ELSEVIER

Materials Science and Engineering A 494 (2008) 68–72

MATERIALS SCIENCE & ENGINEERING A

www.elsevier.com/locate/msea

Gradient-based microstructure reconstructions from distributions using fast Fourier transforms

D.T. Fullwood*, S.R. Kalidindi, S.R. Niezgoda, A. Fast, N. Hampson

Materials Science and Engineering, Drexel University, Philadelphia 19104, USA

Received 8 March 2007; received in revised form 29 June 2007; accepted 15 October 2007

Abstract

Reconstructions are an important step in analyzing the statistics of local state distributions in the internal structure of heterogeneous material systems and in estimating their effective properties using deterministic models. In this paper, we demonstrate the use of fast Fourier transforms (FFTs) and gradient-based algorithms for the reconstruction of microstructure realizations from 2-point statistics. The FFT method greatly improves the computational efficiency of the algorithm, facilitating use of the full set of 2-point statistics in the reconstruction. This approach introduces periodic boundary conditions naturally into the model. The reconstruction of several two-phase 2D structures is demonstrated, resulting in exact replicas of the original microstructures. The limitations of the technique, especially for more complex structures, are also discussed.

Keywords: Microstructure; Reconstruction; FFT; Gradient

1. Introduction

Microstructure information for materials is often available only in a statistical sense rather than an absolute, or deterministic, sense. Structure metrics such as grain size, particle size, composition, etc., generally represent average values, and implicitly indicate that a distribution of values is present in any real sample. A common method of interrogating such information is to reconstruct realizations of the material from statistical information of the structure. Such reconstructions can also be input into deterministic simulation codes (e.g. finite element models [1–6]) to predict the macroscale effective properties or performance characteristics under a broad range of complex loading conditions.

The statistical information itself may be stored and manipulated in various ways. One common approach involves a hierarchy of correlation functions, usually referred to as the n-point statistics [7–11]. A particular advantage of this formalism is that these distributions are ideally suited to evaluating macroscale properties of heterogeneous materials using well-established generalized composite theories [7,12–16]. While these theories are formally exact, they are often expressed as series solutions with each term comprising several highly complicated convolution integrals. Consequently, these theories have not found broad usage. However, with the advances in computational power, and the application of spectral techniques [15,16] it is likely that these theories will find wider application in determining structure-property relations of composite materials in the future.

The most common correlation function used in quantifying the microstructure is the 1-point function, which is essentially equivalent to quantifying the volume fractions of the distinct local states present in the microstructure. The local state at any point in the microstructure, h, may be defined in terms of a set of variables that can be locally defined (for example this includes phase identification, composition, and/or the lattice orientation). The space of all feasible distinct local states is called the local state space, and is denoted by H in this paper, i.e. $h \in H$. The 1-point distribution, $f(h)$, reflects the probability of a randomly placed point in the microstructure being associated with the local state h:

$$P(a \leq h \leq b) = \int_a^b f(h)\,\mathrm{d}h \tag{1}$$

Higher order correlation functions may be defined in a variety of ways [7–11]. The n-point correlation function is defined here to reflect the probability of an n-vertex polygon, randomly placed

* Corresponding author. Tel.: +1 215 895 1216; fax: +1 215 895 6760.
E-mail address: dtf25@drexel.edu (D.T. Fullwood).

0921-5093/$ – see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.msea.2007.10.087

in the material, landing with each vertex being associated with a specified local state. This is more a statement of the general idea behind the functions rather than a strictly correct definition. We will define 2-point correlation functions more rigorously below.

In this work, our focus is on the 2-point correlation function, which contains information regarding the relative separation of specified local states in the material. Since the 1-point function contains no information regarding the morphology of the microstructure, the increase in the amount of information when moving from 1-point to 2-point is quite substantial. Furthermore, recent advances in orientation imaging microscopy (OIM) and related techniques now enable ready determination of the 2-point statistics without undue effort [10].

