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The topologies of contacting grains in two and three dimensions

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ABSTRACT

The topologies of contacting grains were investigated based on large grain datasets from 2D and 3D Monte Carlo simulation, 3D reconstruction of pure iron, and the cross sections of these 3D microstructures. In all systems, the results show the expected trends of high affinity for contact between few- and many-faced or edged grains and avoidance of contact between grains in similar face or edge classes. However, this correlation appears relatively stronger in genuine 2D system than in 2D cross-sectional system and 3D system. This result indicates that the increase in dimension has dampening effect on the contact affinity of curvature-driven grain-growth structure.

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1. Introduction

Cellular structures of polycrystalline materials, foams and biological systems are ubiquitous in nature [1]. Evolution of the overall structure is the combined result of numerous pair- and group-wise interactions among grains/bubbles/cells, termed topological events [2,3]. Due to the fact that the pair-wise interaction among neighboring grains strongly affected the occurrence of topological events and the whole structure, it has been a topic of study for many years [3–16]. For example, the Aboav–Weaire relationship is historically used for describing grain arrangements by the average numbers of edges, M_N, on the first neighbors of N-edged grains [7,8]. Recently, Patterson [2,3] carried out grain growth simulations and proposed a more refined means on the pair-wise interaction analysis by introducing contact affinity term to describe the unbiased tendency for high or low contact between grain-pairs of specific numbers of edges/faces, independent of the frequency of presence of these grains. This methodology provides a significant improvement beyond the Aboav–Weaire approach. However, there is still lack of comprehensive investigations on the contact affinity of grain structures based on large grain datasets both in two and three dimensions.

The main focus of the present work is to compare the affinity properties of two- and three-dimensional microstructures in order to explore the manner in which the introduction of a third dimension changes the structure. We analyzed the pairing of different edge/face classes based on large grain datasets from 2D and 3D Monte Carlo simulation, 3D reconstruction of pure iron, and the cross sections of 3D microstructures. The results show noticeable differences of the affinity features among genuine 2D systems, 3D ones and cross sections of 3D ones.

2. Materials and methods

The Monte Carlo-Potts model was used to simulate 2D and 3D normal grain growth [11–13]. The continuum microstructures are mapped onto 10,000 × 10,000 square lattice and 900 × 900 × 900 cubic lattice with full periodic boundary conditions, respectively. We took steady-state grains at 2500 Monte Carlo Step as research objects in two and three dimensions, i.e., 103864 2D Monte Carlo (MC) grains and 150428 3D MC grains. In addition, 2D cross-sectional grains (210799 grains in total) in the perpendicular cross sections to the axis of 3D simulation system were also sampled for comparison.

Serial sectioning experiment was employed to reconstruct 3D pure iron (99.9% pure) microstructure. The specimen was sectioned from the center of a 30 mm diameter forged bar, and then annealed at 880 °C for 3 h, providing a fully recrystallized grain structure with a mean equivalent-area circle diameter of 32 μm. Microscopic examination on three mutually perpendicular

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surfaces of the specimens showed that the microstructure is essentially isotropic. We investigated 16254 3D grains reconstructed from 300 metallographic pictures. And, at a 15 interval of these metallographic pictures, 38109 2D cross-sectional grains were sampled.

3. Results and discussions

Based on the experiment and simulation grain data, we make statistical analysis on the contact affinity between neighboring grains. The affinity A_{ij} for preferred contact between 2D grains of edge classes i and j is described more accurately by computing the contact frequencies N_{ij} relative to the frequencies that would be expected from random contact N_{ij}^{random} based on the numbers of grains of those classes in the system:

$$A_{ij} = \frac{N_{ij}}{N_{ij}^{\text{random}}} = \frac{N_{ij}}{(i \cdot N_i)\left(\frac{N_j \cdot j}{\sum_{k=3}^{k_{\max}} N_k \cdot k}\right)} \quad (1)$$

where i and j are the number of edges on grains of particular edge classes and N_i is the number of grains in the ith class. N_{ij} is the actual number of i-j grain pairs in system. The ratio in parentheses is the probability of random contact with j-class grains for a given class. Its product with N_i yields the expected number of i-j grain pairs, N_{ij}^{random}. The same definition of A_{ij} in three dimensions is found in [2].

Fig. 1 shows the affinity for contact of i-j edge classes for 2D MC grains, cross-sectional MC ones and 2D cross-sectional pure iron ones. For 2D MC grains (Fig. 1a), the highest and lowest edge classes, 3 and 12, respectively, exhibited the highest affinity for mutual contact, a 14.36 times random occurrence, but an affinity of ~0 for contact with themselves. Intermediate edge class 6 showed an affinity of ~1, random contact, with other classes or with themselves. Such marked tendencies for high or low contact between classes are well addressed by affinity term [3], which is unbiased by the frequency of presence of the neighboring classes as occurs with the Aboav–Weaire approach.

