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An evolutional approach to the numerical construction of polycrystalline structures using the Voronoi tessellation

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ABSTRACT

We developed a method to numerically construct a polycrystalline structure with a specified grain-size distribution by utilizing the genetic algorithm, which is suitable for global optimization of complex parametric space, and the Voronoi tessellation. The computational merits of our new method compared with the conventional optimization method are: (a) it is able to escape more easily from local minima of the penalty function; and (b) it is suitable for parallel processing. The method efficiently creates input data for numerical simulations of microstructural evolution such as recrystallization, grain growth, deformation, and fracture.

1. Introduction

Solid materials in a polycrystalline state or polycrystals consist of many independent grains, and their mechanical properties are closely related to the microstructure, e.g. grain size and misorientation between grains [1]. Thus the computational modeling of polycrystalline materials, such as for grain growth, recrystallization, deformation, and fracture, plays an important role in material science and engineering [2–4]. The results obtained by these numerical methods are often dependent on an initial polycrystalline structure that is an input data set for these models. To numerically reproduce a polycrystal we often resort to the Voronoi tessellation constructed from a random distribution of points, e.g. [5]. Such a tessellation provides a numerical representation of polycrystals with the Poisson–Voronoi grain-size distribution, but real polycrystals often exhibit a log-normal grain-size distribution. In fact, input data with this characteristic is used by some authors to obtain more realistic results, e.g. [6]. Generally speaking, we do not know how much difference of the initial size-distribution influences on the numerical results obtained by various models. One difficulty when conducting such a study is that there is no explicit method for numerically creating a polycrystalline structure with a specified grain-size distribution, including the log-normal distribution.

To overcome this problem, we must resort to an inductive method, which is in practical terms equivalent to applying a numerical optimization method using iterative calculation. Gross and Li [7] use such a technique and succeed in producing a desired grain-size distribution by applying the inverse Monte Carlo method. Xu and Li [8] also use this method to analyze the topological difference between a polycrystal with the Poisson–Voronoi size-distribution, and one with the log-normal size-distribution. However, this optimization is not an easy numerical task because the penalty function has many local minima, and it takes an extremely long time to reach the desired size-distribution, because countless attempts are necessary to escape from such minima. This disadvantage impedes the availability of this method as a handy tool. The problem becomes more serious when an application requires polycrystals composed of a large number of grains.

We proposed a different approach using the genetic algorithm [9,10]. The idea of the genetic algorithm is inspired by Darwinian natural selection: Numerous attempts with different inputs performed simultaneously, and those with excellent performance are allowed to survive while the rest are abandoned. The surviving in-

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puts breed, slightly mutate, and become the next set of attempts. Repetition of this procedure allows the most suitable inputs to prosper and evolve, and leads to an input that satisfies a desired condition. The genetic algorithm is so flexible that it can be applied to many optimization problems related to spatial pattern formation, e.g. [11], and its application to materials science is also becoming popular [12]. In the following we present a successful application of the genetic algorithm to the problem of constructing polycrystalline structures. Refs. [7,8] give a thorough overview of the academic issues and practicalities involved in constructing required polycrystals, but these also lacks sufficient description of computational efficiency, which is extremely important for practical use. This Letter therefore concentrates on quantitative analyses of the computational efficiency of the method.

2. Numerical method

The Voronoi tessellation, commonly used for producing polycrystalline structures, assigns the same number of points to the space as the desired number of grains, and the space is subsequently divided into many polyhedra based on these points. Hereafter we call these points the center points. The simplest use of this method is to choose the center points in a purely random manner. In this case, however, the grain-size distribution $P(d)$, where d is the grain size, always exhibits the Poisson–Voronoi distribution [7]. To obtain a polycrystalline structure with the desired grain-size distribution, it is necessary to somehow rearrange the locations of the center points. A numerical method is required to solve this problem because such a method is not given in an explicit way.

