

3D SIMULATION STUDY OF INHOMOGENEOUS MICROSTRUCTURE AND ITS EVOLUTION (advantages of visual simulation technique in stereological analysis)

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(Accepted October 15, 2003)

ABSTRACT

A 3D Monte Carlo technique has been used to simulate a complex process of recrystallization in a material containing precipitates after graded deformation. By the simulation model, the inhomogeneous deformed microstructure and its evolution during subsequent annealing were directly displayed; moreover, the locally varying recrystallized microstructure was quantitatively analyzed. The simulation results were well verified by experiments with an aluminum alloy containing Al₃Zr particles that had been subjected to deformation and annealing for recrystallization. In the stereological analysis of a non-random microstructure and its evolution kinetics, the visual simulation technique showed apparent advantages for sampling, detection and measuring.

Keywords: 3D computer visualization, inhomogeneous microstructure, Monte Carlo technique, recrystallization, stereology.

INTRODUCTION

Computer visualization of microstructure has been rapidly developed during the past decade in the field of materials science and engineering since Srolovitz *et al.* (1983) for the first time used a 2D Monte Carlo method to simulate normal grain growth. Nowadays, image simulation techniques, mainly including Monte Carlo method (Rollett *et al.*, 1992; Song *et al.*, 2001), cellular automata (Raabe, 2002), vertex model (Enomoto and Kato, 1990) and phase-field theory (Krill and Chen, 2002), have been widely applied to simulate various processes found in materials research & development.

Recrystallization, as a common phenomenon that is observed in most of the metallic materials after plastic deformation and annealing, has been studied with computer modeling by some researchers (see overview by Doherty *et al.* (1997)). A major part of this modeling work has been concentrating on fundamental processes, e.g. recrystallization in single-phase materials, assuming uniform deformation that leads to homogeneous microstructures. However, the uniform deformation cannot be actually attained on the length scale of the sample or even on the length

scale of the grain. Therefore, inhomogeneous recrystallization is very often encountered in industry, especially in materials containing fine particles as a second reinforcing phase.

In the present work, a 3D Monte Carlo technique is developed to model recrystallization after inhomogeneous deformation in a material containing particles. In the complex case where microstructure reveals large scale inhomogeneity and evolves with time, it is difficult and under some circumstances it is impossible to characterize the microstructural features with the conventional stereological methods. It will be shown that, in such cases, 3D visual simulation offers advantages both morphologically and quantitatively.

GRADED DEFORMATION

An Al-0.5wt.%Zr alloy was used in the experiments, containing the dispersed Al₃Zr particles that had formed after precipitation heat treatment at 480°C for 24 hrs. The mean diameter $d_p = 200\text{nm}$ and volume fraction $f_p = 0.04$ of the randomly distributed precipitates were measured with conventional stereological techniques (Exner and Hougardy, 1988; Yu and Liu, 1989) on high resolution scanning microscopy (HRSEM) images.

To study microstructure evolution under the condition of inhomogeneous deformation, a graded deformation was introduced into the sample. A special shape with varying initial height had been designed for the sample which was subjected to subsequent deformation by means of cold rolling. The typical shapes together with the sizes of the sample before and after deformation are shown in Fig. 1. Thus, the rolling reduction (defined as the relative decrease of the height) can be calculated, varying from 60% to 90% along the longitudinal direction of the deformed sample. A number of equidistant straight lines perpendicular to the longitudinal direction were marked on the top surface of the graded part of the undeformed sample (see Fig. 1a) to determine the function of the deformation gradient. Under conditions of volume conservation and a constant width of the sample during deformation process due to cold rolling,

the following relationship should hold,

$$\Delta x_{i+1}^d - \Delta x_i^d = \frac{1}{h^d} (\Delta x^u)^2 \sin \theta \cos \theta, \quad (1)$$

where Δx^u is the initial distance before deformation between equidistant lines, Δx_i^d is a distance measured between two marked lines after deformation, h^d is the constant height of sample after deformation, and θ is the angle of inclination of the graded part of the undeformed sample to the horizontal plane. The right side of Eq. 1 consists only of constants, indicating that after deformation the increase of the distances between the lines is constant. This is approximately confirmed by corresponding measurements on the deformed sample (Fig.1b). Therefore, in the part containing the deformation gradient, the rolling reduction can be characterized as a linearly increasing function of the distance along the rolling direction.

