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Materials

Grain size distribution and topology in 3D grain growth simulation with large-scale Monte Carlo method

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Abstract: Three-dimensional normal grain growth was appropriately simulated using a Potts model Monte Carlo algorithm. The quasi-stationary grain size distribution obtained from simulation agreed well with the experimental result of pure iron. The Weibull function with a parameter β=2.77 and the Yu-Liu function with a parameter ν =2.71 fit the quasi-stationary grain size distribution well. The grain volume distribution is a function that decreased exponentially with increasing grain volume. The distribution of boundary area of grains has a peak at $S/\langle S\rangle$=0.5, where S is the boundary area of a grain and $\langle S\rangle$ is the mean boundary area of all grains in the system. The lognormal function fits the face number distribution well and the peak of the face number distribution is f=10. The mean radius of f-faced grains is not proportional to the face number, but appears to be related by a curve convex upward. In the 2D cross-section, both the perimeter law and the Aboav-Weaire law are observed to hold.

Key words: three-dimensional; grain growth; Monte Carlo simulation; grain size distribution; topology

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1. Introduction

The quasi-stationary state of three-dimensional (3D) grain growth and its associated grain size distribution and topology are fundamental issues of microstructural evolution. However, most of the observations both for the grain size distribution and topology are done on two-dimensional (2D) cuts to perform metallography studies. Owing to the expertise required and the tediousness of the 3D analysis methods such as grain separating [1] and serial section analysis [2-3], to date, only a few experimental studies have been done on the investigation of full 3D grain size distribution and topology. This limits the understanding of 3D grain growth (3DGG). Fortunately, in recent years, significant progress has been made in quantitative understanding of 3DGG using computer simulation techniques, including vertex model [4], surface evolver program [5], phase-field model [6], and Monte Carlo method [7-10]. In order to get high simulation efficiency, the scale of 3D simulations is normally small. However, such small-scale simulation cannot reflect exactly the nature of 3D grain growth. The possibly reason is that there is little grains in the simulation system and the quasi-stationary state cannot be attained in small-scale simulation. Therefore, it is of great importance to develop simulation algorithms in large scale and with high efficiency at the same time.

In this article, large-scale 3D normal grain growth was appropriately simulated using a Potts model Monte Carlo algorithm with high efficiency. The quasi-stationary state of grain growth was attained and the quasi-stationary grain size distribution was investigated. In the aspect of grain size distribution, the computer simulation, experimental result [2] and analytical theory [3, 11-12] are in good consistency. