A study of the influence of input parameters on the microstructure development of polycrystalline materials in Monte Carlo simulations of grain growth

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Abstract

A brief overview is given of the influence of the input parameters on the simulated microstructure development in Monte Carlo simulations for monophase materials and for materials containing static second-phase particles. The second-phase particles do not participate in interaction processes of the grain growth during ceramics sintering or metal annealing. It is commonly known that both these processes are accompanied with secondary recrystallization. On the other hand, they influence microstructure and thus desired properties of the final product. In the work we consider the second-phase particles of various forms (granules, whiskers, fibres) with different mechanical properties, melting temperature and polycrystalline structure other than basic material. We assume that their properties are irrelevant for the grain growth. The presented simulation examples illustrate how the input simulation parameters can influence the resulting structure and hence its properties.

K e y w o r d s: normal grain growth, monophase structure, second phase, whiskers, fibres

1. Introduction

The processing conditions of polycrystalline metallic materials are very important because of their influence on microstructure and properties. The microstructure is characterized by dimensional parameters – the average grain size or the average grain area – and by topological parameters – number of neighbours. Monte Carlo simulations of the grain growth with various input parameters show the way to understand relations between processing conditions and resulting microstructure [1–11].

The aim of the present work is to examine the main influence of the input parameters on the microstructure characteristics of both monophase materials and materials with static second-phase particles. The second-phase particles can be present in the material in the form of granules, whiskers or fibres.

2. Simulation model

The generalized Q-state Pott's spin model is applied to the simulation procedure [1]. The structure development is mapped onto a two-dimensional discrete simulation lattice, which can be either square or hexagonal. An area element of microstructure is represented by one lattice site and is assigned a random number $Q_i\,(1 < Q_i < Q)$ called orientation or spin. The grain boundary lies between two adjacent sites with different orientations. The energy of a lattice site is given by the Hamiltonian

$$E = J \sum_{j=1}^{n} \left(1 - \delta_{Q_i Q_j}\right), \tag{1}$$

where J is a positive constant specifying a measure of the interaction of the evaluated i-th lattice site with

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neighbouring sites, Q_i is the orientation of the i-th lattice site, Q_j is the orientation of the j-th neighbouring lattice site, $\delta_{Q_iQ_j}$ is the Kronecker delta. The sum is given over n vicinal lattice sites.

During the simulation procedure the i-th lattice site orientation is generated randomly and its energy E_1 is calculated according to Eq. (1). Then a new random orientation is generated for the i-th lattice site and energy E_2 after reorientation is again calculated. The reorientation is accepted when $E_2 < E_1$. Otherwise, the reorientation is accepted with the probability

$$P \approx \exp\{-\Delta E/kT\}, \tag{2}$$

where

$$\Delta E = E_2 - E_1, \tag{3}$$

k is the Boltzmann constant and T is the temperature. Let us denote

$$d = \sum_{j=1}^{n} \left(\delta^1_{Q_iQ_j} - \delta^2_{Q_iQ_j}\right), \tag{4}$$

then

$$\Delta E = Jd. \tag{5}$$

The probability of the reorientation acceptance is

$$P \approx \exp\{-Jd/kT\}. \tag{6}$$

The term J/kT can be replaced by α and is called the temperature factor. For the final probability of the reorientation acceptance one obtains

$$P \approx \exp\{-\alpha d\}. \tag{7}$$

If the lattice consists of $N \times N$ lattice sites, $N \times N$ reorientation attempts represent a time unit t called Monte Carlo Step (MCS).

The static second-phase particles do not participate in the energy interaction. In the simulation lattice they are denoted with the orientation Q_s. If during the simulation the lattice point with the orientation Q_s is randomly chosen this trial is ignored. The simulation continues with another trial. Consequently the positions of the static second-phase particles before and after simulation procedure are the same.

3. Simulation results

3.1. Grain growth in monophase structure

The simulations of the grain growth in the monophase structure have been carried out with the aim to investigate the influence of particular input parameters, i.e., the type and the dimensions of the simulation lattice, the number of the orientations and the boundary conditions on the average grain size, which represents the most important characteristics of the resulting microstructure.

In the first experiment we have studied the influence of the size of simulation lattice N on the simulated structure and on the average grain size R.

The examples of structures simulated on the square lattice with the number of orientations $Q = 100$, the temperature coefficient $\alpha = 100$, simulation time $t = 1000$ MCS for two rather different lattice sizes $N = 25$ and $N = 200$ are presented in Figs. 1a,b, respectively. To see more gradually how the size of the simulation lattice affects the structure, in Fig. 1c we introduce the results for sizes $N = 25$, 50, 100, 200, simulated in parallel. From Fig. 1d, which illustrates the development of the average grain size in time, one can conclude that, except for $N = 25$, the size of the simulation lattice does not influence substantially the average grain size. Nevertheless, choosing a greater N can improve the accuracy of the average grain size determination because of substantially greater statistical set is evaluated. From Fig. 1d one can also observe that with increasing simulation time the structure continuously converges to its stable state, i.e., for $t = 1000$ MCS the average grain size practically does not change.

