Article

Chinese Science Bulletin

Materials Science

October 2013 Vol.58 No.30: 3704–3708
doi: 10.1007/s11434-013-5900-5

# Neighborhood topological effect on grain topology-size relationship in three-dimensional polycrystalline microstructures

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Received December 27, 2012; accepted April 1, 2013; published online May 27, 2013

A new grain topology-size relationship in three-dimensional (3D) polycrystalline microstructures has recently been established by considering the effects of non-random first nearest neighbor grains. In this contribution, a generalized form for this relationship is presented by considering the interactions of $k$th ($k$=1, 2, 3…) nearest neighbor grains, and large scale Monte Carlo-Potts model simulation is used to investigate the general neighborhood topological effect on the topology-size relationship. The results show that, unlike their first nearest neighbors ($k$=1), the topological correlations of 3D grains with their $k$th layers ($k\geqslant 2$) of nearest-neighbors may have trivial effect on the topology-size relationship.

**polycrystalline microstructures, grain size, grain topology, neighbors, topological correlations**

**Citation:** Asad U, Liu G Q, Wang H, et al. Neighborhood topological effect on grain topology-size relationship in three-dimensional polycrystalline microstructures. Chin Sci Bull, 2013, 58: 3704–3708, doi: 10.1007/s11434-013-5900-5

Many macroscopic properties such as mechanical, thermal, magnetic and conductive properties of the material can be directly linked to microstructure; therefore, it is very important to predict the grain microstructure and its evolution [1–4]. The size and the shape of grains and their spatial correlation are likely to play a significant role in the microstructural evolution. Therefore, the grain topology-size relationship is of fundamental importance for a better understanding of polycrystalline materials. In 1985, by applying the methods of statistical mechanics to the structure of random, space-filling cellular structures, Rivier [5] revealed that the maximum entropy inference under a few constraints yields structural equations of state, relating the topology of cells to their size. These equations of state are namely Perimeter law (for metallurgical grains) and Lewis's law (for ideal soap froths). According to Perimeter law, the average radius of grains is proportional to the number of their edges. While, in three dimensions (3D), a parabolic relationship exists between the grain size and grain topology. DeHoff and Liu [6] have proposed a linear relationship between the number of grain faces and the mean tangent diameter of individual grains in 3D. Thereafter, Abbruzzese and Compopiano [7] and Thorvaldsen [8] proposed two independent forms of quadratic relationships between the number of grain faces and the sphere-equivalent radius of grains in 3D. The DeHoff-Liu's linear model has been verified experimentally by Liu et al. [9] and strongly recommended it when the mean tangent diameter is used for grain size. Meanwhile, Abbruzzese-Compopiano's quadratic model [7] also agrees well with the experimental results of Liu et al. [9] when the sphere equivalent radius is used for grain size instead of mean tangent diameter. The Abbruzzese-Compopiano's [7] and Thorvaldsen's [8] quadratic models are also consistent with the experimental results of $\beta$-titanium

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alloy [10] and aluminum alloy [11] as well as the results of surface evolver simulation [12]. These studies considered a mean field approach in describing topology-size relationships while neglected the effects of the neighboring grains.

As neighborhood of grains define their topology [13,14] and the interactions of grain neighbors play a vital role within the grain networks, grains should not be considered to exist in a mean field. The nonrandom nearest neighbor correlations in 3D grain structures have been studied both experimentally [10,15] and by simulations [12,16]. Recent studies strongly suggested the importance of considering the effects of first nearest-neighbor grains when studying grain growth [10,16] and also predicting the grain topology-size relationships. More recently, Luan et al. [17] introduced a new grain topology-size equation in three dimensions by considering the interactions of first nearest neighbor grains, which states that the topologically averaged relative grain size $R_f/\langle R\rangle$ depends on the difference between the number of faces of a grain ($f$) and the mean face number of its nearest neighbors ($m_1$), that is

$$R_f/\langle R\rangle = \alpha(f - m_1) + C, \tag{1}$$

where $R_f$ is the sphere equivalent radius (grain size) of $f$-faced grains, $\langle R\rangle$ is the average grain size in 3D system, and $\alpha$ and $C$ are constants.

