International Journal of Plasticity 27 (2011) 1384–1390

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

Chemically and mechanically driven creep due to generation and annihilation of vacancies with non-ideal sources and sinks

F.D. Fischer [a,*], J. Svoboda [b]

[a] Institute of Mechanics, Montanuniversität Leoben, Franz-Josef-Straße 18, A-8700 Leoben, Austria
[b] Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Žižkova 22, CZ-616 62 Brno, Czech Republic

ARTICLE INFO

Article history:
Received 9 September 2010
Received in final revised form 7 March 2011
Available online 2 April 2011

Keywords:
A. Creep
A. Stress relaxation
B. Crystal plasticity
B. Polycrystalline material
Thermodynamic extremal principle

ABSTRACT

The classical concept of Nabarro creep is extended for a general dislocation microstructure. The specific mechanism of the creep consists in generation and annihilation of vacancies at dislocation jogs acting as non-ideal sources and sinks for vacancies. This mechanism causes the climb of dislocations, allowing for local volume and shape change. The final kinetic equations, relating the dislocation microstructure and the local stress state to the creep rate, are derived by means of the thermodynamic extremal principle. Closed-form equations for the creep rate are derived for isotropic polycrystals. Based on the model the creep rate in the ferritic P-91 type steel at very low applied stress is evaluated and compared with experiment.

1. Introduction

As Sai has shown in a recent overview paper, Sai (2011), multi-mechanism models are now widely understood and open for future development. The mechanisms dealt with in his paper are mainly of mechanical type (dislocation slip and creep, hardening, damage, etc.). However, chemical mechanisms may interact with mechanical ones. Recent experimental works on the development of nanoparticles and their influence on creep behavior of intermetallics by Morris et al. (2008) and Muñoz-Morris et al. (2009) show instructive examples for the interaction of mechanics and chemistry. A related process is coarsening of precipitates like carbides via interstitial diffusion and its influence on creep as investigated by Morra et al. (2009).

According to classical text books, motion of dislocations contributes to plastic deformation by two mechanisms:

(i) Usually the dislocations can propagate easily in slip planes by motion of kinks along the dislocation line. As for the motion of kinks diffusion is not needed, slip of dislocations may occur at low temperatures.
(ii) In structural materials like steels a number of obstacles like precipitates exist in the slip plane, which prohibit slip of dislocations. Further motion of dislocations is then possible only by dislocation climb, during which jogs move along the dislocation line. The motion of the jog by one interatomic distance requires generating or annihilating one vacancy. As the vacancies must be transported to or from the jog by lattice diffusion, significant climb of dislocations may occur only at elevated or high temperatures.

Significant plastic deformations can be obtained under steady-state creep conditions, if the strain hardening is compensated by recovery enabled by dislocation climb. Many experimental studies clearly indicate that climb of dislocations is the

* Corresponding author. Tel.: +43 3842 402 4007; fax: +43 3842 46048.
E-mail address: mechanik@unileoben.ac.at (F.D. Fischer).

0749-6419/$ - see front matter © 2011 Elsevier Ltd. All rights reserved.
doi:10.1016/j.ijplas.2011.03.005

controlling mechanism of the steady state creep, and thus, the activation energy of creep corresponds to the activation energy of lattice diffusion mediated by vacancies. Most recently an explicit atomistic detailed study (Kabir et al., 2010) has appeared outlining the interaction of dislocation motion and vacancy diffusion during creep. Predominantly, the contribution of dislocation slip to the total creep deformation dominates the contribution of dislocation climb. Only in the case of an extremely large volume fraction of precipitates like in nickel-base superalloy single crystals, the contribution of slip and climb of dislocations to the creep deformation in steady state is practically the same, see e.g. Eggeler and Dlouhý (1997), Dlouhý and Eggeler (1997), and Svoboda and Lukáš (2000).

The current paper deals with the role of vacancies whose generation and annihilation are combined chemical and mechanical processes. The understanding of the role of vacancies on the deformation process of structural materials is of increasing relevance, see e.g. Svoboda et al. (2005a) or Fischer and Antretter (2009) and concerns specifically the role of creep as outlined above in detail.

