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An efficient algorithm for spatially-correlated random fields generation and its applications on the two-phase material

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ABSTRACT

The properties of material strongly depend on the microstructure, and the development of microstructure is closely related to the phase transition with the temperature-dependent spatial correlation. To consider more realistic microstructures, we have proposed an efficient and simple algorithm for generating the spatially-correlated random field, which is obtained by the weighted average of random fields without spatial correlation according to the spatially-correlated length and anisotropy parameter. By using a mesoscale finite element model with the microstructures generated by our algorithm, an application study on the effective elastic behavior of Al_2O_3–NiAl composite materials is given. Our numerical results are in agreement with the experimental measurements. The proposed method is general and robust, which can be extended to the multi-phase materials.

1. Introduction

It has been a challenge to determine the microstructure of a solid, since the final microstructure depends sensitively on the cooling rate and the depth of quench, which is dictated by dynamics and not by energetics alone [1–3]. However, the feature of material, such as dielectric response [2] and magnetic properties [3], strongly depends on its microstructure. For elastically inhomogeneous alloys, the phase diagram of temperature and composition was numerically obtained, in which the effect of elastic inhomogeneity on the phase transition behavior was also discussed [4]. Recently, dense Al_2O_3–NiAl composites containing 0–100% NiAl were prepared by sintering, with no chemical reactions and negligible mutual solubility between the two materials [5,6]. The elastic and shear moduli obtained experimentally fall within the Voigt–Reuss bounds and close to the lower bound of the Hashin–Shtrikman (H–S) model, while Poisson's ratio of the composites shows strong dependence on their microstructure characteristics.

In general, the elastic properties of two-phase materials can be obtained through solving the relevant governing equations by various numeric algorithms, such as the traditional finite-difference scheme [7] or the popular finite-element technique [8,9]. Employing the lattice Boltzmann method [10], the elastic properties of multiphase composites of complex geometries can be determined by numerically solving the stress–strain relationships in heterogeneous materials, where the random microstructures of the multiphase composites were reproduced by the random generation-growth method [11]. Considering the microstructures of materials, the spatial correlation should be taken into account. For example, the fiber networks exhibited long-range power-law spatial correlations of the density and elastic properties, which can be modeled by the stochastic finite element method [12,13]. In concrete and rock material, different tests of varied ingredients or mixture ratios presented different failure patterns and a large scatter in the softening branch of load–displacement response, which may be due to a great variety of the internal correlation length for these artificial materials [14].

The spatial correlation can be easily calculated when the microstructures are determined. However, the microstructures are not unique for a given spatial correlation and the generation of spatially correlated random field is a typically inverse problem. Till now, several iterative methods have been proposed to generate spatially correlated random field, reflecting the realistic microstructures of the multi-phase materials. Besides the Fast Fourier Transform Method by Yaglom [15] and the Turning Bands Method by Matheron [16], Fenton and Vanmarcke [17] presented the Local Average Subdivision Method for the generation of spatially-correlated random field, which was ideally suited to finite element models. In addition, Fang et al. [18] used a multilevel grid strategy,

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which combined the matrix decomposition method and the screening sequential simulation method. However, all these methods require too much complicated operations for practical applications.

Compared to iterative methods, spatially correlated random field can be generated through stochastic optimizing algorithms [19–21], such as the simulated annealing and genetic algorithm. For given spatial correlations, Yeong and Torquato [19] defined the objective function from a squares error between the candidate ones and the objective one, obtaining the required microstructure by searching the least error via the simulated annealing. Similarly, Matouš et al. [20] constructed a fitness function according to the one- and two-point probability functions and minimized the fitness function, using genetic algorithms combined with simulated annealing. In addition, a stochastic Wang tiling-based technique could be applied to reconstruct the microstructures with given spatial statistics, which utilized a finite set of tiles assembled and accurately reproduced long-range orientation orders with high efficiency [21].

In this paper, we propose a simple and practical algorithm to generate the spatially correlated random field, describing the microstructures with the spatial correlated length and the anisotropy parameter. Starting from a series of random number without spatial correlation, we generate new series with the linear composition of origin series, according to the spatial correlation length and the coefficients which are determined by the calculations of spatially-correlated functions. By using mesoscale finite element models with more realistic microstructures generated by our algorithm, the effective elastic behavior of two-phase material is taken as an application study. Our numerical results of Al_2O_3–NiAl are in agreement with the experimental measurements. The proposed method is general and robust, which can be extended and applied in the multi-phase materials.

2. Methods

The main idea of our algorithm is to generate spatially-correlated random fields from those without spatial correlation, by the weighted average according to the spatially-correlated length and anisotropy parameter. As is known, Ising model has been considered as the typical model to demonstrate the phase evolution, in which the spatial correlation is temperature-dependent following the exponential decay. For simplicity, our method focused on the microstructures with the exponential decaying correlation function. We would investigate the cases with other types of spatial correlations in future work.