One of the main issues with using the higher order correlation functions is that an enormous effort is involved in calculating and manipulating them, due to the sheer size of the computations involved. In this work we first consider fast methods of calculating 2-point correlation functions using fast Fourier transforms (FFTs). Certainly these are already in regular use for the 2-point case in various environments [17]. We briefly review the approach in order to highlight the boundary condition issues inherent to FFTs. We subsequently use the FFTs as the basis for the reconstruction of microstructure realizations from 2-point functions. Various approaches to this problem have been presented in the literature [14,18–20] (and references therein). We explore a gradient-based method and demonstrate a framework for constructing realizations using this technique. However, it is clearly the case that other methods would also benefit from much of the efficiency we introduce by using the FTTs.

2. Correlation functions and FFTs

We first introduce the microstructure function, as previously defined in Refs. [16,21]. This will form the basis for the definition of correlation functions. Consider a material RVE with position vector, $\mathbf{x}$, and a single local state variable, h. Then the microstructure function $M(\mathbf{x}, h)$ is a distribution function on the local state space for each point in the RVE:

$$\int_a^b M(\mathbf{x}, h)\,\mathrm{d}h = P(a \le h(\mathbf{x}) \le b) \tag{2}$$

This is sometimes written in the alternative manner involving the infinitesimal neighborhood, V, of the point $\mathbf{x}$:

$$M(\mathbf{x}, h)\,\mathrm{d}h = \frac{\mathrm{d}V_h}{V} = f(h)|_{\mathbf{x}}\,\mathrm{d}h \tag{3}$$

where $\mathrm{d}V_h$ represents the volume of material in volume element V that is in a state that lies between h and $h+\mathrm{d}h$.

The motivation for this definition stems from the fact that material information is generally derived from data gathered in a neighborhood rather than a single point. This is obvious for a local state such as orientation, which is in fact defined in terms of relative positions of atoms in a neighborhood; but it is also true that instruments gather information from an area or volume determined by their resolution rather than from a single point. Hence a distribution function rather than a well-defined state seems to be appropriate for a given 'point'. The distribution results in a continuous definition of local state rather than the usual discrete description; this view fits better with certain analytical models, such as those required for the gradient-based search algorithms described in this paper. This definition also leads to a concise definition for the 2-point correlation function in the RVE, Ω:

$$f_2(h, h'|\mathbf{r}) = \frac{1}{\mathrm{Vol}(\Omega)} \int_\Omega M(\mathbf{x}, h) M(\mathbf{x}+\mathbf{r}, h')\,\mathrm{d}\mathbf{x} \tag{4}$$

It will be noted immediately that the term on the right hand side of this equation is a convolution of the two functions $M(\mathbf{x}, h)$ and $M(\mathbf{x}, h')$. Thus we may use the usual convolution theorem of Fourier analysis to determine the function f_2. For two functions, f and g, with Fourier transforms, F and G, the Fourier transform of the convolution is equal to the point-wise product of the Fourier transforms:

$$(f \cdot g)(\mathbf{r}) = \int_{\Re^n} f(\mathbf{x}) g(\mathbf{r}-\mathbf{x})\,\mathrm{d}\mathbf{x} = \Im^{-1}(F(k).G(k)) \tag{5}$$

where $\Im^{-1}$ indicates the inverse Fourier transform. We will look at this in more detail below, but first we wish to move to a discrete formulation of the problem for application of the numerical analysis tools used below. The discrete version of the convolution theorem actually allows us to use Fast Fourier Transforms (FFTs), which is the main focus of this effort.

We wish to discretize the function $M(\mathbf{x}, h)$ in the real space, $\Re^n$. The state space, H, is also generally discretized, but this is not necessary to accomplish our current goal. Thus, let us suppose that the real space is discretized into a regular grid, with vertices enumerated by $s = 1{:}S$. We will write $M_s^h = M(\mathbf{x}_s, h)$. The coefficients M_s^h are thus related to the terms D_s^n introduced in a previous paper for the purpose of expanding M in terms of the primitive basis [16,21]. In the previous work an algebraic link was found between the 'discrete' versions of the 2-point correlation function (F'^{nn}_t) and the 'discrete' version of M (D_s^n):

$$F_t^{nn'} = H_{ss't} D_s^n D_{s'}^{n'} \tag{6}$$

This fundamental relationship between the functions enabled inverse design of microstructure as embodied in the terms D_s^n. However, the form of Eq. (6) is very inefficient for calculations, and in part motivates the current move to a framework based upon FFTs.