In the next experiment we have studied the influence of the type of simulation lattice on the simulated structure. The lattice sites can be arranged either in square or hexagonal configuration. While in the previous example we presented the results for square simulation lattice in Fig. 2a, we introduce the structure simulated on a hexagonal simulation array for $N = 100$, $Q = 100$, $\alpha = 100$, $t = 1000$ MCS. In Fig. 2b we present the time dependence of the average grain size for both types of the simulation lattices.

Evidently, the grains grow to larger average sizes in the square simulation lattice rather than in the hexagonal one. This can be related to the greater number of interacting neighbouring lattice sites in the square lattice (8) than in the hexagonal one (6).

Further, we investigated the influence of the orientation number Q on the resulting simulated structure. To illustrate this influence on the shapes of grains, in Figs. 3a,b simulated structures for two extremely different values of $Q = 5$ and $Q = 200$ ($N = 200$, $\alpha = 100$, $t = 1000$ MCS) are presented. In Fig. 3c, the development of the average grain sizes with time for the set of various orientation numbers Q is presented.

For the extremely small number of orientations ($Q = 5$) one can observe abnormal grain growth. The grains have irregular shape and some of them grow much faster than the others. This accounts for larger average size, which is evident from Fig. 3c. This model

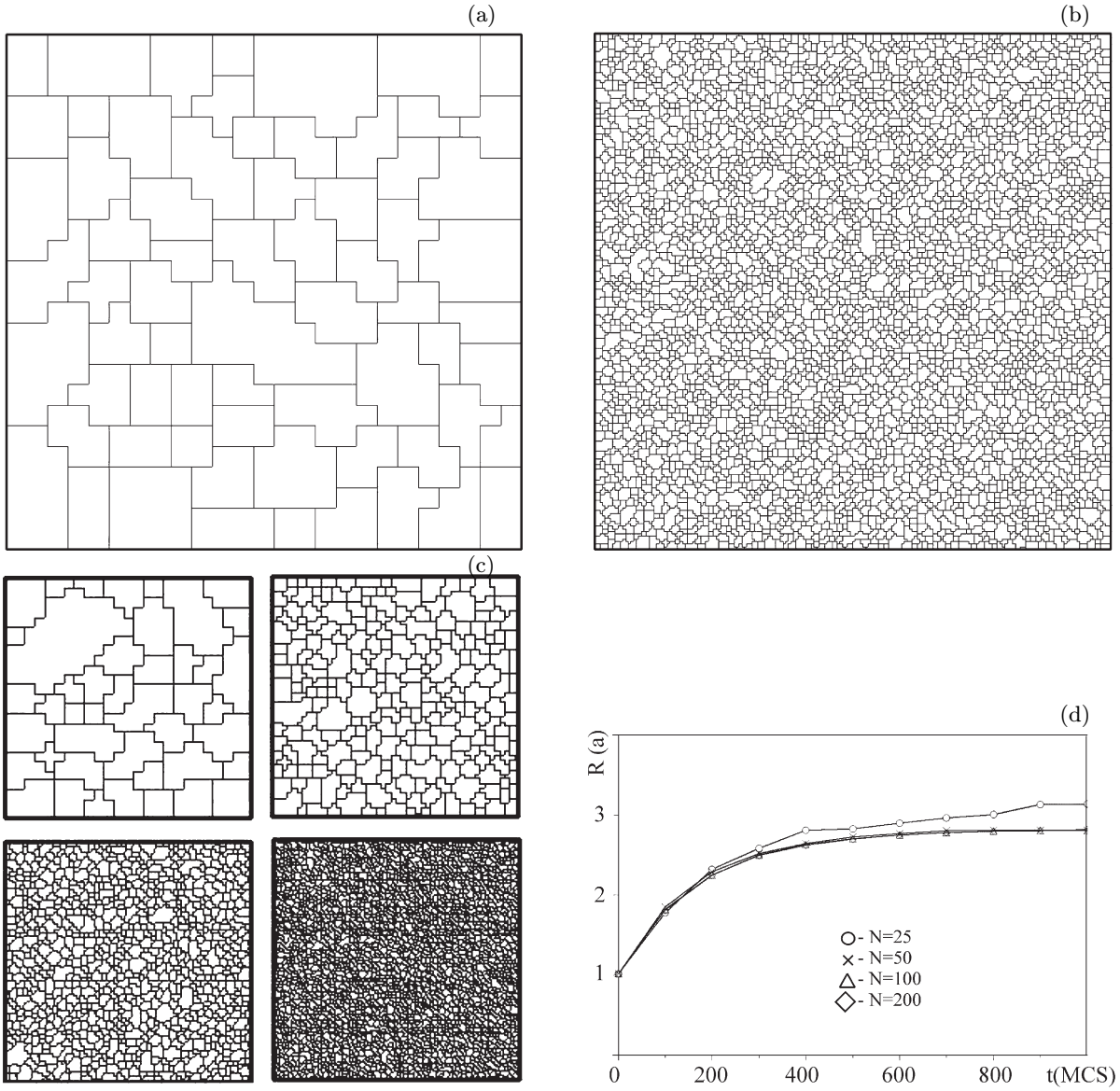

Fig. 1. (a, b) Detail view of normal grain growth simulated on the square simulation lattice with dimensions $N = 25$ (a), $N = 200$ (b) and (c) grouped view for $N = 25$, 50, 100 and 200. (d) The time dependence of the average grain size is shown for various simulation lattice dimensions ($N = 25$, 50, 100, 200). Other simulation parameters were $Q = 100$, α= 100, $t = 1000$ MCS.

can be used for the simulation of grain growth from powders with bimodal distribution of particle sizes. When increasing Q, the simulated structure becomes more homogeneous.

