PHYSICALLY BASED THERMOMECHANICAL MODELING OF METALS OVER A WIDE RANGE OF STRAIN RATES AND TEMPERATURES

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Summary Microstructural physical based constitutive models are developed in this work in order to characterize the thermomechanical response of different types of metals subjected to low and high strain rates and temperatures. The concept of thermal activation energy as well as the dislocations interaction mechanisms is used in the derivation procedure taking into consideration the effect of the mobile dislocation production as well as the dislocation speed on the flow stress of the deformed material. The model is verified using different sets of experimental data for the same material parameters obtained from other independent tests. Good correlation is observed between the model predictions and the experimental observations. The plastic flow is considered in the range of temperatures and strain rates where diffusion and creep are not dominant.

INTRODUCTION

Developing plastic flow models which are physically based, widely applicable and capable of accounting for complex paths of deformation, temperature and strain rate is considered the main desirable goal in constitutive modeling of metals. The understanding of high-strain-rate behavior of metals at elevated temperatures is essential for the modeling and analysis of large deformation problems such as high-speed machining, impact, penetration and shear localization. Deforming a metal beyond the elastic limit activates and moves its dislocations through the crystal. In turn, two types of obstacles that try to prevent dislocation movements through the lattice are encountered; long range and short-range barriers. The long-range barriers are due to the structure of the material and cannot be overcome thus introducing thermal energy through the crystal. On the other hand, the short-range barriers can be overcome by thermal energy activation. Body centered cubic (bcc) and face centered cubic (fcc) metals as well as different types of steel are considered in the present model.

MODEL THEORY AND FORMULATION

In relating the plastic strain rate tensor $\dot{\varepsilon}_{ij}^{p}$ at the macroscale to the plastic shear strain rate $\dot{\gamma}^{p}$ at the microscale (which is related to dislocation density ρ_m, dislocation distance *l*, and Burgers vector *b*), an average form of the Schmidt tensor M_{ij} is assumed since plasticity at the macroscale incorporates a number of differently oriented grains into each continuum point [1]:

$$\dot{\varepsilon}_{ij}^{p} = \dot{\gamma}^{p} M_{ij} \quad \text{where} \quad M_{ij} = (n_i \otimes v_j + v_i \otimes n_j)/2 \quad \text{and} \quad \dot{\gamma}_p = (\partial\gamma^p / \partial\rho_m)\dot{\rho}_m + (\partial\gamma^p / \partial l)v \tag{1}$$

where $\hat{n}$ denotes the unit normal on the slip plane and $\hat{v}$ denotes the unit vector in the slip direction. In a conservative glide, the plastic flow rate defined in Eq.(1) clearly depends on both dislocation production $\dot{\rho}$ and dislocation speed v. Recently, great efforts were made in order to obtain an evolution equation for the dislocation densities in terms of strain rate and temperature. The following equation that describes the mobile dislocation density evolution is proposed [2]:

$$\dot{\rho}_m = (\lambda_1 / b^2 - \lambda_2 \rho_m - \lambda_3 \sqrt{\rho_f} / b)\dot{\varepsilon}_p \tag{2}$$

where ρ_f represents the forest dislocation density and the constant coefficients λ_i are related to the multiplication of mobile dislocations (λ_1), their mutual annihilation and trapping (λ_2), and their immobilization through interaction with forest dislocations (λ_3). The average dislocation velocity *v* can be determined through thermal activation by overcoming local obstacles to dislocation motion. Many authors have introduced velocity expressions for thermally activated dislocation glides. However, the following general expression is postulated [1].

$$v = v_o \exp(-G / kT) \tag{3}$$

where $v_o = d / t_w$ is the reference dislocation velocity, t_w is the time that a dislocation waits at an obstacle, *d* is the average distance the dislocation moves between the obstacles, *G* is the shear stress-dependent free energy of activation which may depend not only on stress but also on temperature and the internal structure, *k* is Boltzmann's constant, and *T* is the absolute temperature. Many authors using different forms have related the activation energy *G* to the thermal flow stress σ_{th}; for example, Kocks et al. [3] suggested the following definition:

$$G = G_o \left(1 - \left(\sigma_{th} / \hat{\sigma}\right)^p\right)^q \tag{4}$$

where G_o is the reference Gibbs energy at T=0, $\hat{\sigma}$ is the threshold stress at which the dislocations can overcome the barriers without the assistance of thermal activation, and *p* and *q* are constants defining the shape of the short-range barrier. The typical values of the constants *q* and *p* are 1.5 and 0.5 respectively [3].