The relationship between 2-point correlation functions and FFTs is well known, and well used for autocorrelations [17]. We briefly review the fundamental relations as a basis for the discussion on boundary conditions.

3. Discrete 2-point correlation function

Let S be the number of points in the finite lattice that covers the RVE. We will momentarily assume that the RVE is a one-dimensional (1D) space for ease of index notation, but it will be obvious how to generalize to higher dimensions. Using the discrete version of the microstructure function, and recognizing that the vectors $\mathbf{r}$ will also take discrete values, enumerated by

t, Eq. (4) becomes:

$$f_2(h, h'|\mathbf{r}_t) = \frac{1}{S}\sum_{s=0}^{S-1} M_s^h M_{s+t}^{h'} \tag{7}$$

where $\mathbf{r}_t$ take values on a lattice of the same spacing as $\mathbf{x}_s$. Take the discrete FT of both sides:

$$\begin{aligned}\Im[f_2(h, h'|\mathbf{r}_t)] &= \frac{1}{S}\sum_{t=0}^{S-1}\sum_{s=0}^{S-1} M_s^h M_{s+t}^{h'} \mathrm{e}^{-2\pi i t k/S} \\ &= \frac{1}{S}\sum_{s=0}^{S-1} M_s^h \sum_{t=0}^{S-1} M_{s+t}^{h'} \mathrm{e}^{-2\pi i t k/S}\end{aligned} \tag{8}$$

Now let $s+t=z$. Then

$$\begin{aligned}\Im[f_2(h, h'|\mathbf{r}_t)] &= \frac{1}{S}\sum_{s=0}^{S-1} M_s^h \sum_{z=s}^{S-1+s} M_z^{h'} \mathrm{e}^{-2\pi i (z-s) k/S} \\ &= \frac{1}{S}\sum_{s=0}^{S-1} M_s^h \mathrm{e}^{-2\pi i (-s) k/N} \sum_{z=s}^{S-1+s} M_z^{h'} \mathrm{e}^{-2\pi i z k/S}\end{aligned} \tag{9}$$

Now let us assume periodicity (cyclicity), i.e. in a single dimension we have $M_z^{h'} = M_{z+S}^{h'}$. Since $\mathrm{e}^{-2\pi i z k/s}$ is also cyclic with the same period, we may re-number the second summation to obtain:

$$\begin{aligned}\Im[f_2(h, h'|\mathbf{r}_t)] &= \frac{1}{S}\sum_{s=0}^{S-1} M_s^h \mathrm{e}^{2\pi i s k/S} \sum_{z=0}^{S-1} M_z^{h'} \mathrm{e}^{-2\pi i z k/S} \\ &= \bar{\aleph}_k^h \aleph_k^{h'}\end{aligned} \tag{10}$$

where $\aleph_k^h = \Im(M_s^h)$ and $\bar{\aleph}_s^h$ is the complex conjugate of $\aleph_s^h$ (since M is real valued, thus $\bar{M}_s^h = M_s^h$). Hence finally we have:

$$f_2(h, h'|\mathbf{r}_t) = \Im^{-1}\left[\bar{\aleph}_k^h \aleph_k^{h'}\right] \tag{11}$$

The result is that in practice we may efficiently obtain the 2-point correlation function using pointwise multiplication of the FFTs of the microstructure function, and an inverse FFT. This is dramatically more efficient than Eq. (6).

