effect of strong shock and is established based on one-dimensional-strain experiments such as the pressure-shear plate impact tests. The other is the regular-pressure models, which does not need to consider the pressure state variable and is established upon the one-dimensional-stress experiments such as the split Hopkinson pressure bar (SHPB) tests. The different stress/strain states in these two types of experiments may result in dissimilar plastic deformation mechanisms since the deviatoric stress and pressure induce different microstructural responses in materials. The authors have investigated the regular-pressure models at the strain rate below 10^6 s^{-1} . They found that the empirical models cannot properly describe some experimental observations, particularly at a high strain rate, such as in the case of high speed machining. This is because the dynamic behavior of a metal at high strain rates is closely related to its microstructural characteristics and evolution during plastic deformation, which is not considered in a conventional phenomenological theory. Physics-based constitutive models have therefore been developed to fill the gap.

Considering that the thermal activation mechanisms of dislocations in metals of different crystalline structures are distinct, Zerilli and Armstrong proposed the ZA model with different constitutive forms for face-centered cubic (fcc), body-centered cubic (bcc) and hexagonal close-packed (hcp) metals which owns mixed characteristics of the bcc and fcc structures. However, Voyiadjis and Abed pointed out that the ZA model is not applicable to high temperature cases and that this model does not include the strain rate effect on thermal activation area. They then proposed a modified ZA model. Nemat-Nasser et al. developed a kind of physical models applicable to both fcc and bcc metals based on their systematic experimental investigation. Follansbee and Kocks proposed a constitutive model for polycrystalline copper with a concept of mechanical threshold stress (MTS, the flow stress at 0 K representing the structural evolution of the material). However, this model needs certain phenomenological expressions and experimental data to determine the thermal component of the MTS which cannot be explicitly expressed, leading to a composite constitutive form inconvenient to use. The authors recently developed a class of dislocation-based Gao-Zhang (GZ) models by using a thermal activation analysis of dislocation motion and a structural evolution of internal state variable MTS, to be applicable to fcc, bcc and hcp metals of different crystalline structures [1, 2]. Furthermore, they introduced the evolution of mobile dislocation density into their fcc model and established a unified fcc model [3], capable of explaining the flow stress upturn phenomenon of fcc metals. This paper will give a brief overview of these constitutive models.

CONSTITUTIVE MODELLING

The plastic deformation of metals can be regarded as the process of dislocation motion and accumulation under a thermally-activated rate-controlled mechanism. In this regime, plastic flow is mainly controlled by the motion of dislocations which is opposed by short- and long-range barriers. The former (e.g., forest dislocations in fcc metals and Peierls stress in bcc metals) may be overcome by thermal activation, whereas the latter are essentially independent of the temperature. Therefore, the flow stress of the materials, which is defined by the material resistance to dislocation motion, can be decomposed as the athermal component (σ_{ath}) reflecting the long-range barriers and the thermal component (σ_{th}) reflecting the short-range barriers. Similarly, the MTS (denoted as $\hat{\sigma}$) can be similarly decomposed. Then the flow stress of the material can be expressed below if the MTS is regarded as a structure parameter,

$$\sigma = \hat{\sigma}_{ath} + f(\dot{\epsilon}, T) \cdot \hat{\sigma}_{th} \quad (1)$$

where $f(\dot{\varepsilon}, T)$ (<1.0) is the influencing function representing the strain rate and temperature effects in the thermal activation process. Based on the Arrhenius expression deduced from the well-known Orowan relation and Johnson-Gilman relation, and the Gibbs free energy expression firstly proposed by Kocks et al., the thermal activation function at the current constant structure can be deduced with the parameters representing the shape of potential barrier of crystals. In reality, a structure will evolve with strain under the influence of strain rate and temperature, and the evolution process is a balancing result of two competing processes – dislocation accumulation and dynamic recovery, which can be described by the strain hardening rate, $\theta = d\hat{\sigma}/d\varepsilon$. The structural parameter MTS can then be determined with the evolution law of the strain hardening rate as follows.