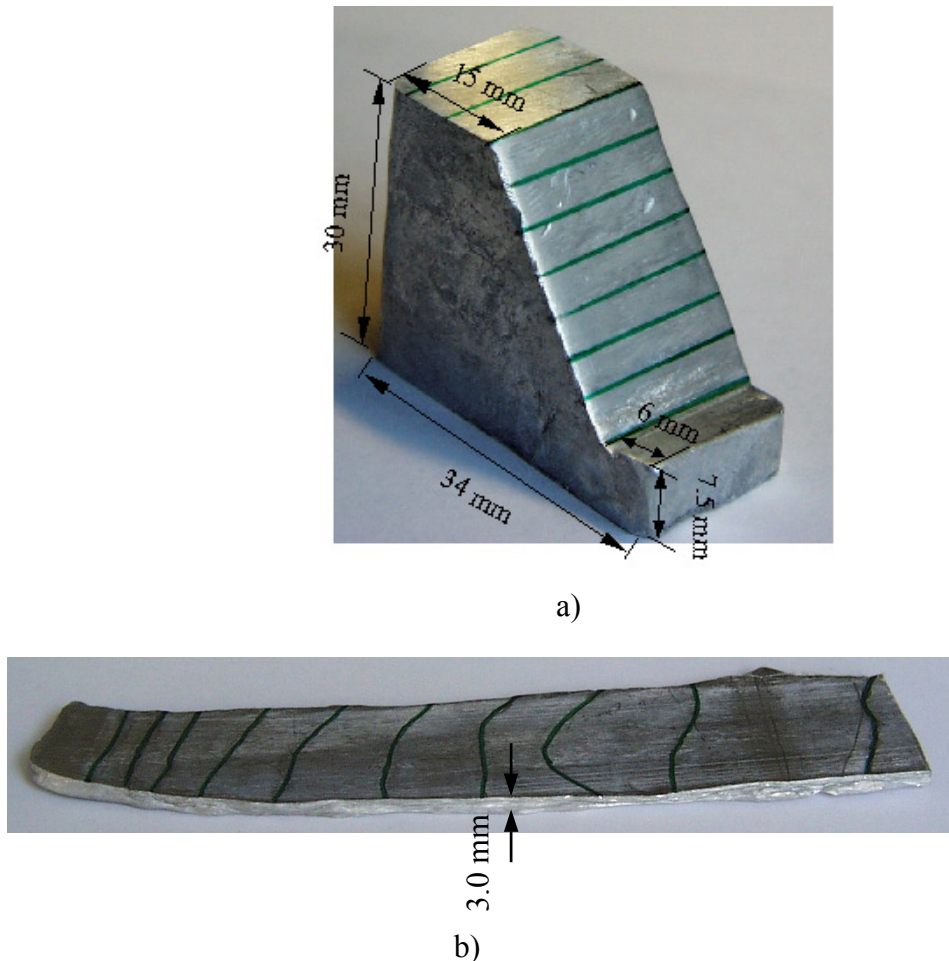


Fig. 1. Pictures of sample before a) and after b) deformation by cold rolling.

SIMULATION MODEL

At first, the initial microstructure with equiaxed grains is generated with a Monte Carlo algorithm for normal grain growth (Song and Liu, 1998). The fine precipitates are distributed randomly in the matrix, which is represented by a cubic micro-unit structure of uniform size. The deformed grain structure is then generated by tracing the positions of micro-units which belong to the same grain before deformation and whose positions are changed according to the local rolling reduction. As a result of locally varying reductions, the deformed grains at the transition zone

from lower deformation to higher deformation will have an upward macroscopic curvature. This is demonstrated by the shape change of a circular zone representative of an ideal equiaxed grain, as shown in Fig. 2. The geometry of the simulated domain with a shape equivalent to that of the experimental sample is shown in Fig. 3a, with the corresponding deformed microstructure in Fig. 3b. To restrict computing time, only a part (1113×30×100 cubic units) of the total volume (2463×30×100 cubic units) is used that contains the deformation gradient plus parts of the adjacent zones with approximately uniform deformation.