However, eq. (1) is only concerned about the interactions of first nearest neighbor grains (short range topological correlations). For a more precise and unbiased estimation of grain size or topology it would be better to consider the interactions of other neighboring grains (long range topological correlations) as well. In order to consider the effects of $k$th ($k$=2, 3…) neighbor grains along with first neighbors, a generalized form for eq. (1) is required. In this article, a generalized form for grain topology-size relationship (eq. (1)) is presented by considering the interactions of $k$th ($k$=1, 2, 3…) nearest neighbor grains, and large scale Monte Carlo-Potts model simulation is used to investigate the correlations between grains and their different types of neighbors for an ultimate object of studying the general neighborhood topological effect on the topology-size relationship of 3D grains.

## 1 Methods and parameters

To investigate the long range topological correlations of grains, a definition of second, third and even $k$th nearest neighbor grains is desired. As for as we are aware of, there exist different opinions about the definition of second and third nearest neighbors of grains (or bubbles, cells). Some define them as, the grains which can be connected with the central grain by a single edge are second nearest neighbors and the third nearest neighbors are those which require two edges to connect [18–20], while others define them as in closed concentric layers of grains around the central grain and Some neighbor grains were defined as defects [21,22]. In a previous paper [23], the authors introduced a new definition of second, third or $k$th nearest neighbors to investigate the topological correlations of 3D grains, which is more suitable to study the interactions of $k$th ($k$=2, 3…) nearest neighbors as compared to other definitions because this definition covers the largest number of nearest neighbors in each layer, which is more suitable to study the contribution of all nearest neighbors. In what follows, we adopt the same definition.

A grain structure divides space into $N$ individual grains. The neighborhoods of a grain can be thought of as in closed concentric layers of grains around it (shell structure). The $k$th layer of a given grain is the set of its $k$th nearest neighbors. It is well understood that the grains which are adjacent to a given grain are its first nearest neighbors. For $k$>1, the $k$th nearest neighbors are those adjacent to ($k$–1)th layer, but do not belong to ($k$-2)th layer (0 layer means the given grain itself). For the sake of simplicity, we illustrated this definition here in two dimensions (2D) by using a micrograph of pure iron, Figure 1 shows the first, second and third nearest neighbors (colored orange, green and red respectively) of a grain colored purple in concentric layers of grains around it. In 3D, the definition of $k$th nearest neighbors is exactly the same as in 2D. We consider there are $c_k$ neighboring grains in $k$th layer and $F_k$ is their total number of faces, so the average number of faces of $k$th neighbor grains will be

$$m_k = F_k/c_k\,. \tag{2}$$

We define $L_{1-n}$ as the mean face number for all neighbor grains in (1–$n$)th layers, i.e.

$$L_{1-n} = \frac{\sum_{k=1}^{n} F_k}{\sum_{k=1}^{n} c_k} = \frac{1}{P_n}\sum_{k=1}^{n} c_k m_k \tag{3}$$

where $P_n$ is the total number of grains in (1–$n$)th layers, which equals the summation of $c_k$ ($k$=1–$n$). For example, for first nearest neighbors ($n$=1), $L_{1-1}=m_1$; for both first and second nearest neighbors ($n$=2), $L_{1-2}=(c_1m_1+c_2m_2)/P_2$; and similarly for first, second and third nearest neighbors ($n$=3), $L_{1-3}=(c_1m_1+c_2m_2+c_3m_3)/P_3$ and so on. Thus, with the help of eq. (3), we can suggest a generalized form for the grain topology-size relationship to consider the effect of both the long and short range topological correlations of grains,

$$R_f/\langle R\rangle = \alpha\left(f - L_{1-n}\right) + C. \tag{4}$$

Here for $n$=1, we get $L_{1-1}=m_1$, which is the mean face number of first nearest neighbor grains i.e. for $n$=1, eq. (4) takes the form of eq. (1), the proposed grain topology-size equation in [17]; which can serve as a special case of this general grain topology-size equation (eq. (4)).