In what follows we have studied the influence of the temperature coefficient α on the development of the simulated structure. In our experiment we have set parameters $N = 200$, $Q = 100$ and for $\alpha = 1.2$, 1.4, 1.5, 1.8, 2, 3, 5, 10, 100 we have carried out simulations during 10 000 MCS. The resulting structures in Fig. 4a illustrate this influence. The development of the average grain sizes as a function of time for $\alpha = 1.2$, 1.5, 5, 50, 100 is given in Fig. 4b. One can see that for $\alpha = 5$ and higher, the courses of the average size developments are practically identical. To see the influence for small values of α in detail, in Fig. 4c we scanned the region between $\alpha = 1$ and $\alpha = 2$. In Fig. 4d the dependence of the average grain size on both number of orientations Q and temperature coefficient α is presented.

From Figs. 4a,b it is apparent that for $\alpha = 1.2$ (and less) grains do not grow. In Fig. 4a, for $\alpha = 1.4$ one can observe rapid growth of few grains accompanied with simultaneous melting on grain boundaries. The indications of melting are still visible even for $\alpha = 1.5$, however, the grains grow more slowly. This trend continues with increasing α. In Fig. 4a, for $\alpha = 1.8$ one can observe that the melting on grain boundaries disappears and for $\alpha = 5$ we obtain a homogeneous structure. Increasing α to higher values does not change

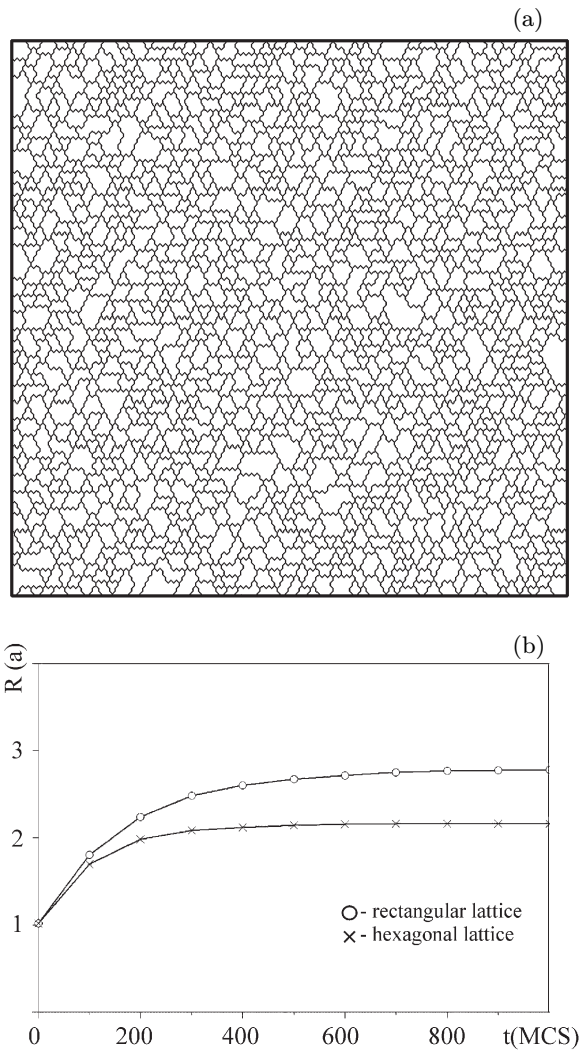

Fig. 2. Hexagonal simulation lattice with simulation parameters $Q = 100$, $\alpha = 100$, $t = 1000$ MCS (a) and time dependence of type of simulation lattice on the average grain size (b).

substantially the characteristics of the simulated microstructure.

Finally, we investigated the influence of the boundary conditions. During the simulation it can happen that the investigated point i is positioned at the edge of the simulation lattice. In this case two algorithms of interactions can be employed. The point can interact either only with the points inside of the lattice (finite simulation array or edge interaction) or for outside neighbours the interaction can be extended to the points on the opposite side of the lattice (infinite simulated array or so-called band effect). Simulation experiments proved that the resulting average grain size is practically independent of the chosen algorithm (edge interaction or band effect) for N greater than 50.