For fcc metals, Gao and Zhang proposed a quasi-power-type law, instead of the linear Voce law, for the strain hardening rate. By using the equation describing the saturated MTS, they obtained the thermal component of MTS. On the other hand, the athermal stress includes an initial yield stress reflecting the influence of solute and initial defects, and a constant stress reflecting the size effect of grain boundaries in polycrystals which is limited for conventional coarse-grained materials but quite obvious for nanocrystalline materials. The grain's size effect obeys the Hall-Petch relationship and can be regarded as constant if there are no physical changes to alter the average grain diameter during plastic deformation. After determined the MTS, the constitutive model for fcc metals was then established.

There exists an important difference between bcc and fcc metals in their thermally-activated dislocation mechanisms due to their different crystalline structures. The thermal activation area is closely related with strain for fcc metals but not for bcc metals. In other words, the strain hardening of bcc metals is not coupled in the thermal stress but belongs to the athermal stress. The athermal stress of bcc metals can be firstly determined by using empirical power law for strain hardening. The saturated value of the thermal component of MTS is the same as itself since it is independent of strain; besides, the saturation stress equation for fcc metals can be assumed to be applicable to bcc metals too. So the thermal component of MTS can be known. Then the constitutive model for bcc metals was determined.

Considering that hcp metals may own partial structural characteristics of both bcc and fcc metals, Gao and Zhang proposed a new mixed model by combining the fcc and bcc models to describe the intermediate behavior of hcp metals. To be noticed is that the deformation twinning, which is prone to occur in the plastic deformation of hcp and bcc metals at high strain rates, has been considered in this model by a way similar to grain boundaries.

On the other hand, Follansbee and Kocks found that the flow stress of oxygen-free high conductivity copper (OFHC Cu) increases dramatically when strain rate exceeds 10^4 s^{-1} . That is to say, there appears a continuous and fast rise in the rate sensitivity of flow stress. For fcc metals, the plastic models based on thermally-activated dislocation glide kinetics have satisfactorily described the viscoplastic behavior in deformation at strain rates up to 10^4 s^{-1} . However, the kinetics of viscoplastic flow may be controlled by different mechanisms at higher deformation rates. Gao and Zhang pointed out that the dislocation density evolution (DDE), which results in a remarkable multiplication of mobile dislocations, should be considered in the existing thermal activation mechanism under very high strain rates. Although some models [4] have been proposed based on DDE, the physics of the dislocation kinetics at extremely high strain rates is still not very clear. Gao and Zhang therefore developed a new fcc model by incorporating an evolution equation of mobile dislocation density into their previous fcc model to successfully explain the flow stress upturn at extremely high strain rates. Furthermore, a unified fcc model was proposed for a broad strain rate range by combining the new fcc model with its reduced form at relatively low strain rates.

Finally, the predictions of these constitutive models summarized above were provided. These models have been compared with experimental data as well as with other typical models for validation, as discussed respectively in the primary literature in detail.

CONCLUSIONS

In the authors' work, a class of dislocation-based models has been established for fcc, bcc and hcp metals, including a unified model for fcc metals to cover a wide strain rate range $10^{-4} - 10^6 \text{ s}^{-1}$. The adiabatic shear effect and deformation twinning effect can be included in these models. The one-dimensional constitutive relations developed can easily be converted to ones of three-dimensional materials by replacing the true stress and strain with the von Mises equivalent stress and strain defined by the tensor's invariants.

References

- [1] Gao C. Y., Zhang L. C.: A constitutive model for dynamic plasticity of FCC metals. *Mater. Sci. Eng. A* **527**:3138-3143, 2010.
- [2] Gao C. Y., Zhang L. C., Yan H. X.: A new constitutive model for HCP metals. *Mater. Sci. Eng. A* **528**:4445-4452, 2011.
- [3] Gao C. Y., Zhang L. C.: Constitutive modelling of plasticity of fcc metals under extremely high strain rates. *Int. J. Plasticity* DOI: 10.1016/j.ijplas.2011.12.001.
- [4] Voyiadjis G. Z., Almasri A. H.: A physically based constitutive model for fcc metals with applications to dynamic hardness. *Mech. Mater.* **40**:549-563, 2008.