Available online at www.sciencedirect.com
ScienceDirect
Acta Materialia 56 (2008) 5285–5292
Acta MATERIALIA
www.elsevier.com/locate/actamat

Delineation of the space of 2-point correlations in a composite material system

S.R. Niezgoda [a], D.T. Fullwood [b], S.R. Kalidindi [a,*]

[a] Department of Materials Science and Engineering, Drexel University, 32nd Chesnut Street, Philadelphia, PA 19104, USA
[b] Mechanical Engineering Department, Brigham Young University, Provo, UT 84602, USA

Received 4 March 2008; received in revised form 30 June 2008; accepted 1 July 2008
Available online 3 August 2008

Abstract

The complete set of 2-point correlations for a composite material system with a large number of local states (e.g. polycrystalline metals) forms a vast and unwieldy data set containing a large amount of redundant information. The interrelations in these correlations have been well characterized for composite material systems with two local states, but only a small number have been delineated for the composite systems with many local states. This paper presents an analysis of interrelations between the complete set of 2-point correlations for composite material systems through their spectral representations via discrete Fourier transforms. These interrelations are used to delineate a compact and convex space that bounds the set of all physically realizable 2-point correlations called the 2-point correlations hull. The representation of any given microstructure in this hull, and the techniques to produce a representative volume element are also explored in this paper.

Keywords: 2-Point correlation; Microstructure; Discrete Fourier transform; Pair correlation function; Statistics

1. Introduction

At its core, the field of materials science and engineering is concerned with understanding and modeling the relationships between a material's internal structure, its macro-scale properties and its processing history. Fundamental to establishing these relationships is the quantitative representation of the material's internal structure, which includes not only an identification of the constituent local states, but also their spatial placement. As interest is typically in the micro-scale features, the material's internal structure is referred to as the microstructure in this paper. However, the approach and the results presented here can be applied at any length scale.

It is not usually practical or even necessary, to quantify completely the microstructure of a large sample in its full spatial extent. The assumption of statistical homogeneity permits one to approximate the relevant statistics of interest in the sample as an average from an ensemble of subdomains extracted randomly from the sample. A rigorous framework defining the statistics of the microstructure is available in the literature in the form of n-point correlations or n-point statistics [1–5]. These correlations provide a hierarchy of statistical measures of the microstructure. The simplest of these are the 1-point correlations, $f(h)$, which essentially reflect the volume fractions of the various distinct constituents (denoted by h and also referred to as local states; the complete space of local states is referred to as the local state space H). These are termed 1-point statistics because they reflect the probability density associated with finding a specific local state of interest at a point selected randomly in the microstructure. Expanding on this basic concept, the 2-point correlations, $f(h, h' \mid \mathbf{r})$, capture the probability density associated with finding an ordered pair of specific local states at the head and tail of a randomly placed vector $\mathbf{r}$ into the microstructure. In a very similar manner, n-point statistics can be extracted

* Corresponding author.
E-mail address: skalidin@coe.drexel.edu (S.R. Kalidindi).

1359-6454/$34.00 © 2008 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
doi:10.1016/j.actamat.2008.07.005

from the microstructure through the placement of a complete set of n-vertex polyhedra.

This paper focuses on the 2-point correlation functions for composite material systems. Two-point correlations have been the focus of several investigations in current literature [6–10]. They capture the first-order information on the morphology of the microstructure. There is a tremendous leap in the amount of information contained in the 2-point correlations, when compared with the 1-point statistics. For most real microstructures, the 2-point correlations form a very large and unwieldy set of data. For example, in single-phase polycrystalline samples, the local state is defined by the lattice orientation g, which is often defined by a set of three angles called the Bunge–Euler angles [11]. Thus, for this relatively simple class of materials, the 2-point correlations need to be defined in a space consisting of nine independent variables. The continuous orientation and spatial spaces spanned by these variables are often discretized by binning. For example, a coarse discretization of the orientation space into 512 bins produces 262,144 2-point distributions, each of which is a function of the three-dimensional vector $\mathbf{r}$. Fortunately, this complete set of 2-point correlations has a large number of interdependencies, only some of which have been outlined by prior studies in this field [12–14]. This paper presents a rigorous treatment of the interdependencies among the complete set of 2-point correlations, leading to the establishment of a compact high-dimensional space wherein each point represents a complete set of 2-point statistics. This is accomplished largely through spectral representation of these correlations, and exploiting several of the known properties of discrete Fourier transforms (DFT). Although, every physically realizable microstructure[1] will have a representation in this high-dimensional space, it is not true that every point in this space will correspond to a physically realizable microstructure. The set of points in this space that correspond to all physically realizable 2-point correlations is referred to in this paper as the 2-point correlations hull. In other words, a point inside the 2-point correlation hull will correspond to one or more physically realizable microstructures, whereas points outside this hull will not correspond to any physically realizable microstructure.

In recent work [15–18], a novel mathematical framework called Microstructure Sensitive Design (MSD) was formulated for establishing invertible structure–property–processing linkages in materials. In a parallel effort, it was found to be quite efficient to quantify the microstructure using 2-point correlations [9,10,15]. Second-order structure–property linkages for elastic response of multi-phase and polycrystalline microstructures were successfully established. MSD aims to identify the complete set of microstructures that are theoretically predicted to exhibit a designer-specified combination of macro-scale properties or performance characteristics. A critical element of MSD is the delineation of the complete space of physically realizable microstructures, which for several of the problems being currently studied amounts to the delineation of the space of physically realizable correlations or the 2-point correlation hull mentioned earlier. This paper, using the established interdependencies among the 2-point correlations in a given microstructure, demonstrates the delineation of the 2-point correlation hull for a highly simplified class of one-dimensional microstructures. To the best of the authors' knowledge, this is the first report of the successful delineation of the 2-point correlation hull. Although the example selected for this demonstration deals with a grossly simplified microstructure, the underlying mathematical framework presented is quite general and easily extendable to a much broader class of material systems and microstructures.

The concepts presented in this paper also have significant implications for the notion of a representative volume element (RVE). In characterizing the microstructure of a material system, it is necessary to collect microstructure information from different samples produced with nominally the same processing history, and from different locations in each sample. The benefit of obtaining multiple microstructure data sets is that the averaged statistics from this ensemble of micrographs is expected to represent more accurately the overall microstructure statistics for the material system. It should be recognized, however, that it is not necessarily possible to produce a single instantiation of the RVE that exhibits the ensemble averaged 2-point correlations. With a simple example case study, it is demonstrated here that it is often impossible to identify a single RVE that reflects precisely the ensemble averaged 2-point correlations. Viable alternatives for constructing RVEs from an ensemble of microstructures are discussed in this paper.

2. Microstructure function, 2-point correlations and DFT

The application of DFT techniques to the rapid calculation of 2-point statistics has been discussed previously [19,20] and will be reviewed briefly here. Consider a microstructure data set extracted from a material sample. Let the spatial position in the microstructure be identified by the vector $\mathbf{x}$, and the local state of interest by h. One can define the microstructure function $m(\mathbf{x},h)$ as a distribution on the local state space for each spatial position as[2] [9].

[1] Physically realizable microstructures include all those that can be imagined (or digitally created). It is recognized that a very large fraction of these have not yet been realized by currently employed materials processing routes.

[2] In some prior work, M was used to denote the microstructure function. In this paper, the authors choose to follow the conventions used in the signal processing literature and use m for the microstructure function in real space and the M for the Fourier transform of the microstructure function. In addition, the Einstein summation convention for repeated indices is not used. For clarity, all summations will be explicitly indicated with Σ notation.