Similar trends of high affinity for contact between few- and many-edged grains and avoidance of contact between grains in similar edge classes are observed in Fig. 1b and c for 2D cross-sectional microstructures. However, the differences in affinity between genuine 2D systems and cross sections of 3D ones are also obvious. As an example, grains from high- and low-face classes, say 3 and 12, have affinities A_{3-12} of 2.61 and 2.25 times random occurrence for 2D cross sectional MC and pure iron grains respectively, which are far less than the corresponding affinity value in 2D system, 14.36. It is clear that the contact affinity correlation appears relatively stronger in 2D system than in 2D cross-sectional system. The reason is supposed to be the difference in the evolution mechanism of 2D system and cross sections of 3D one. The genuine 2D systems evolve through the decrease of grain boundary energy with no constraint in a third dimension. However, the evolution of cross sections is not governed by the same energy-minimization considerations due to the constraint of the spacing-filling requirement in 3D. The constraint inhibits the ideal 2D topology evolution in the cross sections, which resulted in notable differences in the affinity property between genuine 2D system and cross sections, as well as differences in edge distributions observed before. The affinity term thus appears to be a potential feature to distinguish different cellular microstructures.

Fig. 2 shows the affinity for contact of i-j face classes for 3D MC grains and pure iron ones. For 3D MC grains (Fig. 2a), face classes 4 and 6 show very low contact with other few-faced grains and higher contact with high classes; face classes 11 and 13 show

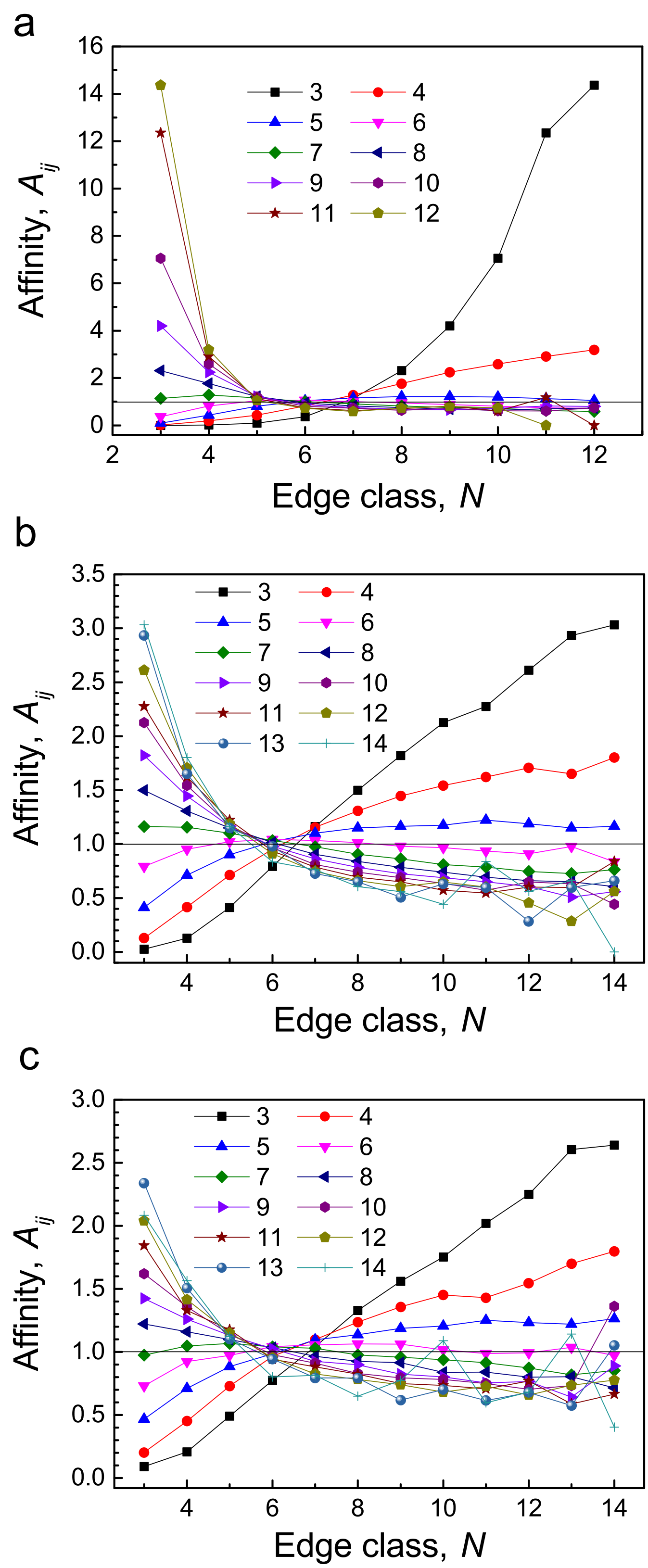

Fig. 1. Contact affinity between M-edged grains and N-edged neighbors for 2D MC grains (a), cross-sectional MC grains (b) and cross-sectional pure iron grains (c). Lines are included to guide the eye.

random contact with all other grains; face class 24 shows onset of preference for contact with few-faced grains and decreased contact with higher face classes; face class 32 shows still stronger preference for few-faced grains and lower contact with many-

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