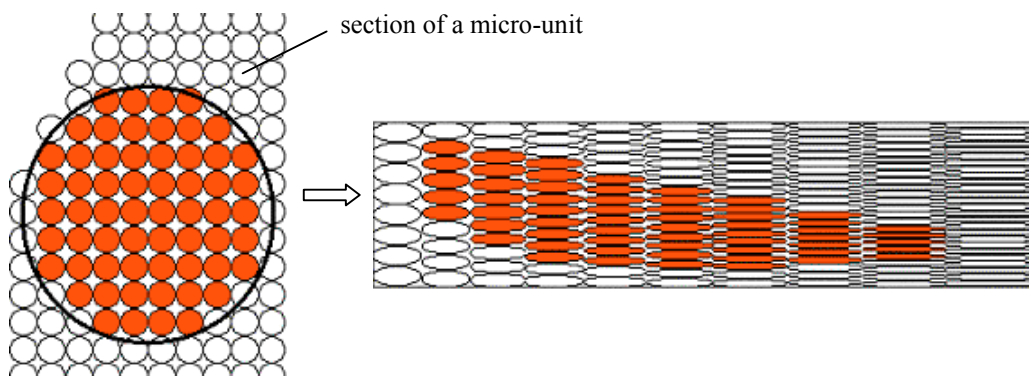


Fig. 2. Demonstration of deformed geometry due to cold rolling of a circular zone, representing an equiaxed grain; the reduction varies from 25% to 80% at the left and right borders respectively.

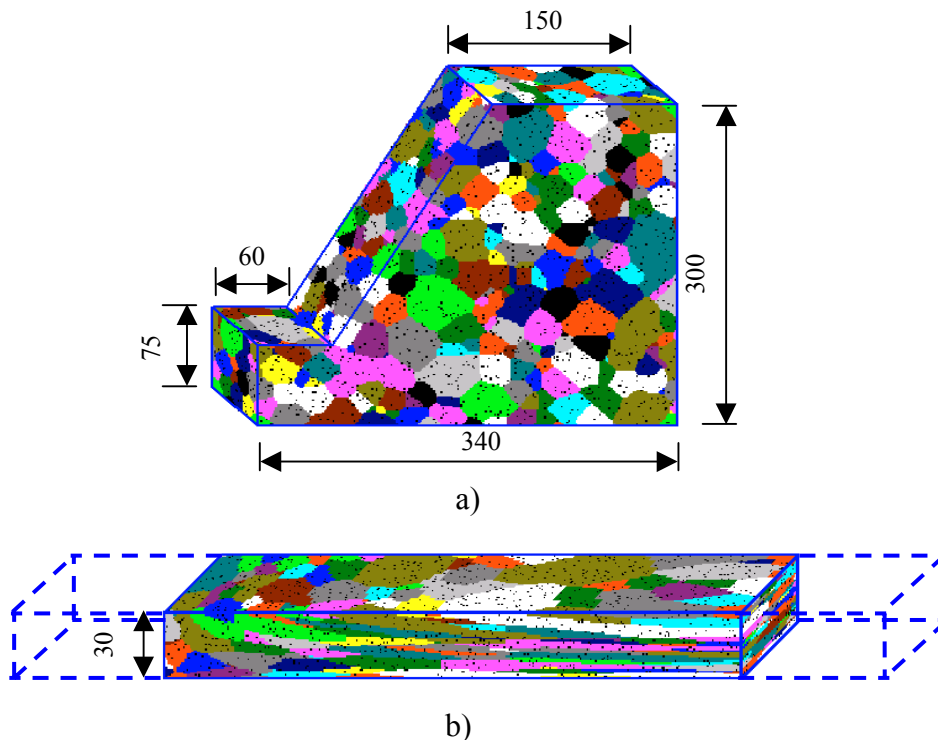


Fig. 3. Simulated 3D microstructures before a) and after b) deformation; both geometries are equivalent to those of the experimental sample. Dimensions are given as numbers of Monte Carlo micro-units.