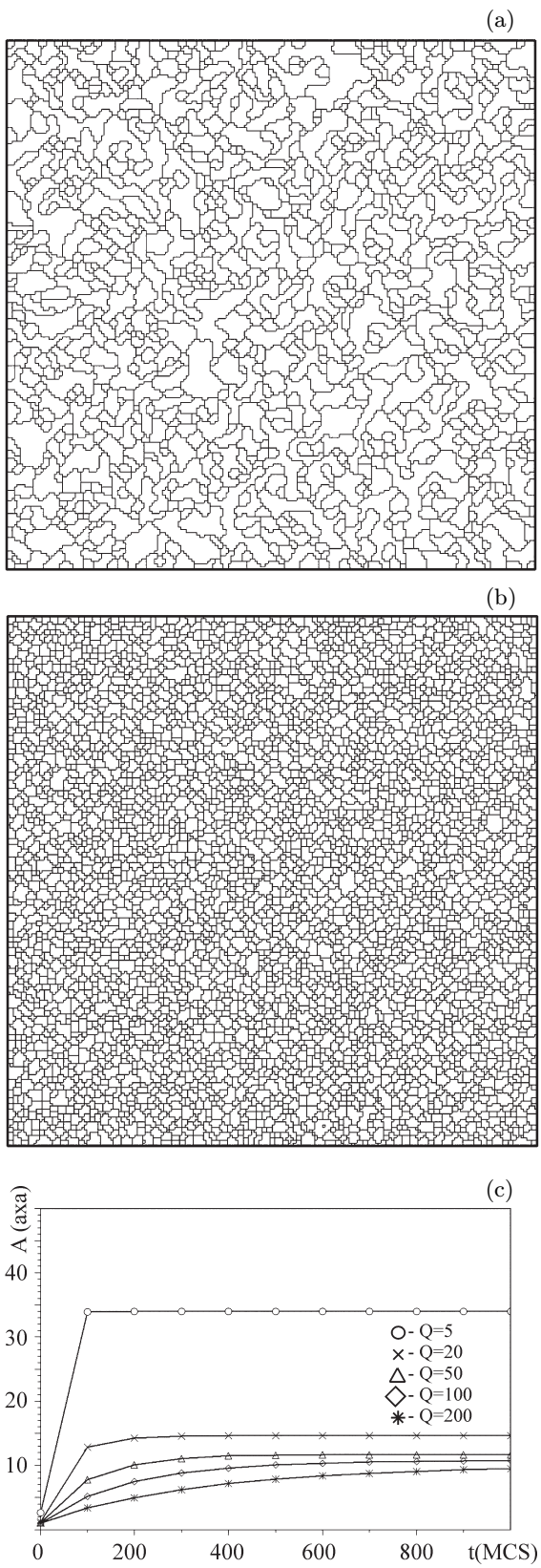

Fig. 3. Simulated structures with parameters $N = 200$, $\alpha = 100$, t= 1000 MCS with Q= 5 (a), 200 (b) and time dependence of average grain area on Q parameter (c).

