Available online at www.sciencedirect.com
ScienceDirect
Computer-Aided Design 40 (2008) 293–310
COMPUTER-AIDED DESIGN
www.elsevier.com/locate/cad

CAD-based reconstruction of 3D polycrystalline alloy microstructures from FIB generated serial sections

S. Ghosh*, Y. Bhandari, M. Groeber

Mechanical Engineering, The Ohio State University, Columbus, OH-43210, USA

Received 6 October 2006; accepted 3 November 2007

Abstract

This paper develops a robust CAD-based methodology for simulating 3D microstructures of polycrystalline metals using crystallographic input data on sections created by a focused ion beam (FIB)–scanning electron microscopy (SEM) system. The method is able to construct consistent polycrystalline microstructures with control on the resolution necessary for meaningful computational analysis in microstructure-property estimation. The microstructure simulation methodology is based on a hierarchical geometrical representation using primitives used in CAD modeling. It involves steps of data cleanup, interface point identification, polynomial and NURBS function-based parametric surface segments construction, generalized cell decomposition, geometric defeaturing, and gap and overlap removal. The implementation of the entire procedure described above is performed with the aid of user-programming facilities of a commercial CAD package Unigraphics NX3. The microstructure simulation algorithm is validated using various error criteria and measures for an extracted microstructure of a nickel superalloy.

Keywords: FIB–SEM; 3D microstructure simulation; Parametric surface; NURBS; Gap-overlap removal

1. Introduction

Advanced metallic materials used in many industrial applications have complex multi-colony, multi-phase polycrystalline aggregates in their microstructure as shown in Fig. 1. The mechanical behavior and fatigue failure response are intricately governed by microstructural features that include morphological and crystallographic characteristics, e.g. shape, size and location of phases in the colony structure, relative colony size and locations, crystal orientations and misorientations, grain boundary geometry etc. Detailed micromechanical computational models are being used to understand deformation and damage mechanisms and throw light on the stochastic nature of failure and fatigue phenomena of these materials [1–10]. While, the computational models of polycrystalline materials implementing crystal plasticity models are making great strides in predicting the stress–strain behavior with reasonable accuracy, ductility and fatigue failure predictions with high fidelity are still far from mature. Morphological and crystallographic heterogeneities in the microstructures result in strong anisotropy and localized non-homogeneous deformation, which impose severe challenges to these computational models. Experimental studies [11] suggest that the growth of crystallographic microslip bands along active slip systems of plastic flow causes localized instability due to compatibility requirements between interacting grains. They continue to grow across grain boundaries due to grain structure instability and eventually manifest as macroscopic shear bands. The interaction of microscopic shear bands with transverse grain boundaries also leads to grain boundary microcracking, which grows in size and merge to cause fracture.

It is important for computational models to capture the 3D geometric and crystallographic details of grain morphology, as well as their distribution in the polycrystalline aggregate for robust prediction of their properties. An automated approach of characterizing 3D microstructure using a dual beam focused ion beam (FIB)–SEM system has been recently developed [26] to acquire 3D orientation data of a succession of sections in the material microstructure. Using a FIB column in the microscope, highly localized micromachining and ion imaging is conducted. Following this, high resolution electron back-scatter diffraction (EBSD) images are acquired by a SEM column for grain orientations. These experimental advancements have made

* Corresponding author. Tel.: +1 614 292 2599; fax: +1 614 292 3163.
E-mail address: ghosh.5@osu.edu (S. Ghosh).

0010-4485/$ - see front matter © 2007 Elsevier Ltd. All rights reserved.
doi:10.1016/j.cad.2007.11.003

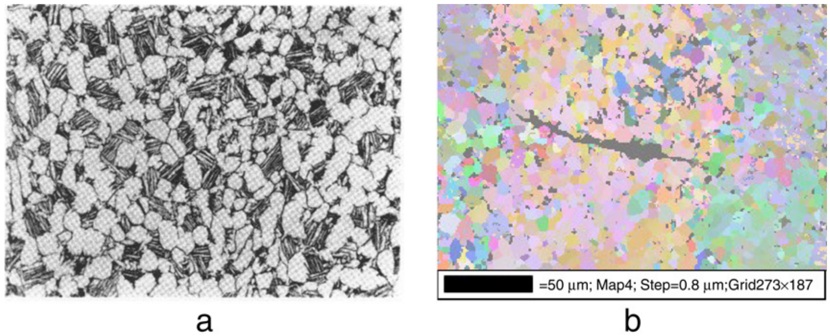

Fig. 1. (a) Optical micrograph α/β forged Ti-6242 alloy; (b) an orientation imaging microscopy image of the alloy showing a fatigue crack.