4. Boundary conditions

As indicated above (Eq. (10)), using FFTs to calculate correlation functions implicitly assumes periodic boundary conditions. A different boundary condition may be applied by using padding (see, for example [22] for a discussion of padding). Continuing with a 1D example, assume a discrete domain of S points where $\mathbf{x}$ takes the values from 0 to $S-1$. One commonly used definition of the 2-point correlation function that does not involve periodic boundary conditions is given by [21]:

$$f_2(h, h'|\mathbf{r}) = N_{\Omega|\mathbf{r}} \int_{\Omega|\mathbf{r}} M(\mathbf{x}, h) M(\mathbf{x}+\mathbf{r}, h')\, \mathrm{d}\mathbf{x} \tag{12}$$

where $\Omega|\mathbf{r} = \{\mathbf{x} \in \Omega | \mathbf{x}+\mathbf{r} \in \Omega\}$. In the continuous case the normalization factor is given by $N_{\Omega|\mathbf{r}} = 1/V_{\Omega|\mathbf{r}}$. In the discrete 1D case of S points, the normalization factor is given by 1/(number of points sampled); i.e. $N_{\Omega|\mathbf{r}} = 1/(S-t)$ where t takes the integer values from 0 to $S-1$. If we pad our discrete 1D example with $S-1$ zeros then the resultant calculation for f_2 effectively calculates the integral in Eq. (12) without the normalization factor; hence the FFT results must be normalized by $1/(S-t)$. Note that one issue with these boundary conditions is that the values of $f_2(h, h'|\mathbf{r})$ for larger value of $|\mathbf{r}|$ are sampled with significantly less frequency than those for smaller values of $|\mathbf{r}|$; nevertheless, they are given equal importance. For example, in the discrete 1D case, the vector between the first and last point on the domain is only sampled once. To deal with this issue, it may be assumed (for example) that values of $|\mathbf{r}|$ above 1/2 the size of the domain should be ignored, as being insufficiently sampled to be statistically meaningful (the value of 1/2 is an arbitrary value that may be chosen more carefully depending upon the level of statistical confidence required). If this same approach is taken in the case of the unpadded FFT, it will also reduce the effect from the assumed periodicity, since the smaller $\mathbf{r}$-vectors will cross the boundary of the domain for a smaller proportion of the S sample points.

Another approach, if our sample size is not large enough to comfortably ignore the larger $\mathbf{r}$-vectors, is to artificially increase the sample size using a collage of the original RVE created from random translations. This effectively increases the size of the sample with a layer of material having the same statistics as the original sample, but not in a periodic manner. The approach will, of course, not be valid if the assumption of homogeneity cannot be invoked. Such an approach will be investigated in future work.

5. Gradient-based reconstruction methods

Reconstruction approaches from 2-point statistics involve the minimization of an error function defined on the trial microstructure. As mentioned above, in practice both the real and state spaces are discretized, leading to an error function:

$$E(M) = \sum_{h_i, h_j \in H} \sum_{\mathbf{r}_t \in R(\Omega)} \left\{ f_2^M(h_i, h_j|\mathbf{r}_k) - f_2^I(h_i, h_j|\mathbf{r}_t) \right\}^2 \tag{13}$$

where M indicates the trial microstructure, and I indicates the original microstructure that we are trying to reconstruct. The inner sum may be calculated rapidly since the FFT approach provides the values of f_2 for all values of $\mathbf{r}$ simultaneously. This makes it efficient to calculate error between trial and original microstructure in terms of the full 2-point correlation function. Previous methods have chosen subsets of the 2-point function (for example using only values of $\mathbf{r}$ in the direction of the axis vectors [14]) in order to reduce the computational burden. In fact, further efficiencies may be achieved by calculating the error in Fourier space, thus removing the requirement for the inverse transform in Eq. (11). However, some weighting may be needed to balance the size of the contributions from different frequencies in Fourier space. The predominant contribution is generally from the zero frequency term. Using the notation in Eq. (11):

$$E_f(M) = \sum_{h_i, h_j \in H} \sum_k \omega_k \left\{ \bar{\aleph}(M)_k^h \aleph(M)_k^{h'} - \bar{\aleph}(I)_k^h \aleph(I)_k^{h'} \right\}^2 \tag{14}$$

where ω_k is a weighting term.

