Available online at www.sciencedirect.com
ScienceDirect
Journal of the Mechanics and Physics of Solids 56 (2008) 1105–1125
JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS
www.elsevier.com/locate/jmps

Characterization of macroscopic tensile strength of polycrystalline metals with two-scale finite element analysis

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Received 22 March 2007; received in revised form 4 June 2007; accepted 6 June 2007

Abstract

The objective of this contribution is to develop an elastic–plastic–damage constitutive model for crystal grain and to incorporate it with two-scale finite element analyses based on mathematical homogenization method, in order to characterize the macroscopic tensile strength of polycrystalline metals. More specifically, the constitutive model for single crystal is obtained by combining hyperelasticity, a rate-independent single crystal plasticity and a continuum damage model. The evolution equations, stress update algorithm and consistent tangent are derived within the framework of standard elastoplasticity at finite strain. By employing two-scale finite element analysis, the ductile behaviour of polycrystalline metals and corresponding tensile strength are evaluated. The importance of finite element formulation is examined by comparing performance of several finite elements and their convergence behaviour is assessed with mesh refinement. Finally, the grain size effect on yield and tensile strength is analysed in order to illustrate the versatility of the proposed two-scale model.

Keywords: Multi-scale methods; Tensile strength and ductility; Crystal plasticity; Continuum damage model; Polycrystalline metals

1. Introduction

In this work, we propose an elastic–plastic–damage constitutive model for crystal grain and apply it to two-scale analysis method for characterization of the macroscopic stiffness degradation caused by microscopic damage.

For almost half a century, continuum damage mechanics has been used for description of the stiffness degradation of material. Since the pioneering work by Kachanov (1958) and Rabotnov (1963), a substantial number of publications have been devoted to the formulation of constitutive models to describe the internal degradation of solids within the framework of continuum mechanics. For example, Leckie and Hayhurst

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0022-5096/$ - see front matter
doi:10.1016/j.jmps.2007.06.001

(1974) have proposed their model for creep-rupture under multiaxial stresses. The anisotropic damage model for creep-damage is proposed by Chaboche (1978, 1981, 1984) and Murakami (1988). Within the theory of elastoplasticity, Gurson (1977) has proposed a void damage model for ductile damage. Micromechanically based damage model was derived by Krajcinovic and Fonseka (1981) for brittle material, which is characterized by planar penny-shaped microcracks. Later, the model was endowed with a thermodynamical structure and extended to account for ductile damage (Krajcinovic, 1983). Also, Lemaitre (1985a, b) has suggested a phenomenological damage model which is defined on the basis of the influence that internal degradation exerts on the macroscopic properties of the material for ductile damage in metallic material. In any continuum damage model, even micromechanical-based model, the internal variable for damage model represents some average of the microscopic defects which characterize the state of internal deterioration. Although it is well known that the metallic materials are mainly composed of polycrystalline aggregate, a detailed consideration of these microscopic heterogeneities in the description of the damaging process seems to be lacking.

A considerable number of studies have been conducted on multiscale modelling for polycrystalline metals. The modelling normally involves an averaging of microscopic heterogeneities and microscopic constitutive response within a representative volume element (RVE) to characterize the behaviour of the crystal grain. Taylor model (Taylor, 1938) and self-consistent model (Kröner, 1961; Hill, 1965) are well-known averaging methods for polycrystalline metals, in which the microscopic heterogeneity is characterized by crystallographic orientations with single crystal plasticity (Asaro, 1983). Two-scale modelling based on finite element discretization of the microstructure enables us to consider morphology of crystal grain and allows for the intergranular and intragranular behaviour of polycrystalline aggregate to be incorporated into numerical analysis (Miehe et al., 1999; Watanabe et al., 2005). The consideration of such microscopic heterogeneities results in complicated macroscopic behaviour, such as kinematical and anisotropic hardening, to be naturally depicted by these multiscale approaches with much simpler constitutive relations at the micro-scale (Iwakuma and Nemat-Nasser, 1983; Watanabe et al., 2005). Besides, two-scale finite element analysis allows not only the macroscopic behaviour to be estimated but also captures important information about the deformation state of the microstructure. One should note, however, that the accurate characterization of realistic material behaviour depends crucially on the accuracy of the constitutive models adopted at the microscopic level. To address this issue, a number of studies have recently been performed on innovative constitutive models based on detailed microscopic mechanisms such as moving dislocation field (Gao et al., 1999; Gurtin, 2002). In this context, a two-scale finite element methodology with an elastic–plastic–damage constitutive model for crystal grain enables us to characterize material failure at both micro- and macro-scale. Single crystal plasticity models coupled with a continuum damage model have been proposed in some publications (Qi and Bertram, 1999; Feng et al., 2002, 2004) but, to the authors' knowledge, it has not been reported in the context of two-scale analysis. We remark, though, that the constitutive model itself and the computational methodology for coupling plasticity with damage are still open to discussion.

In this paper, an elastic–plastic–damage constitutive model for single crystal is developed and incorporated into a two-scale finite element analysis framework to characterize both the deformation characteristics and the strength of polycrystalline metals. Numerical simulations are carried out in order to validate the response of the proposed model.

The paper is organized as follows:

First, in Section 2 we present two-scale boundary value problem (BVP) in the framework of mathematical homogenization method for nonlinear heterogeneous solids.

Section 3 addresses the microscopic constitutive equations. We propose an elastic–plastic–damage constitutive model by combining standard rate-independent finite strain single crystal plasticity equations and an energy-based continuum damage theory coupled to hyperelasticity. After describing the relevant kinematics associated with the multiplicative decomposition of the deformation gradient into elastic, plastic and damage parts, we derive the evolution equations of the corresponding internal variables within the framework of multi-surface plasticity. Due to the nature of the damage model adopted, the underlying damage evolution equation is cast in a very simple format as an extra unilateral constraint (a damage surface) added to the rate equations of plasticity. The associated state update algorithm is derived along with the corresponding consistent tangent moduli.