Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
International Journal of Solids and Structures 42 (2005) 971–1007
INTERNATIONAL JOURNAL OF SOLIDS and STRUCTURES
www.elsevier.com/locate/ijsolstr

A three-dimensional, higher-order, elasticity-based micromechanics model

Todd O. Williams *

Theoretical Division, T-3, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Received 1 April 2003; received in revised form 18 June 2004
Available online 3 September 2004

Abstract

The three-dimensional (3D) version of a new homogenization theory [A Two-Dimensional, Higher-Order, Elasticity-Based Micromechanics Model, in print] is presented. The 3D theory utilizes a higher-order, elasticity-based cell model (ECM) analysis for a periodic array of 3D unit cells. The unit cell is discretized into eight subregions or subcells. The displacement field within each subcell is approximated by a (truncated) eigenfunction expansion of up to fifth order. The governing equations are developed by satisfying the pointwise governing equations of geometrically linear continuum mechanics exactly up through the given order of the subcell displacement fields. The specified governing equations are valid for any type of constitutive model used to describe the behavior of the material in a subcell. The specialization of the theory to lower orders and to two-dimeinsions (2D) and to the exact one-dimensional (1D) theory is discussed.

Since the proposed 3D homogenization theory correctly reduces to both 2D and 1D the validation process applied to the 2D theory [A Two-Dimensional, Higher-Order, Elasticity-Based Micromechanics Model, in print] directly applies to the current formulation. Additional comparisons of the predicted responses obtained from the 3D ECM theory with existing published results are conducted. The good agreement obtained shows that the current theory represents a viable 3D homogenization tool. The improved agreement between the current theory results and published results as compared to the comparison of the MOC results and the published results is due to the correct incorporation of the coupling effects between the local fields. Additional results showing the convergence behavior of the average fields as a function of the order of the analysis is presented. These results show that the 1st order theory may not accurately predict the local averages but that consistent and converged behavior is obtained using the higher order ECM theories.

The proposed theory represents the necessary theoretical foundations for the development of exact homogenization solutions of generalized, three-dimensional microstructures.

* Tel.: +1 505 665 9190; fax: +1 505 665 5926.
E-mail address: oakhill@lanl.gov

0020-7683/$ - see front matter
doi:10.1016/j.ijsolstr.2004.06.056

Keywords: Micromechanics; Elasticity-based cell model (ECM); Particulate composites; Homogenization; Method of cells; Periodicity; Elasticity

1. Introduction

Most materials when viewed at the microstructural level, can be considered to have three-dimensional microstructures. Examples are polycrystalline metals, particulate composites, and high explosives. Three-dimensional (3D) homogenization based approaches are one method for modeling the effective behavior of such materials (Christensen, 1979; Aboudi, 1991; and Nemat-Nasser and Hori, 1993). Such models are capable of accounting directly for geometric effects within the microstructure, providing the concentration factors (Hill, 1963) that relate the local fields to the global fields, and predicting the material response under complex loading conditions. A particular homogenization approach which has proven highly successful is the 3D method of cells (MOC) analysis (Aboudi, 1991, 1996). One shortcoming of the 3D MOC theory is the lack of coupling between the local normal and shearing fields. This coupling between the different deformation phenomena is due to the presence of material property mismatches at the microstructural level as well as the geometric arrangement of the microstructure. The need for coupling the local fields is discussed more fully by Williams and Aboudi (1999).

Previous efforts, based more or less loosely on the original method of cells or generalized method of cells (GMC) analyzes (Paley and Aboudi, 1992), have been developed to address the need for coupled local effects in two-dimensional (2D) microstructures. The first effort by Williams and Aboudi (1999) carried out a weak solution analysis based on a general expansion for the displacement field within the subcells in a unit cell. A second theory was developed by Aboudi et al. (2001). This work also utilized a weak solution approach in conjunction with a partial, second order expansion for the displacement field in a subcell to analyze general microstructures. The above solution approaches are "weak" in the sense that both efforts apply a method of moments to the equilibrium equations approach in conjunction with integration by parts and the traction continuity equations to obtain the approximate governing equilibrium equations. Such an approach has been shown to be consistent with variational solution approaches, i.e. virtual work (Soldatos, 1995; Gilat, 1998) and thus the solution does not attempt to satisfy the pointwise governing equations. There are a number of considerations in the use of these approaches. In addition to the use of a weak formulation approach, the initial work by Williams and Aboudi (1999) introduced overly restrictive assumptions on the continuity behavior. The more recent weak solution approach pursued by Aboudi et al. (2001) has a number of differences from the original MOC/GMC type of analysis. First, while this approach has been formulated for complex microstructures it is not capable of analyzing the original microstructure associated with the MOC analysis due to the use of a second order expansion for the displacement field. Second, the approach is based on the use of the concepts of asymptotic homogenization (Bensoussan et al., 1978).

More recently, Williams (2004) has developed a elasticity based cell model (ECM) approach based on the use of eigenfunctions to describe the displacement field within a subcell which are part of a repeating unit cell. This work is based on a strong solution approach, i.e. on the solution of the pointwise governing equations of geometrically linear continuum mechanics as opposed to a variationally based solution approach. Consistent with the original MOC theory, this theory is based on the original microstructure proposed by Aboudi and provides all of the different concentration factors directly and simultaneously.

To date, no 3D analyzes equivalent to the above discussed 2D analyzes have been presented. The purpose of the current work is to extend the 2D analysis of Williams (2004) to three dimensions. In particular, the formulation for a new three-dimensional micromechanical theory utilizing an higher-order,