Since we are now assuming discretization of both real and state spaces let us normalize the parameters M_s^n that define the microstructure, M.

$$\sum_{n=1}^{N} M_s^n = 1, \quad 0 \leq M_s^n \leq 1 \tag{15}$$

for each s. Then the optimization routine involves minimization of the error function (Eq. (13) or (14)), subject to the constraint Eq. (15). It should also be noted at this point, that in most previous work (e.g. [14,20]), the coefficients M_s^n are assumed to only take the values 0 or 1. Thus at each spatial point, s, the material occupies a single state given by the unique non-zero M_s^n.

A popular technique to solve this optimization problem involves simulated annealing [14]. One of the advantages of this technique is that it is designed for problems with many local optima. Gradient-based methods, on the other hand, are notoriously poor at finding global optima in such problems [23]. Nevertheless, in cases where the gradient methods are applicable, they will generally converge faster than other techniques. For the examples given below, we apply a sequential quadratic programming (SQP) routine as contained in Ref. [24].

6. Results and discussion

A checkerboard-type test case was used to demonstrate the results of the methodology. In this case the sample size is 32×32, with square white phase 1 'grains' in a matrix of black phase 2. For a two-phase structure the full 2-point correlation function is uniquely determined by the autocorrelation function of either of the phases. Thus only the autocorrelation function of phase 1 is required to define the error. The starting microstructure was assumed to be random ($M_s^n = 0.5$ for all s, n). Convergence took approximately 7 h, and accurately reproduced the original microstructure up to a translation (Fig. 1; note that without the FFT approach the convergence was taking several days. All calculations were performed on a standard PC with a single 3 MHz processor).

A more varied microstructure was generated and reconstructed using the same approach. The original and final microstructures are shown in Fig. 2. Again, the reconstructed structure appears to be an exact replica of the original, except for a translation. The time taken for the reconstruction was similar to that for the previous example.

In summary, calculation of the 2-point correlation functions using FFTs greatly improves the efficiency of reconstruction algorithms, and facilitates use of the full 2-point correlation in the description of error. The FFT approach introduces periodic boundary conditions that the user must be aware of, although such conditions are commonly used anyway. A gradient-based optimization routine has been successfully used for the reconstructions, and appears to perform at least as well as some other methods reported in the literature, although direct comparison of computational effort is difficult due to the lack of accurate data. The authors implemented simulated annealing [14] (without full optimization of the method suggested in the reference)