Body cubic centred (bcc) and face cubic centred (fcc) models

The behavior of bcc metals shows a strong dependence of the thermal yield stress on the strain rate and temperature. The thermal stress is attributed to the resistance of the dislocation motion by the Peierls barriers (short-range barriers) provided by the lattice itself. On the other hand, the emergence and evolution of a heterogeneous microstructure of dislocations as well as the long-range intersections between dislocations dominates and controls the mechanisms of thermal activation analysis in fcc metals. Thus, the thermal activation is strongly dependent on the plastic strain. Utilizing Eqs.1 to 4 and using the additive decomposition of the thermal and athermal stresses, the equivalent flow stress in terms of the equivalent plastic strain, equivalent plastic strain rate and temperatures is given as follows:

for bcc metals $$\sigma = \hat{Y}(1-(\beta_1 T - \beta_2 T \ln \dot{\varepsilon}_p)^{1/q})^{1/p} + B\varepsilon_p^n + Y_a \quad (5)$$

for fcc metals $$\sigma = B\varepsilon_p^n(1-(\beta_1 T - \beta_2 T \ln \dot{\varepsilon}_p)^{1/q})^{1/p} + Y_a \quad (6)$$

The parameters β_s are related to the microstructure quantities as follows:

$$\beta_1 = \frac{k}{G_o}\ln\left(\frac{\tilde{m}b\rho_m v_o}{1-\tilde{m}l(\lambda_1/b-\lambda_2 b\rho_m-\lambda_3\rho_f^{0.5})}\right) \quad \text{and} \quad \beta_2 = \frac{k}{G_o} \quad \text{where} \quad \tilde{m} = (2M_{ij}M_{ij}/3)^{1/2} \quad (7)$$

RESULTS & CONCLUSIONS

The effectiveness of the foregoing models is tested using independent experimental data obtained in the literature [4, 5] for different bcc and fcc metals (e.g. Vanadium, Molybdenum, Niobium, Tantalum and OFHC Copper) over a wide range of strain rates and temperatures. The comparison of the theoretical isothermal and adiabatic flow stress show very good correlations with the experimental results (see Figs.1 and 2 for example). A combination of the above two models is used in modeling the thermo-mechanical response of different types of steel (e.g. AL-6XN stainless steel and DH-36 structural steel) which is a combination of bcc and fcc crystal components. The agreement between the experimental results and those obtained using the present model was found excellent (see Fig.3 for example). It's found that the contribution of the generation of the mobile dislocation density during the plastic deformation in the proposed model shows considerable effect on the prediction of the flow stress particularly in the case of high strain rates and temperatures. On the other hand, ignoring the mobile dislocation density rate from the present formulation causes additional hardening that overpredicts the experimental data. The parameter β_l plays an important task in determining the temperature and strain rate behavior of the proposed model during the plastic deformation since it contains the effects of dislocation densities as well as the dislocation distance which represents crucial aspects in controlling the scale effect of the internal deformation behavior. In the case of bcc metals, the physical quantities that define the proposed model parameters, are related to their initial values while, the thermal hardening behavior of fcc metals shows strong coupling between the plastic deformation and the effects of strain rates and temperatures, thus, the mobile dislocation densities are accumulated up to their saturated values as the plastic hardening evolves.

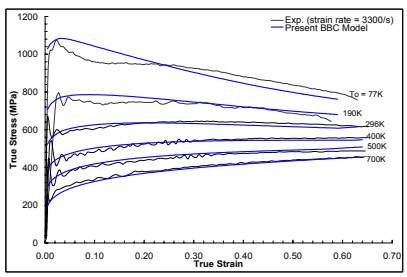

Figure 1 Adiabatic stress-strain curves for the proposed bcc model, for Niobium (Nb), and compared to the experimental results at 3300s^{-1} strain rate and for different initial temperatures.

$$\sigma = 1350(1-(0.00193T - 0.0000937T\ln\dot{\varepsilon}_p)^{2/3})^2 + 440\varepsilon_p^{0.25} + 60$$

$$T = T_o + 0.44\int \sigma d\varepsilon_p$$

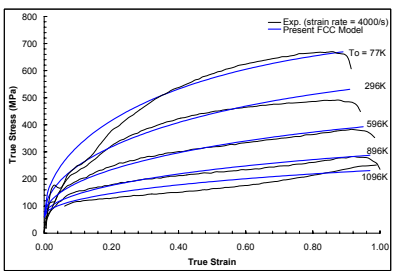

Figure 2 Adiabatic stress-strain curves, for the proposed fcc model, for OFHC Copper, and compared to the experimental results at 4000s^{-1} strain rate and for different initial temperatures.

$$\sigma = 950\varepsilon_p^{0.47}(1-(0.0006739T - 0.0000355T\ln\dot{\varepsilon}_p)^{2/3})^2 + 60$$

$$T = T_o + 0.262\int \sigma d\varepsilon_p$$

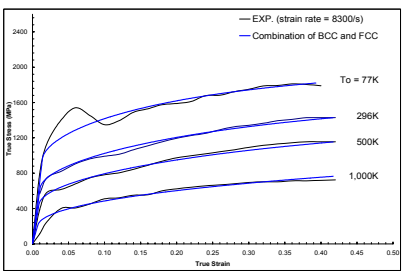

Figure 3 Adiabatic stress-strain curves, for the proposed models, for AL-6XN stainless steel, compared to the experimental results at 8300 s^{-1} strain rate and for different initial temperatures.

$$\sigma = 139 + 800\varepsilon_p^{0.45} + 1100\left(1-\left(0.00121T - 0.0000618T\ln\dot{\varepsilon}_p\right)^{2/3}\right)^2 + 2190\varepsilon_p^{0.71}\left(1-\left(0.00113T - 0.000051T\ln\dot{\varepsilon}_p\right)^{2/3}\right)^2$$

$$T = T_o + 0.252\int \sigma d\varepsilon_p$$

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