it possible to seamlessly reconstruct high fidelity 3D grain and subgrain microstructures of polycrystalline materials. The high fidelity 3D microregions can then be discretized and analyzed by computational methods like the finite element analysis methods for an accurate and reliable prediction of material properties. This paper develops a CAD-based method of creating 3D grain structures through post-processing of the FIB–SEM generated OIM data. A seamless reconstruction process will have certain characteristics and features that are summarized below.

- *Input/output data*: The input to the process is crystallographic orientation data of a metallic specimen in a 3D square grid. The output is a collection of solid bodies, with each body representing an individual grain. A requirement is that there be no overlap or gaps between them.
- *Data uncertainty*: Uncertainty corresponding to un-indexed points, incorrectly indexed points, misalignment, scatter marks etc. are to be expected in the experimentally acquired data, and has to be effectively dealt with.
- *Process automation*: The entire process from reading of the experimentally generated orientation maps to the creation of grain geometries in the aggregate should be automated, such that no, or minimum, additional user input is required.
- *Robustness*: The grain ensemble reconstruction procedure should be adequately robust to deal with different material microstructures, for which the sectional data is available. This requires identification of unstable operations and their removal.
- *Requirements for finite element mesh*: Typically crystal plasticity simulations of polycrystalline microstructures require prohibitively high computations, especially for models that represent microstructural details. It is therefore desirable to generate the microstructural details, keeping in mind both accuracy and efficiency considerations. Optimal representation with respect to the number of nodes and elements in the finite element mesh should be generated to retain both accuracy and efficiency of the eventual computational analysis.

This paper addresses the development of a seamless methodology for simulating polycrystalline metal microstructures from FIB–SEM generated serial sections using primitives used in CAD methods. A unique strength of this method is that it is entirely possible to monitor and control the resolution of the simulated microstructure for accuracy and efficiency needed for materials modeling. A commercial CAD package Unigraphics NX3 [31] (henceforth referred to as NX3) is used to perform all operations in the polycrystalline microstructure reconstruction. NX3 allows direct access to most of its geometric modeling and manipulation facilities through Open C API interface. A special module has been developed through this interface to reconstruct microstructure without any user intervention. Section 2 reviews some of the related work in this general area. Section 3.1 discusses steps for data collection and cleanup procedures, while Sections 3.2–3.4 describes the reconstruction process. Finally validation of this method with respect to microstructural characteristics is discussed in Section 4.

2. Brief review of microstructure reconstruction methods

Since polycrystalline deformation is predominantly 3D in nature, it is essential that the microstructural models be developed with detailed 3D information. Techniques based on ultrasonics or its variants, such as acoustic microscopy or laser ultrasonics [12,13] rely on good reflection properties and have limited application in metals. While X-ray-based computed tomography [14,15] methods are widely used in 3D solid model generation, they are generally deficient in achieving the resolution desired for the detailed study of polycrystalline metals. Synchrotron-based CT technology have been developed to yield tomographic images with considerably high resolution [16]. However, this method is still not commercially available and in generally is quite expensive. A few notable recent developments in microstructure representation are showing considerable promise. Of these, models that involve statistical extrapolations from 2D surface or section images [17], and the morphologically ‘precise’ models of 3D reconstruction from FIB–SEM generated serial-section data [18] are gaining considerable attention. The former approach [17] has the advantage of not relying on exhaustive (often destructive) experiments to obtain the crystallographic information. However, the reliability of these methods in reproducing important microstructural characteristics depends on the accuracy of the statistical interpolators and methods. This is a non-trivial task and can sometimes cause large errors if sufficient constraints are not developed in the statistical interpolation space. Reconstruction methods from 3D sections [18], on the other hand can be experimentally challenging and are generally destructive in nature.