A numerical optimization method introduced by Gross and Li [7] makes this rearrangement of the center points using the inverse Monte Carlo method: They define a penalty function W^2 that is the square of the distance between the desired grain-size distribution and that given by the Voronoi tessellation as:

$$W^2 = \frac{1}{N}\sum_{i=1}^{N}\left[P_r(d_i) - P(d_i)\right]^2, \tag{1}$$

where N is the number of discretized values of the grain size; d_i the discretized value of the grain size; and $P_r(d_i)$ the desired grain-size distribution. Their algorithm of optimization involves the following steps: (a) Take a set of the center points randomly; (b) Construct the Voronoi tessellation using these center points and compute the size-distribution $P(d)$ and the penalty function W^2; (c) Move a center point randomly and recalculate W^2; (d) If W^2 is smaller, keep the move; If W^2 is larger, keep the move only if $e^{-W/\alpha} < \rho$ is satisfied where ρ is a random number in the range of $(0, 1]$ and α is a small number, otherwise abandon the move; (e) Go to step (c). The iteration of this algorithm continues until the penalty function becomes less than a certain criterion. Although they report that the method is successful, there is a technical concern with this method: The searching process is likely to be frequently trapped by local minima of the penalty function. The larger α is the greater the possibility of escaping from the traps is, but the risk of losing good candidates also increase, thus the optimum value of α is difficult to determine. This algorithm can also make only one new attempt per step while the searching space is tremendously large and complex. This poses a serious disadvantage especially when creating a polycrystal composed of a large number of grains.

Our new method, which uses the Voronoi tessellation in a similar fashion to the method of Gross and Li, introduces a genetic algorithm instead of the inverse Monte Carlo method. In our genetic algorithm, we treat these center points as a set of genes, a polycrystalline structure produced by the set of the center points as an individual, and a ensemble of polycrystals as the population (shown in Fig. 1).

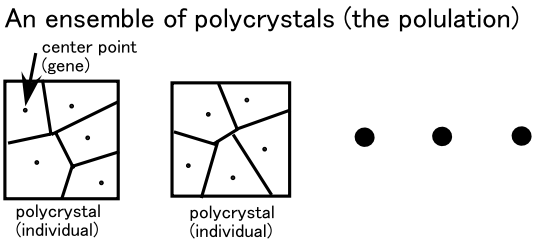

Fig. 1. The basic concept of the application of the genetic algorithm to constructing polycrystalline structures: The words in the parentheses are the corresponding roles in the genetic algorithm.

To begin the genetic algorithm, an initial set of individuals, i.e. an ensemble of initial different polycrystals must be ready. Each initial individual, a polycrystal with a certain configuration of grains, is constructed by selecting the center points in a purely random manner; i.e. all initial individuals are an assembly of different polycrystals with the Poisson–Voronoi size-distribution and ready to be the first generation of the algorithm. To obtain the second generation, the fitness function F of each individual of the first generation must be calculated. The fitness function is a measure that indicates how exactly the grains made by the Voronoi tessellation, arrange themselves in the desired grain-size distribution. We define this as the inverse of the penalty function, such as $F = 1/W^2$. Individuals in the second generation are randomly selected from those of the first generation, but the probability of being selected is proportional to the fitness function. A newly selected polycrystal must go through a mutation of randomizing genes or shifting randomly center points; a center point to mutate is randomly selected, and the selection probability is proportional to the grain volume the center point belongs to. The mutation occurs at a constant rate at each center point selected, with some new individuals experiencing many mutations while others experience none. We consider two types of mutations: a new center point is selected completely randomly; and it randomly shifts a short distance. The first type of mutation plays an important role in accelerating global optimization because it efficiently allows the searching process to escape from local minima of the penalty function. The second type of mutation is useful for fine adjustments in the evolutional process. Each time a mutation is requested, one of the two types of mutation is selected with the same probability. The mixing of two individuals, called the gene crossover, was not used, because it did not improve computational efficiency. Consequently each infant of the new generation is produced from a single mutated parent without gene input from another parent. Fitness gradually increases as the population evolves or higher generations are created by repeating this procedure. The iteration continues until one individual satisfies a certain criterion.

In this genetic algorithm, we also adopted the elitism strategy; a few of the fittest individuals, that is the elites, are kept without mutation thus avoiding the accidental loss of the best individuals, which can occur in the inverse Monte Carlo method.

A new computer program was developed specifically for evaluating the above method. In the program, we define the cubic lattice space with lattice points that have an integer state indicating the grain each point belongs to. The integer value of each lattice point is determined by the closest center point for the Voronoi tessellation. Grain size is given by the cubic root of the total number of lattice points inside the grain. The most time-consuming part of the program is the computation of the Voronoi tessellation, i.e. determining of the integer state of all lattice points. Fortunately a parallel processing technique can be applied, and we can create