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Strongly-coupled Finite Element Method Approachto Multi-scale Modelingof Polycrystalline Solids

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ABSTRACT

A multi-scale (macro-micro) finite element framework for analysis of polycrystalline solids is suggested. The proposed frame work is strongly-coupled in a sense that the two scale calculation is performed at the same time. The issue of averaging micro-scale material stress and stiffness is addressed and a strategy is proposed. The proposed framework is implemented and applied to two examples having different geometries and loading modes. It is concluded that the proposed multi-scale framework can be used for more detailed and accurate analysis compared with the single-scale finite element analysis.

Keywords: *multi-scale modeling, polycrystalline solids, finite element, parallel computation.*

1. Introduction

This paper proposes a strategy for solving multi-scale problems of polycrystalline solids linking continuum (macro) and crystal (micro) scales. The method suggests a computational framework for transferring information between two scales at run time using a strongly coupled approach. Particularly, a solution strategy is investigated for a finite element (FE) representation of microstructure coupled with a FE representation of continuum scale mesh.

2. Macro- and micro-scale linking process

In a multi-scale analysis, how to transfer one information at a scale to another scale should be determined. Strong coupling of a point in a continuum and aggregate of single crystals requires two aspects; (a) how to transfer input loading at the macro-level to micro-level as a boundary condition (*localization process*), and (b) once the micro-scale calculation is performed, how to average responses of

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the aggregate of single crystals and feed them back to the macro-level (*homogenization process*).

Linking between macro-scale (continuum) and micro-scale (crystal) finite element calculations are briefly summarized here. In the formulation, crystallographic slip is assumed to be the only source of plastic deformation. Dislocation motion through the crystal lattice causes the slip, then the material can experience rotations and elastic strains. Only the proposed linking assumption is described here, and the detailed formulations for each length scale are described in Marin and Dawson (1998).

At each integration point of macro-scale finite element calculation, the following linking procedure is performed:

(1) *Localize.*

Set macro-scale velocity gradient at the integration point to micro-scale velocity gradient at boundaries for the micro-scale calculation.

(2) Initialize or restore database (velocity, coordinates, and state variables) for micro-scale calculation.

(3) Perform the micro-scale finite element calculation with the velocity gradient applied to boundaries of the micro-scale finite element mesh.

(4) Update and save the database from micro-scale calculation.

(5) *Homogenize.*

Return stress to integration point at the macro-scale using volume average of micro-scale stresses:

$$\bar{\sigma} = <\sigma> = \frac{1}{V}\int_B \sigma dv.$$

Determine macro-scale material stiffness at the integration point by averaging material (not structural) stiffness obtained from constitutive equation evaluation during the micro-scale finite element calculation and return to the integration point at the macro-scale.

The described computational methodology was implemented using Fortran 95 and Message Passing Interface (MPI) with the module-based programing technique. The module-based programing approach made the implementation of the complex idea possible in a relatively short amount of development time. Implementation of the FE-FE calculation, which has recursive nature, benefited significantly from the module-based programing available in Fortran 95. The macro-scale mesh is divided among processors, and the micro-scale simulation is performed on the local processor of the parent element.

3. Application

The dimension of the plate is 2×8×30 mm. The bottom of the plate is fixed, and positive velocity is applied to the top of the plate in z-direction (Figure 1(a)). Other surfaces of the plate are free. The plate is assumed to be composed of Fe/Cu (33/67%) alloy. The micro-scale finite element mesh used in the simulation is shown in Figure 1(b), which has 8 elements per grain. Material properties and modeling parameters shown in Table 1. The proposed multi-scale calculation (FE-FE) results are compared with the Taylor-FE calculation (Marin and Dawson, 1998) where Taylor-type computation is performed at micro-scale.

Macro-scale stress-strain response up to about 0.3% strain is shown in Figure 2(a). In the figure,

macroscale response of the FE-FE calculation is more flexible than that of the FE-Taylor calculation. The difference comes from explicit representation of the spatial distribution of the multiphase polycrystals at the micro-scale using finite elements. Around 150MPa, macro-scale stress-strain response from the FE-FE calculation deviates from the Taylor-FE calculation results, where the yielding of the weaker phase (Cu-phase) occurs. Transition from elastic behavior to yielding of stronger phase (Fe-phase) from the FE-FE calculation is smoother compared with that from the Taylor-FE calculation. These are attributed to the fact that the finite element analysis can capture local stress concentration from spacial phase morphology and crystal orientation distribution while the Taylor-type calculation can not.