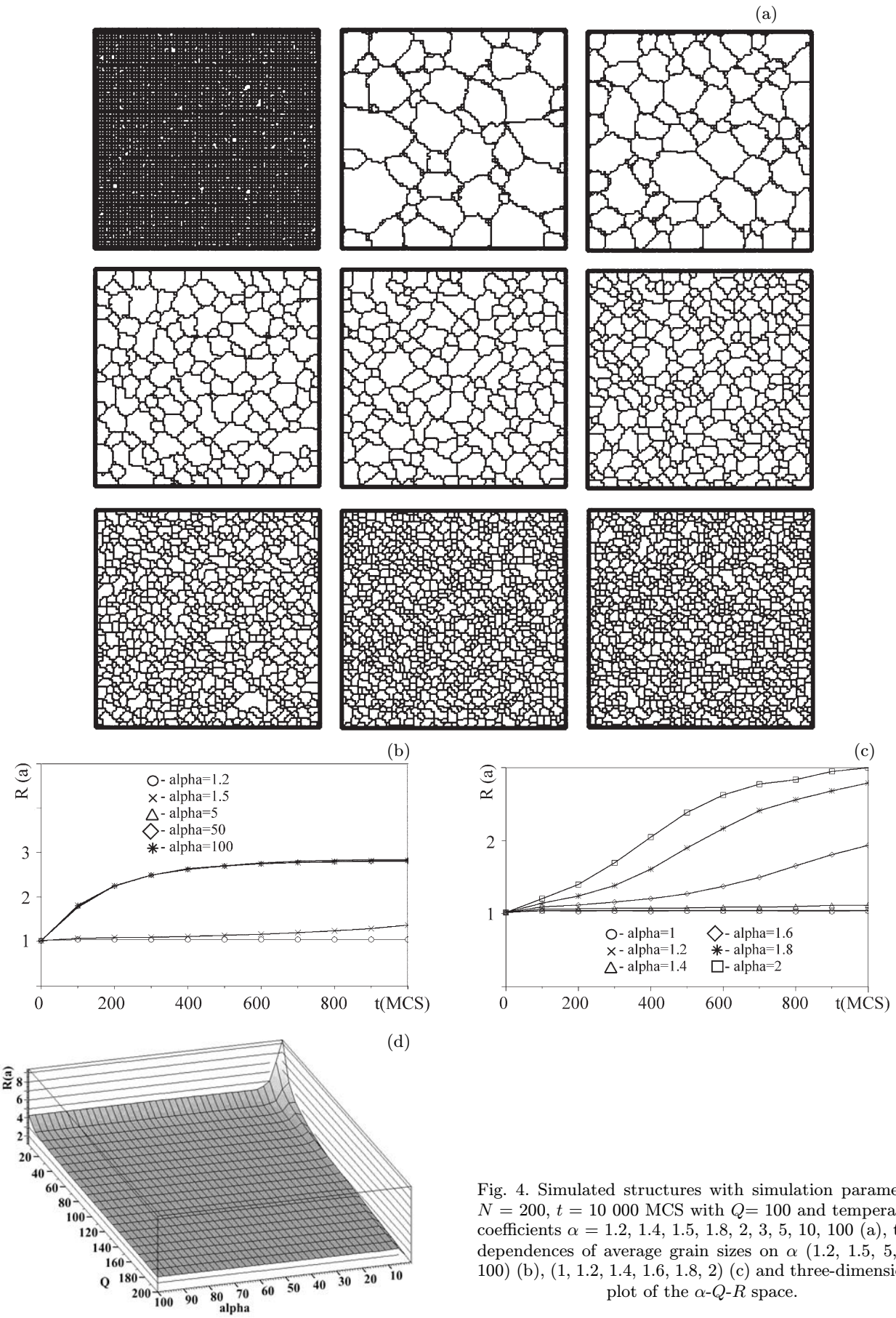

Fig. 4. Simulated structures with simulation parameters $N = 200$, $t = 10\,000$ MCS with Q= 100 and temperature coefficients α = 1.2, 1.4, 1.5, 1.8, 2, 3, 5, 10, 100 (a), time dependences of average grain sizes on α (1.2, 1.5, 5, 50, 100) (b), (1, 1.2, 1.4, 1.6, 1.8, 2) (c) and three-dimensional plot of the α-Q-R space.