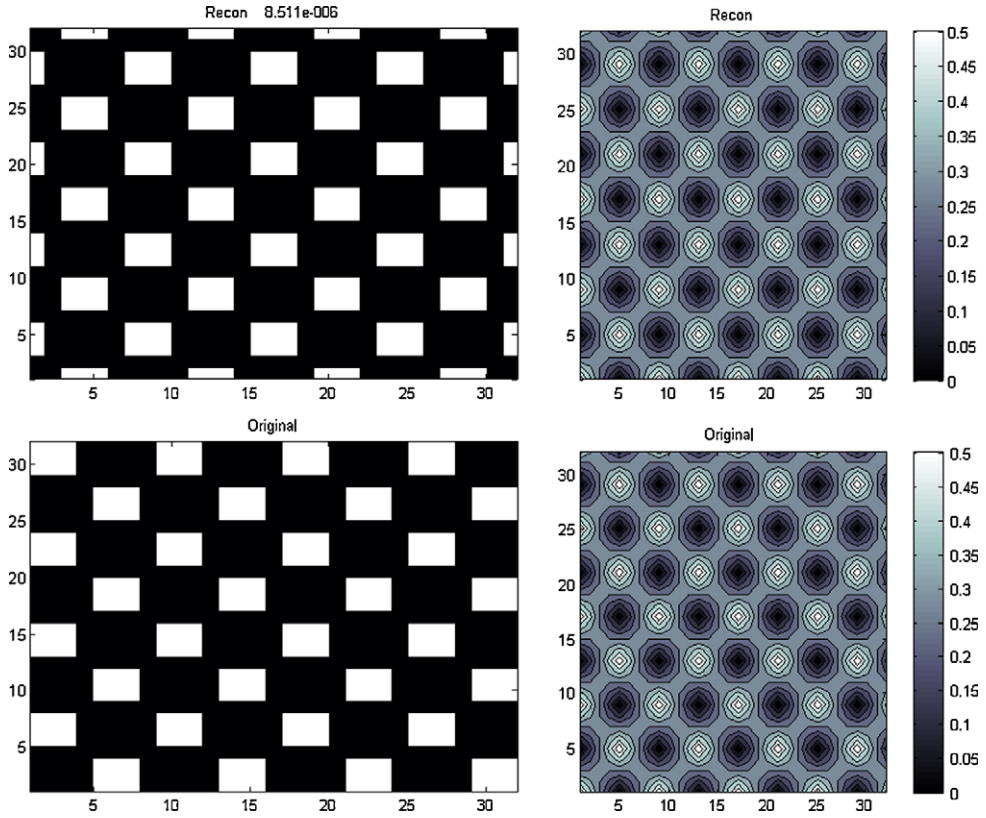

Fig. 1. Clockwise from bottom left: original two-phase microstructure, autocorrelation function for the white phase, autocorrelation function for the reconstructed structure, and actual reconstructed microstructure.

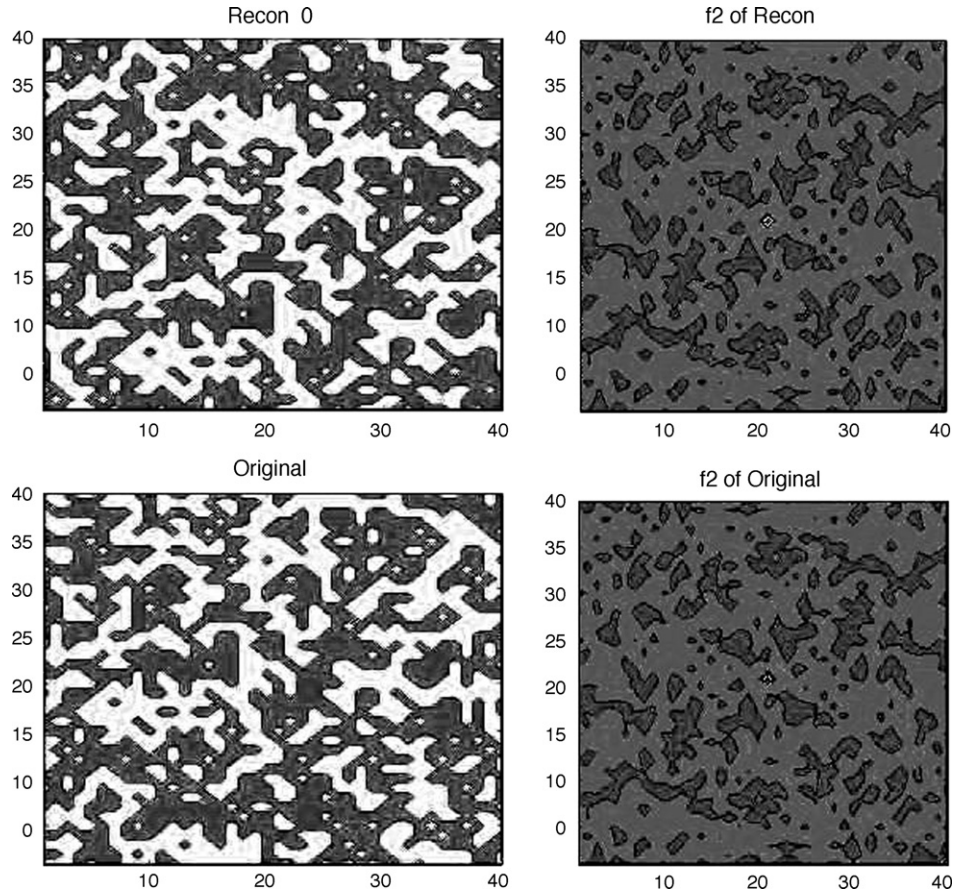

Fig. 2. Anti-clockwise from bottom left: original two-phase microstructure, autocorrelation function for the white phase, autocorrelation function for the reconstructed structure, and actual reconstructed microstructure.