The usual picture of creep is based on slip and climb of dislocations subjected to a mechanical driving force. Recent treatments (Svoboda et al., 2006; Svoboda and Fischer, 2009; Fischer and Svoboda, 2010), however, have shown that also the chemical driving force may significantly contribute to creep via generation and annihilation of vacancies at sources and sinks (note the prominent Kirkendall effect). Up to now it was accounted for isotropic swelling and shrinkage of representative volume elements being sensitive only to the value of hydrostatic stress σ_H.

The goal of the current model is now to show that vacancies, located at jogs of dislocations and acting as non-ideal sources and sinks for vacancies, are activated in a different amount by the local stress state and lead to a creep rate yielding both a volume change and a shape change. In the paper only the contribution of the generation/annihilation of vacancies at jogs on a fixed dislocation structure to the creep strain is taken into account. The amount of vacancies described by their site fraction is changed by their generation/annihilation and also by the flux of vacancies which balances the fluxes of the substitutional components situated in the lattice positions. In the case of chemically inhomogeneous alloys with multiple substitutional components, significant deviation of vacancy site fraction from its equilibrium value and also formation of significant internal stresses can occur due to diffusion. In pure materials, where no diffusion occurs, only the applied stress plays a role. The reader can take the kinetics of vacancies from Svoboda et al. (2006) and the recent paper Fischer and Svoboda (2010) demonstrating details how to calculate the distribution of vacancies.

2. Model

As a first step a scalar generalized chemical potential for vacancies is introduced; see the open literature or Svoboda et al. (2006) for a rigorous derivation:

$$\mu_0^* = \mu_0 - \sigma_H \Omega. \tag{1.1}$$

Ω is the volume corresponding to one mole of lattice positions taken to be equal to the partial molar volume of vacancies. μ_0 is the chemical potential of vacancies given by

$$\mu_0 = R_g T \ln(y_0/y_0^{eq}) \tag{1.2}$$

with R_g being the gas constant, T the absolute temperature, y_0 site fraction of vacancies and y_0^{eq} their equilibrium value in the stress free state. The role of strain energy is neglected in (1.1); for details see Svoboda et al. (2006), Section 3.1.

Local generation (annihilation) of vacancies is always coupled with the local inelastic swelling (shrinkage). In the case of generation/annihilation of vacancies at jogs on a dislocation line with the Burgers vector $\boldsymbol{b}$ the material swells/shrinks just only in the direction of $\boldsymbol{b}$. If the generation/annihilation of vacancies occurs at jogs on dislocations with randomly distributed Burgers vectors and the jogs are activated in an equal amount, then the swelling/shrinkage strain is addressed only to a hydrostatic component dependent on μ_0^* and no deviatoric components. Such an assumption has been used in the past and also in all our previous treatments. We develop now a concept introducing the sensitivity of sources and sinks for vacancies on the whole stress tensor with the goal to obtain a corresponding generalized creep strain rate tensor including both the hydrostatic component and also deviatoric components. We consider a representative volume element of unit volume subjected to a homogeneous stress state $\boldsymbol{\sigma} = \sigma_{ij}$ and having a homogeneous chemical composition and a homogeneous chemical potential of vacancies μ_0. For simplicity, any effects of segregation of some components at dislocations are neglected. Furthermore, let us assume that dislocations with different (normalized) Burgers vectors $\boldsymbol{b}^{(k)}$, $k = 1, \ldots, K$, exist in the representative volume element, and there are $H^{(k)}$ jogs corresponding to each k in the representative volume element,

$$\boldsymbol{b}^{(k)} = b_i^{(k)}, \quad i = 1,2,3, \quad \sum_{i=1}^{3} (b_i^{(k)})^2 = 1. \tag{2}$$

The motion of $H^{(k)}$ jogs along the dislocation line with normalized Burgers vectors causes the shrinkage or expansion just in the direction of the Burgers vector $\boldsymbol{b}^{(k)}$, and, thus, the generalized creep strain rate due to activity of $H^{(k)}$ jogs is given by

$$\dot{\boldsymbol{\varepsilon}}^{(k)} = \dot{\varepsilon}_{rs}^{(k)} = \alpha^{(k)} b_r^{(k)} b_s^{(k)}. \tag{3}$$

$\alpha^{(k)}$ is the kinetic parameter expressing the rate of moles of vacancies generated in the representative volume element at jogs corresponding to Burgers vector $\boldsymbol{b}^{(k)}$ related to the total number of moles of site positions in the representative volume