Now, to investigate the effects of $k$th nearest neighbors

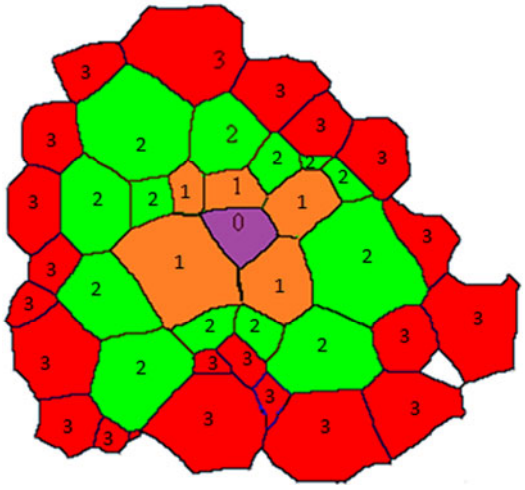

**Figure 1** Representation of neighbors as concentric layers around a central grain (0) colored purple.

on the central grain (here we take the average number of faces of neighbors to describe the neighboring effects), we use large scale Monte Carlo-Potts model simulation as described in earlier works [24,25]. A continuum microstructure is mapped onto a cubic lattice with full periodic boundary conditions and with $N$ (400×400×400) sites. Each site in the lattice is assigned an index $S_i$(1–$N$) sequentially, corresponding to the orientation of the grain that it belongs to. Sites with the same index are considered to be part of the same grain and grain boundary only exists between neighbors with different orientations. The simulation temperature is 0.5, and complete details of simulation are described in ref. [24]. Large number of grains are sampled in steady-state grain-growth structures at different simulation time. The grain volume $V$ is determined by counting the lattice sites with the same index. The grain size $R$ is defined as the sphere-equivalent radius, $R=(3V/4\pi)^{1/3}$. Here, the normalized sphere equivalent radius $R/\langle R\rangle$ is used to represent the grain size. The number of faces $f$ for a grain is obtained by counting the grains which are adjacent to it. The average number of faces of each grain's first, second and third nearest neighbors ($l_1$, $l_2$, and $l_3$ respectively) are counted and the average values of $l_1$, $l_2$ and $l_3$ for $f$-faced grains are then obtained which are denoted by $m_1$, $m_2$ and $m_3$ respectively.

## 2 Results and discussion

The relationship between the number of grain faces $f$ and topologically averaged values of $m_1$, $m_2$ and $m_3$ are shown in Figure 2(a)–(c) respectively. It is obvious from Figure 2(a) that there exist a strong correlation between grains and their first nearest neighbors, i.e. grains with many faces tend to surround the grains that have fewer faces; grains with fewer faces tend to surround the grains that have many faces, in other words, large grains tend to be surrounded by smaller

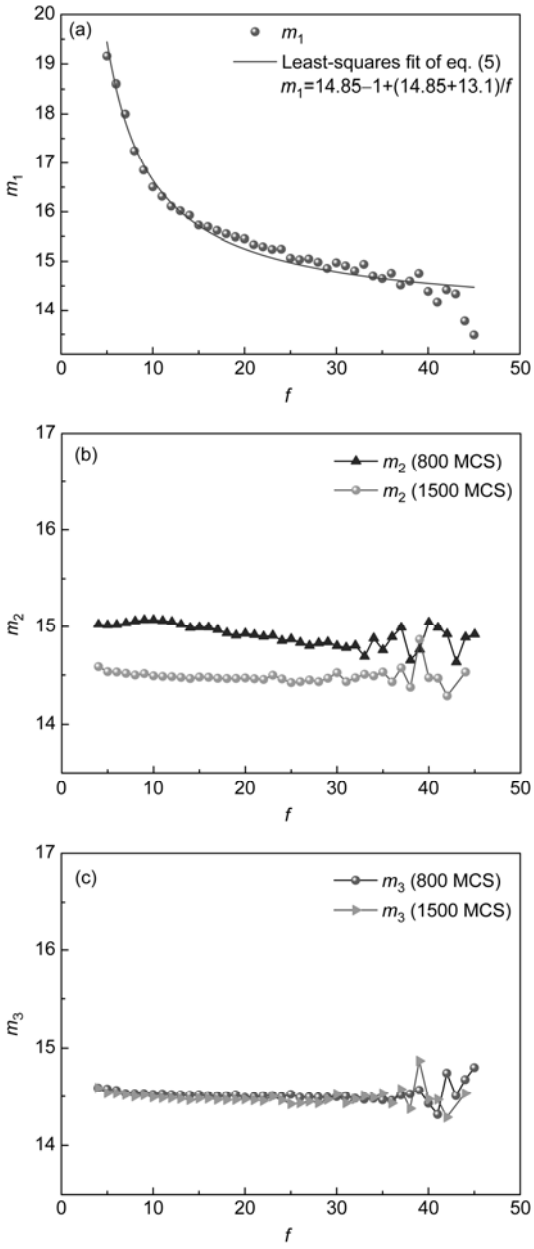


**Figure 2** Plots of the number of faces $f$ of grains vs. average number of faces of their first neighbors $m_1$ (a), second neighbors $m_2$ (b), and third neighbors $m_3$ (c).

