International Journal of Plasticity 27 (2011) 707–727

Contents lists available at ScienceDirect

International Journal of Plasticity

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

Modeling the viscoplastic micromechanical response of two-phase materials using Fast Fourier Transforms

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ARTICLE INFO

Article history:
Received 9 October 2009
Received in final revised form 31 August 2010
Available online 15 September 2010

Keywords:
Micromechanical modeling
Composite materials
Stress and strain-rate fields
Viscoplasticity
Microstructure–property relationship

ABSTRACT

A viscoplastic approach using the Fast Fourier Transform (FFT) method for obtaining local mechanical response is utilized to study microstructure–property relationships in composite materials. Specifically, three-dimensional, two-phase digital materials containing isotropically coarsened particles surrounded by a matrix phase, generated through a Kinetic Monte Carlo Potts model for Ostwald ripening, are used as instantiations in order to calculate the stress and strain-rate fields under uniaxial tension. The effects of the morphology of the matrix phase, the volume fraction and the contiguity of particles, and the polycrystallinity of matrix phase, on the stress and strain-rate fields under uniaxial tension are examined. It is found that the first moments of the stress and strain-rate fields have a different dependence on the particle volume fraction and the particle contiguity from their second moments. The average stresses and average strain-rates of both phases and of the overall composite have rather simple relationships with the particle volume fraction whereas their standard deviations vary strongly, especially when the particle volume fraction is high, and the contiguity of particles has a noticeable effect on the mechanical response. It is also found that the shape of stress distribution in the BCC hard particle phase evolves as the volume fraction of particles in the composite varies, such that it agrees with the stress field in the BCC polycrystal as the volume of particles approaches unity. Finally, it is observed that the stress and strain-rate fields in the microstructures with a polycrystalline matrix are less sensitive to changes in volume fraction and contiguity of particles.

1. Introduction

It is well known in Materials Science that the properties of materials are a function of their microstructural parameters. In studying microstructure–property relationships, it is crucial to map the microstructural parameters obtained from materials characterization to the desired materials property. Conventionally, materials characterization is based on data obtained from two-dimensional plane sections because of the opacity of most crystalline materials. However, many problems related to the properties of materials are three-dimensional in nature (Becker and Panchanadeeswaran, 1995; Lin et al., 1995; Patton et al., 1998; Shan and Gokhale, 2001; Suresh, 1998) because most materials of technological relevance have a polycrystalline or multi-phase structure with significant complexity in the spatial arrangement of their microstructural units. Even though stereology (Underwood, 1970) can be used to deduce the three-dimensional microstructure from conventional two-dimensional characterization, its statistical approach inevitably requires various spatial and morphological assumptions about the structural units. For example, even though the contiguity of particles can be easily measured in two-dimensional

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0749-6419/$ - see front matter
doi:10.1016/j.ijplas.2010.09.002