Next, the local stored energy that is calculated from the local strain is mapped onto the micro-units that build the deformed microstructure. Nucleation of recrystallization is assumed to occur instantaneously at positions where the local stored energy $E_D(x)$ is higher than the sum of the critical stored energy for recrystallization E_D^C and the pinning force from the precipitates F_p . The local nucleation rate $\dot{N}(x)$ can therefore be expressed as

$$\dot{N}(x) = C_0(E_D(x) - E_D^C - F_p) \exp\left(\frac{-Q}{RT}\right). \quad (2)$$

Q is the activation energy of nucleation, R is the gas constant, and T is the absolute temperature. C_0 is the rate constant that is used here as a fitting parameter. During the first simulation time unit (Monte Carlo Step, MCS), the local nucleus density is calculated with Eq. 2. Initially, the nuclei are given the uniform size of the micro-unit.

The microstructure evolution with time is then simulated by tracking the re-orientation tendencies of each micro-unit with respect to the orientation state of one of its randomly selected neighbors. Micro-units that represent precipitates are excluded from selection as reorienting or neighboring units. The local energy E_t at time t of a micro-unit is determined using the formalism

$$E_t = g(S_i)E_D(x) + \sum_{K=1}^{N_K} \sum_{j \in K} J(1 - \delta_{S_i S_j}), \quad (3)$$

where S_i is the orientation index of unit i , and $g(S_i)$ is a step function of S_i . $g(S_i)$ equals unity or zero when unit i is an unrecrystallized or a recrystallized micro-unit, respectively. The second term on the right side of Eq. 3 represents the local interface energy (Song and Liu, 1998). At time $t + \Delta t$, when unit i strives to reorient to a new orientation with index as S'_i , the tentative new energy state of unit i is calculated by

$$E_{t+\Delta t} = \sum_{K=1}^{N_K} \sum_{j \in K} J(1 - \delta_{S'_i S_j}) + F_p. \quad (4)$$

The reorientation probability depends on the change of the energy $\Delta E = E_{t+\Delta t} - E_t$. To characterize the varying migration velocities of the recrystallizing grain boundaries due to the graded stored energy, the relationship between the reorientation probability and

the energy change is determined quantitatively. When the new energy state according to Eq. 4 is lower than the original energy state (Eq. 3), the orientation change is effectuated with a probability that corresponds to the ratio between the absolute value of ΔE and the maximum possible decrease of energy when the highest local stored energy is released. If the new energy state is exceeding the old one, the former orientation is maintained.

RESULTS

The simulated recrystallizing microstructures can be displayed in 3D at any simulation step. Hence, the microstructure evolution during recrystallization can be directly observed. Two simulated 3D microstructures representing an intermediate state and the stabilized recrystallization state are shown in Fig. 4a and 4b, respectively. The recrystallized grains can be identified in the deformed matrix with elongated grains by the approximately equiaxed shape. The two-dimensional microstructures in sections including the rolling direction and the direction normal to the rolling surface (i.e. those parallel to XOY plane, as indicated in Fig. 4) are microstructures generally investigated in metallography. Additionally, microstructures in sections parallel to the rolling surface (i.e. those parallel to XOZ plane in Fig. 4) and perpendicular to the rolling direction (i.e. those parallel to YOZ plane in Fig. 4) are also displayed.

The three-dimensional perspective effect of simulation provides an appropriate and efficient way to study inhomogeneous microstructures as well as their evolution. The gradually increasing nucleus density with distance from the end of the lowest deformation state is reflected by the microstructure at an early stage of recrystallization, and also by the distribution of recrystallizing grains at intermediate stages (Fig. 4a). The locally varying grain growth velocities result in different increases in the size of the recrystallizing grains at different locations after the same time interval, as shown by a sequence of microstructures revealed by YOZ sections (Fig. 4a). After long simulation times, the local (and, hence, the total) recrystallized volume fraction remains essentially constant as a result of the energy balance between the stored energy, acting as the driving force for nucleation and the growth of recrystallizing grains, and the dragging force from the fine particles. Consequently, a final stabilized microstructure with the graded sizes and volume fractions of the recrystallized grains is obtained (Fig. 4b).