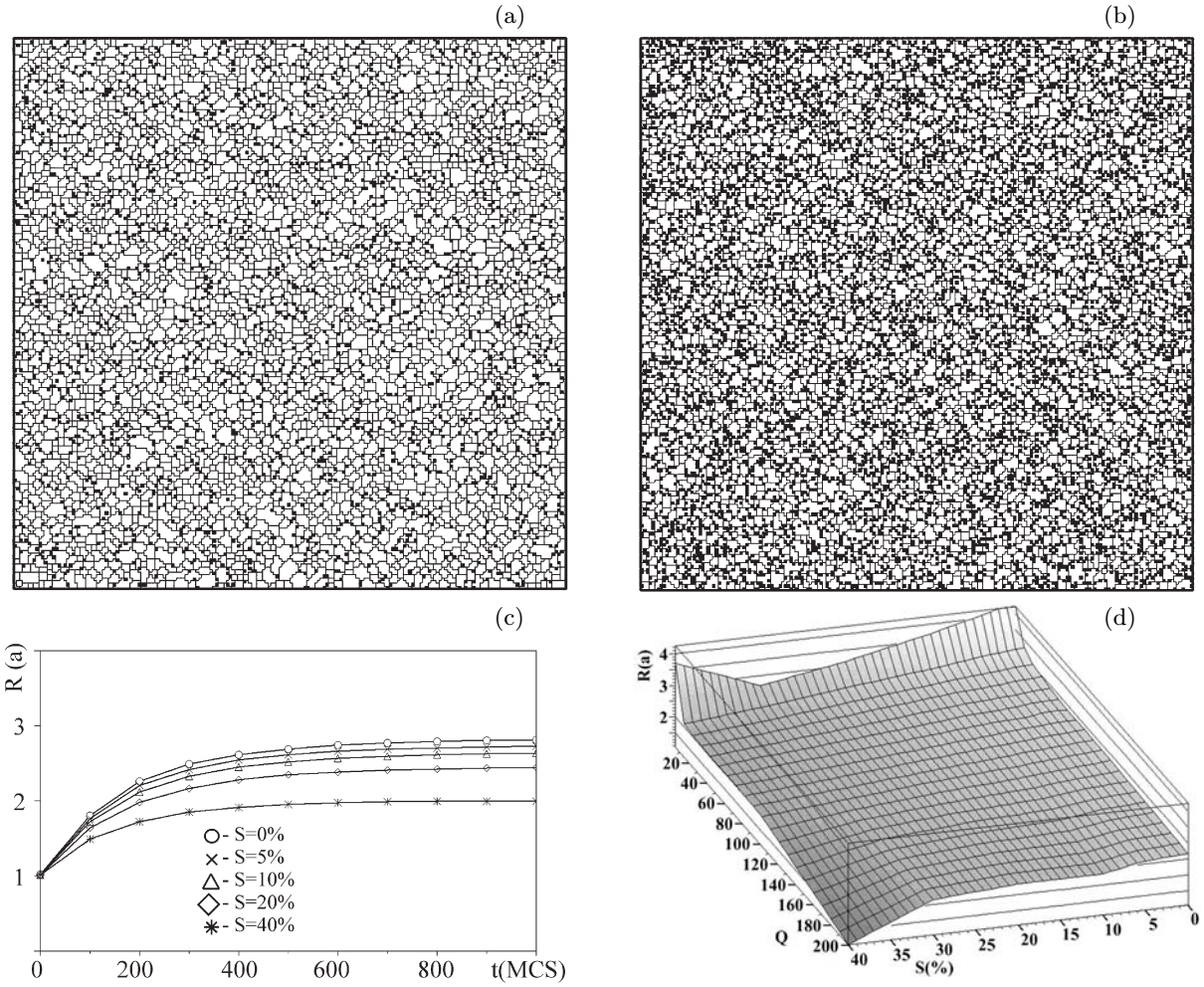

Fig. 5. Simulated structures with granular second-phase particles with parameters $N = 200$, $Q = 100$, $t = 1000$ MCS, $\alpha = 100$ and $S = 5$ % (a), $S = 20$ % (b), time dependences of the average grain sizes on the second-phase volume fraction (c) and three-dimensional plot of S-Q-R space (d).

3.2. Grain growth with static second phase

Static second-phase particles can have the shape of small granules – inclusions, or small needles – whiskers or contiguous fibres stretched entirely throughout the structure [12–17].

In a first experiment we have studied the influence of the volume fraction S of second-phase particles in the form of granules. We assumed the size of the second-phase granules to be equal to the size of lattice site. The second-phase particles were introduced into material randomly (having the orientation Q_s) in volume fraction S. We carried out a sequence of simulations with the parameters $N = 200$, $Q = 100$, $\alpha = 100$, $t = 1000$ MCS step by step for the concentrations $S = 2$ %, 5 %, 10 %, 20 %, 30 % and 40 % of the second phase. For the sake of illustration, in Figs. 5a,b we present the simulated structures for $S = 5$ % and 20 %. From the dependences of the average grain sizes on time given in Fig. 5c it is obvious that the second-phase particles impose a considerable braking effect to the grain growth. From Fig. 5d one can see how various combinations of number densities of second-phase particles and number of orientations, i.e., the homogeneity of initial powders, influence the average grain size of the simulated structure.

Next, we have investigated the influence of the volume fraction of second-phase particles presented in the form of whiskers with the width equal to the size of lattice site. In the carried out simulations the input parameters were set to be $N = 200$, $Q = 100$, $\alpha = 100$ and $t = 1000$ MCS. Before the simulation starts, the whiskers can be initialized with either random or regular distribution having lengths in a given range. The examples of simulated structures with whiskers initialized randomly with the length $10a$ (a is the basic lattice parameter) and the volume fractions $W = 5$ % and 20 % are shown in Figs. 6a and 6b. Figure 6c illustrates the simulated structure with whiskers initialized with regular distribution, with $W = 5$ % and the length equal to $5a$.