and branch and bound algorithms [25] with comparable computational effort to the gradient method. However, some attempts at three-dimensional reconstructions using the same method, and not reported in this paper, were highly dependent upon the chosen initial microstructure, demonstrating the effects of local minima. Similarly attempts at reconstructing structures with a higher number of phases had more issues with local optima. These issues will be studied further and reported in a later paper.

Acknowledgments

The authors acknowledge financial support for this work from the DARPA-ONR Dynamic 3D Digital Structure project, Award No. N000140510504 (Program Manager: Dr. Julie Christodoulou).

References

[1] A.P. Roberts, E.J. Garboczi, J. Mech. Phys. Solids 47 (1999) 2029–2055.
[2] L.O.E. Santos, P.C. Philippi, M.C. Damiani, C.P. Fernandes, J. Petrol. Sci. Eng. 35 (2002) 109–124.
[3] B. Biswal, R. Hilfer, Physica A 266 (1999) 307–311.
[4] P.-E. Øren, S. Bakke, J. Petrol. Sci. Eng. 39 (2003) 177–199.
[5] I.F. Vasconcelos, I. Cantat, J.A. Glazier, J. Comput. Phys. 192 (2003) 1–20.
[6] Z. Liang, M.A. Ioannidis, I. Chatzis, Chem. Eng. Sci. 55 (2000) 5247–5262.
[7] E. Kröner, in: J. Gittus, J. Zarka (Eds.), Modeling Small Deformation in Polycrystals, Elsevier, 1986.
[8] P.I. Etingof, D.D. Sam, B.L. Adams, Phil. Mag. A 72 (1995) 199.
[9] N. Sheehan, S. Torquato, J. Appl. Phys. 18 (2001) 53–60.
[10] X. Gao, C.P. Przybyla, B.L. Adams, Metall. Mater. Trans. A 37 (2006) 2379–2387.
[11] T.A. Mason, B.L. Adams, Metall. Mater. Trans. A 30 (1999) 969–979.
[12] M.J. Beran, T.A. Mason, B.L. Adams, T. Olsen, J. Mech. Phys. Solids 44 (1996) 1543–1563.
[13] G.W. Milton, The Theory of Composites, Cambridge University Press, Cambridge, 2002.
[14] S. Torquato, Random Heterogeneous Materials, Springer–Verlag, New York, 2002.
[15] S.R. Kalidindi, M. Binci, D. Fullwood, B.L. Adams, Acta Mater. 54 (2006) 3117–3126.
[16] D.T. Fullwood, B.L. Adams, S.R. Kalidindi, Comput. Mater. Sci. 38 (2007) 788–799.
[17] B. Rust, D. Donnelly, Comput. Sci. Eng. 7 (2005) 74–78.
[18] B. Bochenek, R. Pyrz, Comput. Mater. Sci. 31 (2004) 93–112.
[19] C.L.Y. Yeong, S. Torquato, Phys. Rev. E 58 (1998) 224–233.
[20] V. Sundararaghavan, N. Zabaras, Comput. Mater. Sci. 32 (2005) 223–239.
[21] B.L. Adams, X. Gao, S.R. Kalidindi, Acta Mater. 53 (2005) 3563–3577.
[22] J.S. Walker, Fast Fourier Transform, CRC Press, Boca Raton, FL, 1996.
[23] J.A. Snyman, Practical Mathematical Optimization: An Introduction to Basic Optimization Theory and Classical and New Gradient-Based Algorithms, Springer, New York, 2005.
[24] Matlab, In: The Mathworks Inc., 2006.
[25] B.L. Hansen, B.L. Adams, M.E. Lyon, A.J. Henrie, J. Comp. Aided Mater. Des. 10 (2003) 163–173.