ones and vice versa. This is what the Aboav-Weaire law [13,14] tells us about the grains and their first nearest neighbors:

$$m_1 = \langle f \rangle - 1 + \frac{\langle f \rangle + \mu_f}{f}, \quad (5)$$

where $m_1$ is the average face number of first nearest neighbors for $f$-faced grains, $\mu_f$ is second moment in the distribution of the number of faces in the system, and $\langle f \rangle$ is average number of faces in the system. The least squares fit of Aboav-Weaire law shows a close correlation to the data of 800 Monte Carlo Steps (MCS) with a correlation coefficient

of 0.975 (Figure 2(a)).

Figure 2(b) and (c) plot the relationship between grains and their second and third neighbors respectively at different simulation time (800 and 1500 MCS). It is clear that, unlike first nearest neighbors, the grains have a very little correlation with their second and third nearest-neighbors. However, the fluctuation in data for large *f*-faced grains ($f$ >35 on average) is most related to the scatter of the data, this is most likely due to a smaller set of statistics for large faced grains since they have a much lower likelihood of occurrence in the sample. It can also be observed from Figure 2 that, with increase in topological distance ($k$) the correlation between grains and their $k$th neighbors decreases.

The evidence of strong correlations between grains and their first nearest neighbors and very weak (negligible) correlations between the grains and their second and third nearest neighbors from the above investigation confirms the feasibility of neglecting the topological correlations beyond first nearest neighbor grains in obtaining eq. (1) from the general grain topology-size relation (eq. (4)). Figure 3 shows the relationship between topologically averaged relative values, $R_f/\langle R\rangle$, and the difference between the grain face numbers and the mean face number of their neighbors in (1–3) layers, ($f$–$L_{1-3}$). This relationship is similar to that obtained between $R_f/\langle R\rangle$ and ($f$–$m_1$) in [17], this further confirms that the effects of long range topological correlations are trivial. The least squares fit of eq. (4) to the data of 800 MCS (17521 grains) depicts a linear relationship with a correlation coefficient of 0.997. The values of $\alpha$ and $C$ are 0.05 and 0.99 respectively. Here, we have included a large number of grains (17521) than [17] to study the correlations between grains more clearly. The results support the feasibility of eq. (1), which considers only the interactions of first nearest neighbor grains. Hence eq. (1) may be a suitable choice for the estimation of grain topology or grain size in 3D polycrystalline microstructures.

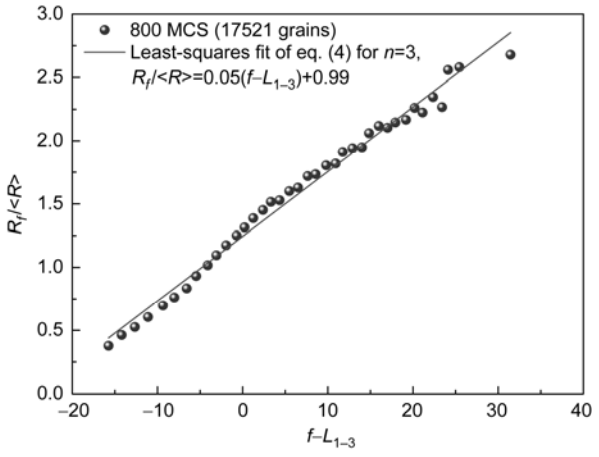


**Figure 3** Relationship between the topologically averaged values, $R_f/\langle R\rangle$, and the difference between the grain face numbers and the mean face number of their neighboring grains in (1–3) layers.

## 3 Conclusions

In this contribution, the general neighborhood topological effect on the topology-size relationship of grains in 3D polycrystalline microstructures is investigated by using large scale Monte Carlo-potts model simulation. The results revealed that a strong correlation exist between grains and their first nearest neighbors, while there exist very little (negligible) correlation between grains and their $k$th ($k\geqslant 2$) nearest neighbors (on average). This confirms that the topological correlations of 3D grains with their $k$th layers ($k\geqslant 2$) of nearest-neighbors may have trivial effect on the topology-size relationship, and thus provides support to a new grain topology-size equation [17] that only considered the non-random first nearest-neighbor interactions.

*This work was supported by the National Natural Science Foundation of China (51071019, 50901008 and 50871017).*

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