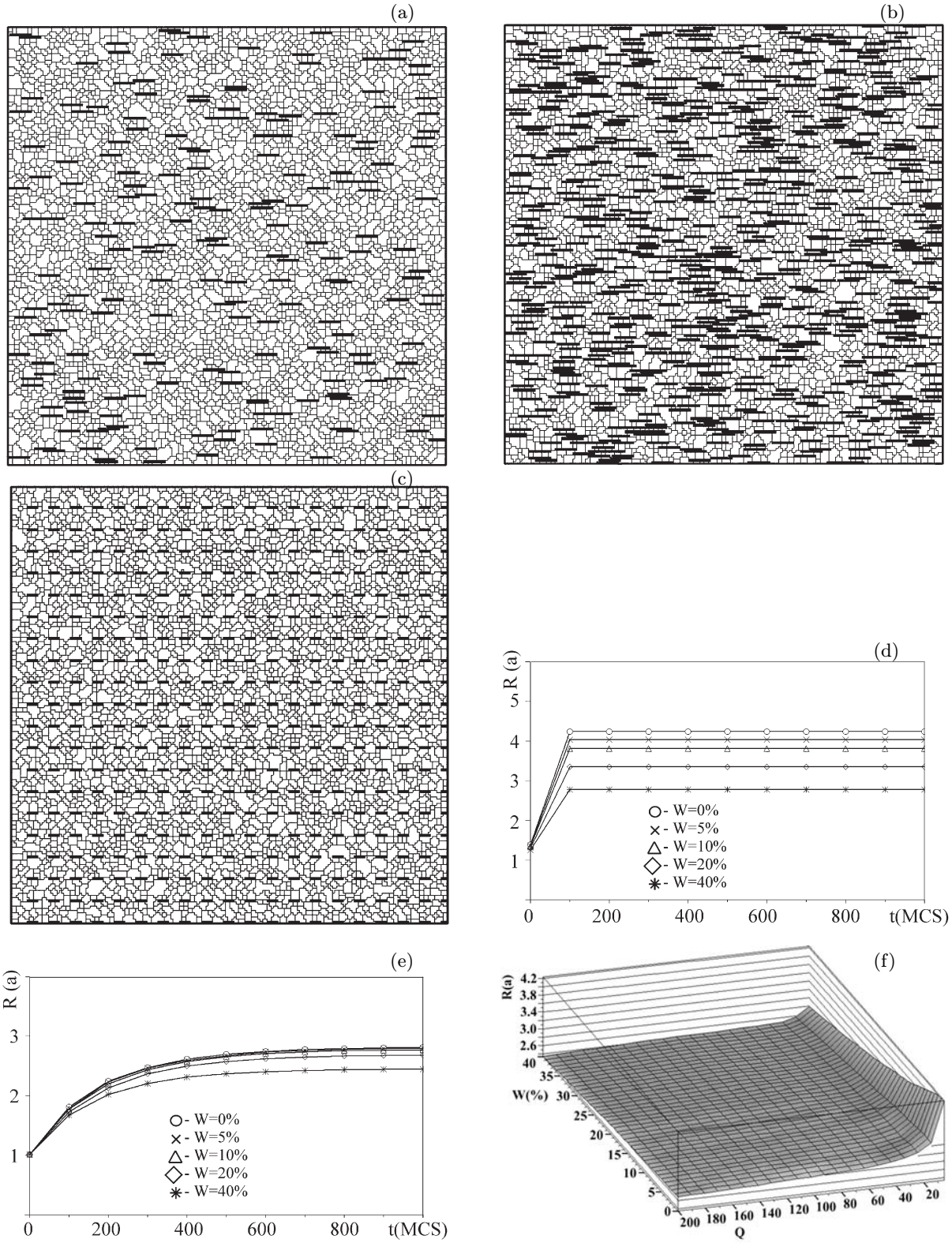

Fig. 6. Simulated structures with whiskers and simulation parameters $N = 200$, $Q = 100$, $t = 1000$ MCS, $\alpha = 100$, $W = 5$ % (a), $W = 20$ % (b) included randomly, $W = 5$ % with length $l = 5a$ included regularly (c), time dependence of the average grain size on W ($W = 0$ %, 5 %, 10 %, 20 %, 40 %) with length $l = 10a$ and with $Q = 5$ (d) and $Q = 100$ (e) and three-dimensional plot of W-Q-R space (f).

In Figs. 6d and 6e one can see the time dependences of the grain growth in the structures with various values of W of randomly initialized whiskers with the length equal to $10a$ for numbers of orientations