For the two-phase material, we firstly consider a one-dimensional random series without spatial correlation $a_i = \pm 1$, $i=1, 2, \ldots, n$, where 1 and -1 indicate the two components. Thus, we have

$$\langle a_i a_{i+d}\rangle = \frac{1}{n}\sum_{i=1}^{n} a_i a_{i+d} = \begin{cases} 1, & d=0 \\ 0, & d\neq 0 \end{cases} \tag{1}$$

where d is the distance between a_{i+d} and a_i. With the linear composition of a_i and certain parameters c_i, we construct a new series b_i ($i=1, 2, \ldots, n$):

$$b_i = c_0 a_i + \sum_{k=1}^{n} c_k a_k r^{d(k)} \tag{2}$$

where $d(k)$ is the *effective* distance between a_i and a_k, and $r=\exp(-(1/L))$, in which L denotes the spatial correlation length. Applying the periodical boundary condition, we have $a_{i+n}=a_i$. Note that using a linear transformation of the vector of independent random variables is a general technique to produce random variables with a specified covariance matrix, such as the Cholesky decomposition [22].

For the isotropic material, $d(k)$ is the absolute value of $(k-i)$ in the one dimensional case. The correlation of b_i can be calculated as:

$$\langle b_i b_{i+k}\rangle = \frac{1}{n}\sum_{i=1}^{n} b_i b_{i+k} = \begin{cases} c_0^2 + O(r), & k=0 \\ \sum_{j=0}^{k} (c_j c_{k-j}) r^k + O(r^{k+1}), & k\neq 0 \end{cases} \tag{3}$$

where $O(r)$ and $O(r^{k+1})$ are the ignored terms of higher order than r and r^{k+1}, respectively. Thus, we should have $c_0^2=1$ and $\sum_{j=0}^{k}(c_j c_{k-j})=1$, which confirm

$$\langle b_i b_i\rangle : \langle b_i b_{i+1}\rangle : \langle b_i b_{i+2}\rangle \ldots \langle b_i b_{i+k}\rangle \ldots = 1 : r : r^2 : \ldots : r^k. \tag{4}$$

We set c_0 to be 1 and thus c_1 should be 0.5, since $c_0 c_1 + c_1 c_0 = 1$. With $c_0=1$ and $c_1=0.5$, we can obtain c_2 from $c_0 c_2 + c_1 c_1 + c_2 c_0 = 1$. Similarly, the c_i of larger indices can be obtained. As shown in the inset of Fig. 1(a), the parameters c_i decrease as the index i increases. Note that we use the truncation to simplify the calculation of c_i, which would also induce the discrepancies compared to analytical functions. However, the strict deduction of c_i is much more complicated.

In the construction of spatial-correlated random field, there are two factors to be determined: the parameter c_i and the *effective* distance of d. Similar to one dimensional case, we construct the new series b_{ij} for two dimensional cases to maintain the spatial

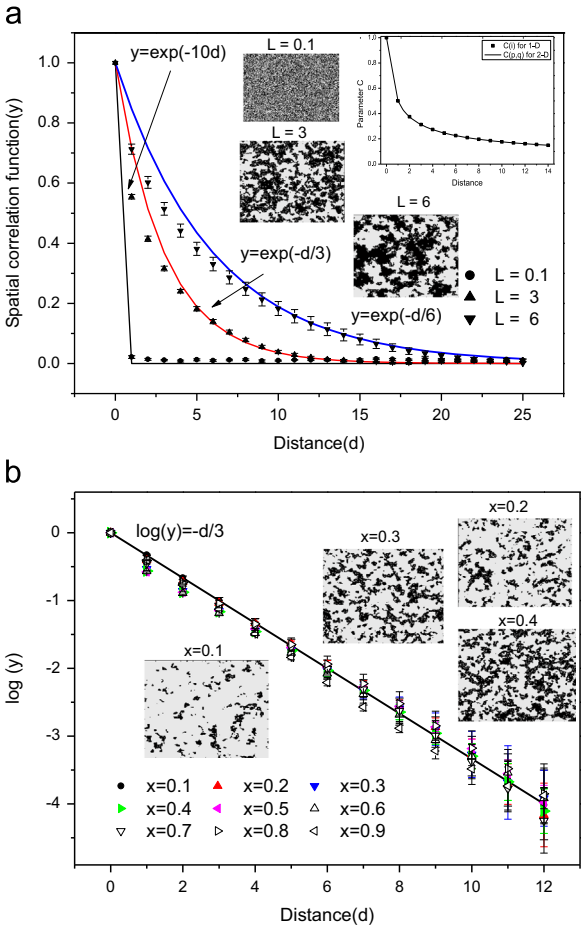

Fig. 1. (Color online) The spatial correlation functions and microstructures obtained by the algorithm for two-dimensional case with various spatial correlation lengths (L) and composition (x): (a) $x=0.5$, $L=0.1$, 3, and 6; (b) $L=0.3$, $x=0.1$–0.9. The results of analytical calculations are plot in solid lines for comparison, with typical microstructures shown in the inset. The parameters c_i and $c_{d(p,q)}$ are shown in the inset of (a).