Experiments were carried out for validation purpose. The deformed sample shown in Fig. 1b was at 380°C during 3 hours annealed for recrystallization. Afterwards, a series of parts of the sample were prepared metallurgically for the optical microscope and the scanning electron microscope (SEM). The inhomogeneously recrystallized microstructure was observed. Many stereological techniques that require random sampling for generating unbiased estimates (Yu and Liu, 1989) cannot be applied to microstructures with non-randomly distributed features. To describe as completely as possible the characteristics of such an inhomogeneous microstructure, 90 pictures were taken of sections that included the rolling direction and the direction normal to the rolling surface of the sample. As an example, Fig. 5 depicts a transition zone with respect to the deformation gradient. The macroscopic curvature of the deformed grains, the lower nucleus density and the smaller sizes of recrystallizing grains in the zones closer to the low

deformation end, are in qualitative agreement with the simulation predictions (see Fig. 4). The recrystallized volume fractions as a function of position, obtained separately from experiments and simulations, are compared in Fig. 6. Good quantitative agreement between the experimental and simulation results is found.

It is worth pointing out that, a traditional stereological technique as serial sectioning (Exner and Hougardy, 1988; Yu and Liu, 1989) perpendicular to the rolling direction (referring to Fig. 4a), would be more precise for characterizing the inhomogeneous microstructure in experiments. However, it will be enormously time- and energy-consuming (thus, impractical) to acquire the microstructural features of the whole sample with sufficient accuracy. Thus, in this respect, the visual simulation technique is obviously superior to the experimental methods.

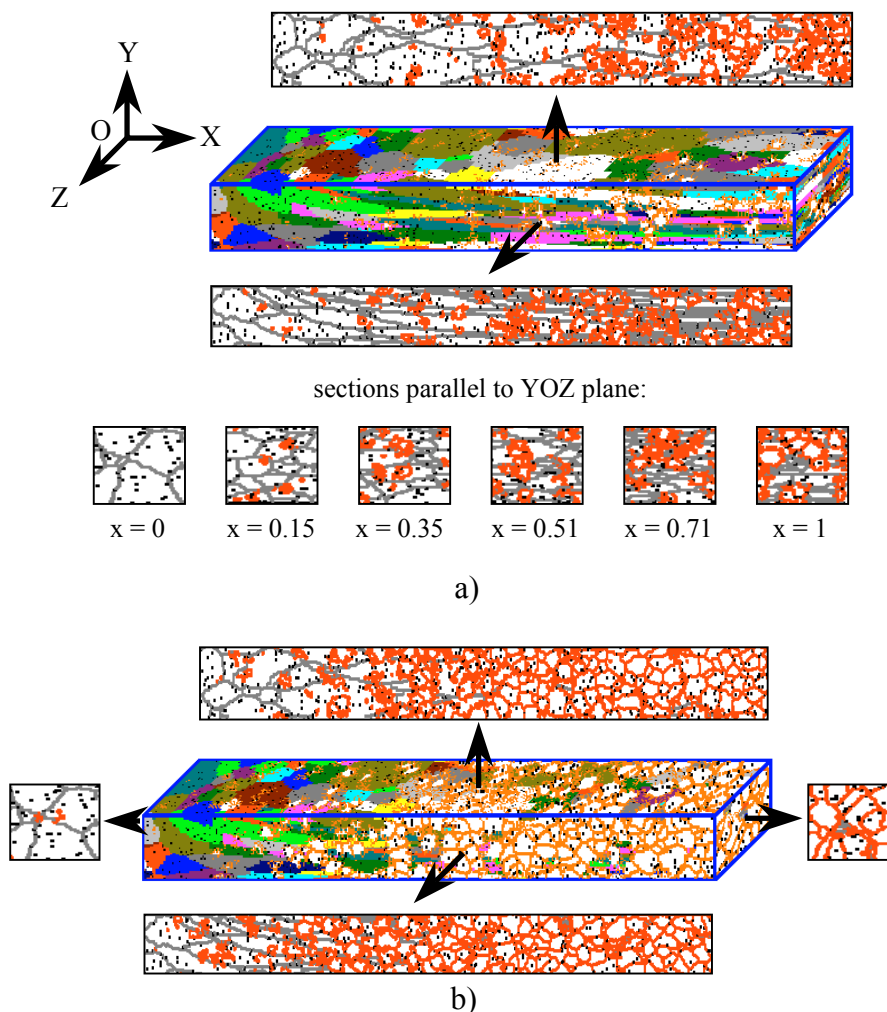


Fig. 4. Simulated microstructure evolution during recrystallization: a) intermediate state, with x as the relative distance from the low deformation end; b) final stabilized state.