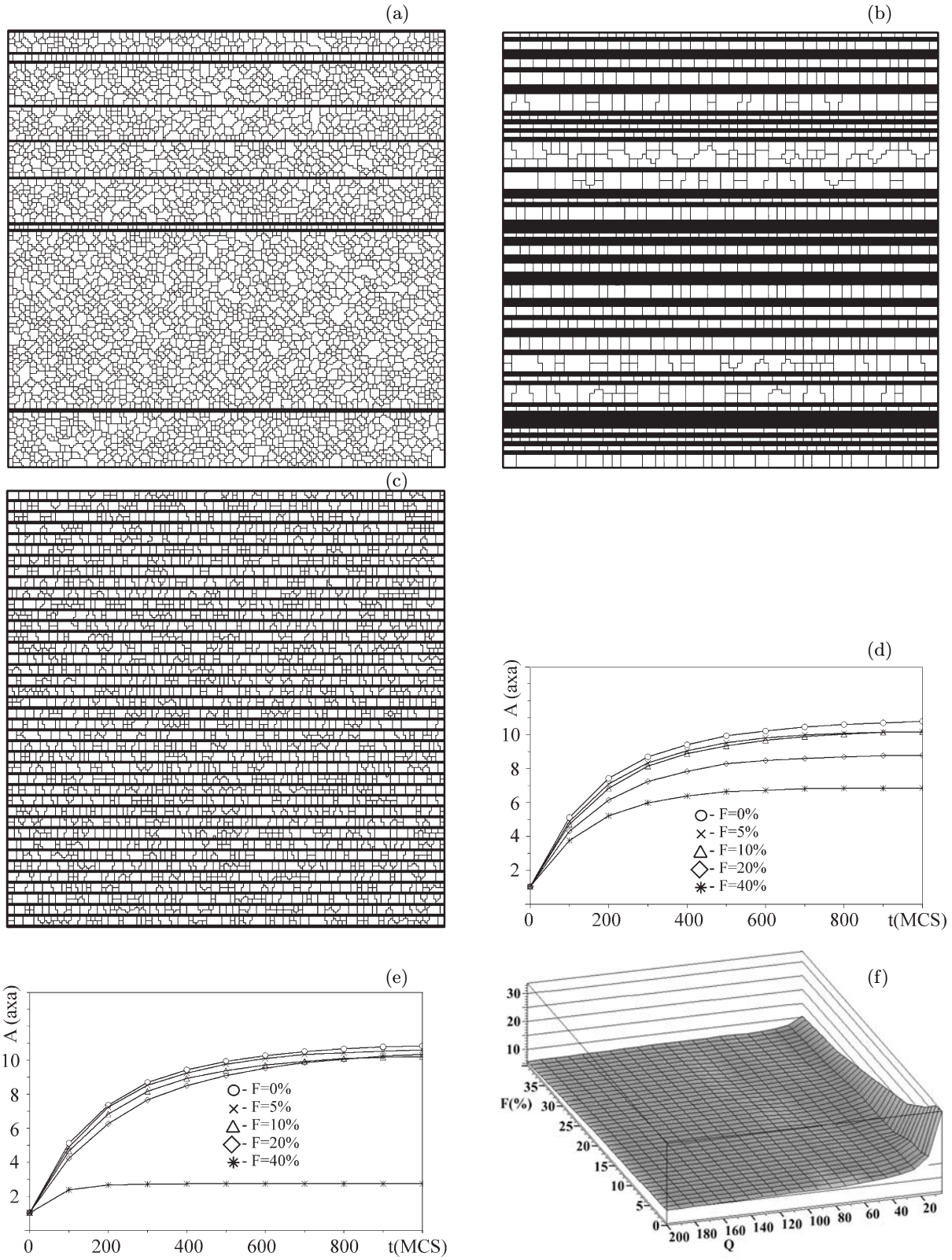

Fig. 7. Simulated structures with randomly initiated fibres with simulation parameters $N = 200$, $Q = 100$, $t = 1000$ MCS, $\alpha = 100$ and $F = 5$ % (a), $N = 100$, $F = 40$ % (b) $N = 200$ and $F = 20$ % (c). Time dependences of average grain areas in the simulated structures with fibres initiated randomly (d), regularly (e) and three-dimensional plot of the F-Q-R space (f).

$Q = 5$ and $Q = 100$. One can conclude that whiskers influence considerably the average grain size for small number of orientations while for large values of Q this influence is negligible. To determine the influence of

various combinations of Q and W on the average grain size $\overline{R}\,(Q, W)$, we scanned the range given in Fig. 6f.

Finally, we carried out similar experiment with fibres. Like in the investigation of whiskers, we studied how the volume fraction of fibres and number of orientations influence the grain growth of the basic material. Again, to illustrate the influence of various parameters we introduce a few examples. In Fig. 7a ($N = 200$, $Q = 100$, $\alpha = 100$ and $t = 1000$ MCS) we show the simulated structure for $F = 5$ % initialized with random distribution. Next in Fig. 7b ($N = 100$, $Q = 100$, $\alpha = 100$ and $t = 1000$ MCS) we increased the volume fraction of fibres to $F = 40$ %. In Fig. 7c ($N = 200$, $Q = 100$, $\alpha = 100$, $t = 1000$ MCS and $F = 40$ %) the fibres were distributed regularly. For large values of F (Figs. 7b,c) one can observe that the grains grow only in the direction parallel to the fibres because grain growth in the other direction is suppressed by the fibres. Time dependences of average grain areas for both randomly and regularly distributed fibres for various volume fractions are given in Figs. 7d and 7e, respectively. In accordance to Figs. 7c,e the above-mentioned effect is more apparent for regularly distributed fibres and for higher volume fractions. The dependence of average grain areas on both number of orientations Q and fibre fractions is presented in Fig. 7f.

4. Conclusion

We have investigated the influence of individual simulation parameters as well as their combinations to resulting simulated structure. Taken together this study reveals the relation of simulated and real structures to simulation parameters and shows their possible impact on the preparation of particular materials in practice.

The type of simulation lattice (rectangular or hexagonal) clearly proved its influence on resulting structure and thus average grain size. Materials crystallizing in hexagonal lattice have structure with finer grains than materials crystallizing in other types of lattices, simulated with rectangular lattice.

Modality (number of orientations) of initial powders proved to influence on homogeneity and thus properties of sintered material as well. High values of Q guarantee more homogeneous structure and therefore the material becomes mechanically more resistant. Small values of Q make it possible to simulate structures with multimodal distribution of initial powders.

The temperature coefficient α is the parameter unambiguously affecting the sizes of grains. Polycrystalline ceramics as well as metals are sintered (or recrystallized) at the temperatures specific for a particular material. In principle, for a given material one can determine the optimal value of α. Too small values of α represent a situation when the melting temperature of the material has been exceeded.

In general for materials containing static second-phase particles, one can conclude that their volume fraction influences the average grain size and hence final properties of the material. As expected with increasing volume fraction of static particles of the second phase, the average grain size obtained under otherwise identical conditions decreases. Their interaction properties can be simulated under various simulation conditions by changing several input parameters.

For materials with second-phase particles in the form of whiskers or fibres one can conclude that their presence influences granularity of the simulated structure and consequently increases the strength of the material. This influence is dominant in the structures simulated with large values of Q and high volume fraction of inclusions. The resulting structures are as fine-grained as if we sintered materials with monomodal distribution, i.e., with initial powders without second-phase inclusions.

There are many possibilities how to put into context structures simulated under specific input parameters with real materials sintered under specific conditions. In this paper we have presented the influence of various input simulation parameters as well as the influence of the number density of static second-phase inclusions on the final grain size of simulated structures.

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