The lattice strains in the loading and the transverse directions are shown in Figure 2(b) for the Fe-phase {111} crystals parallel to scattering vector [100] (E1 in Figure 1(a)). As in the macro-scale response, the FE micro-scale structure is more flexible, and has lower strength. Although not shown here, the FE calculation results have higher standard deviations than the Taylor-type calculation results. In fact, the standard deviation for the Taylor-type calculation is zero before yielding of crystals. Even from the brief presentation provided in this paper, it can be shown that the proposed multi-scale approach can be used to link two distinct scales more accurately compared with the Taylor-FE type approach. For detailed results and discussions, readers are referred to Han and Dawson (2006).

4. Summary

A multi-scale simulation strategy for polycrystalline solids is proposed. Linking hypothesis between the macro-scale and micro-scale (localization and homogenization) is suggested. The proposed strategy is implemented and the feasibility of the proposed model is verified with two examples. The FE-FE calculation results are compared with the FE calculation combined with the Taylor-type micro-scale calculation results. The comparison showed that there are differences between the two modeling approaches at the macro-scale and the micro-scale levels alike using the same modeling parameters, and the proposed method can be used for more detailed and accurate sub-grain analysis.

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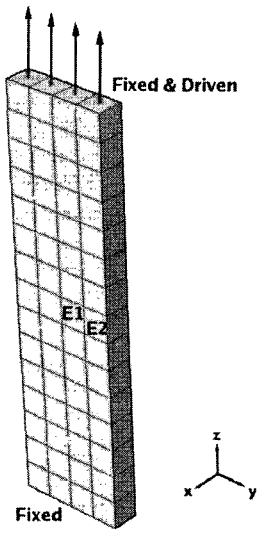
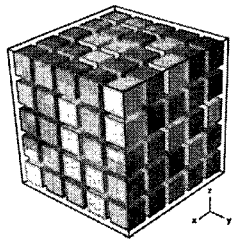
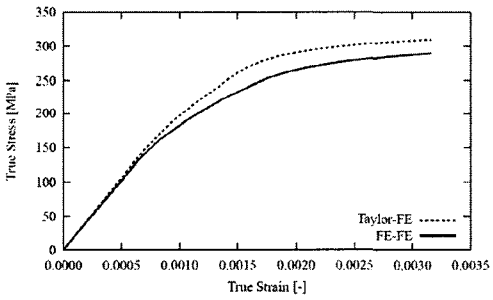


(a) Macro-scale mesh

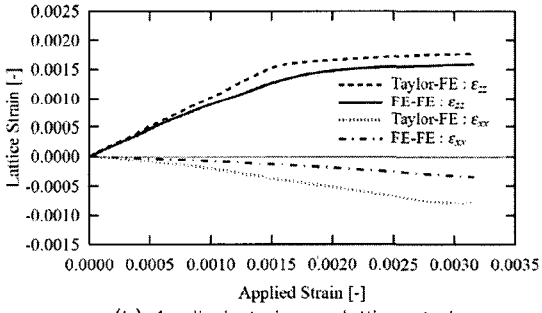


(b) Micro-scale mesh

Figure 1 Finite element meshes



(a) Macro-scale stress vs. strain



(b) Applied strain vs. lattice strain
(Fe-phase, c{211}//q[100])

Figure 2 Stress-strain responses (Note: Lattice strain result from E1 in Figure 1 is presented.)

Table 1 Slip system strain hardening parameters and elastic moduli
(Note: For notation, see Dawson and Mariin (1998))

Phase	Slip Parameters						Elastic Moduli [Gpa]		
	h_0[MPa]	g_0[MPa]	g_s[MPa]	$\dot{\gamma}_0[s^{-1}]$	m	n	c_{11}	c_{12}	c_{44}
Fe	300.0	180.0	225.0	1.0	0.02	1.0	168.4	121.4	75.2
Cu	250.0	50.0	130.0	1.0	0.02	1.0	228.0	132.0	111.5