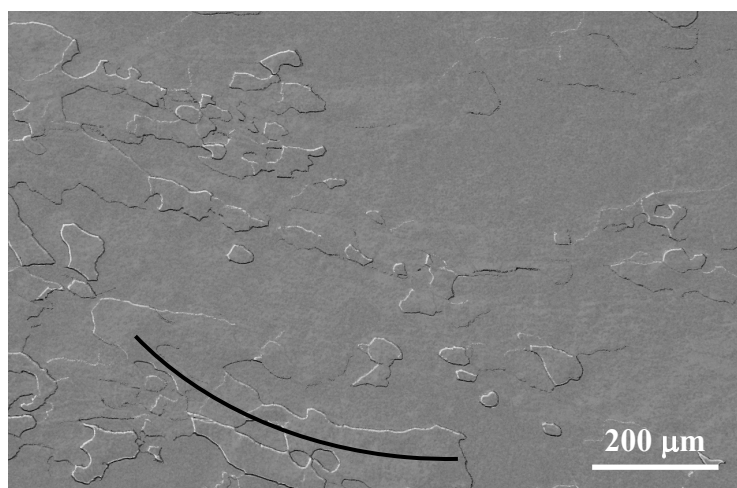


Fig. 5. Partially recrystallized microstructures of Al-0.5%Zr sample, taken at a relative distance $x = 0.05$ from the low deformation end. The line indicates the curved shape of deformed grains.

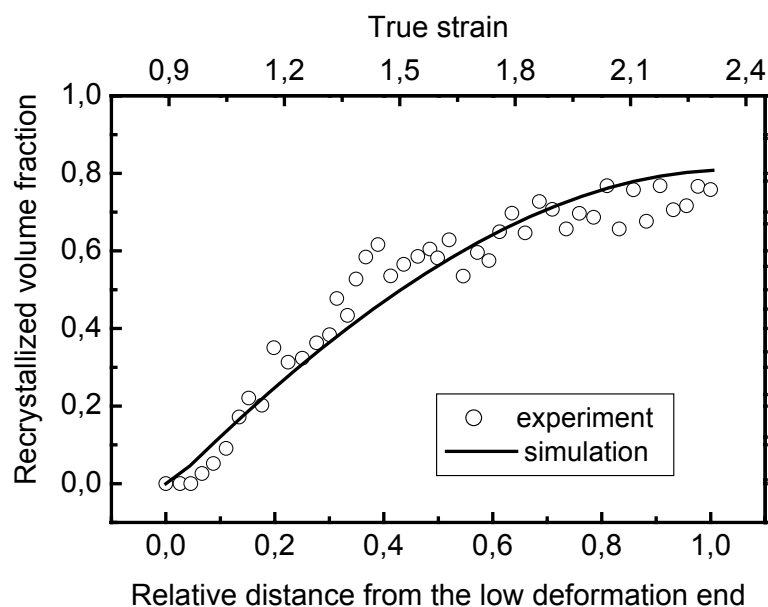


Fig. 6. Variation of the recrystallized volume fraction with position.

CONCLUSIONS

A 3D Monte Carlo model that correlates the stored energy, nucleus density and migration velocity of recrystallizing grain boundaries, to the local deformation, has been developed to simulate the recrystallization behavior in a material containing particles. The evolving microstructures were displayed both in three-dimensions and at different sections, guaranteeing an accurate description of characteristics of the inhomogeneous microstructures. The simulation results agree well both morphologically

and quantitatively with experiments of an Al-0.5wt.%Zr alloy containing Al_3Zr precipitates that has been subjected to graded deformation and annealing. In the case of large scale inhomogeneities in the microstructure, the technique of 3D computer visualization shows advantages for sampling, detection and measuring.

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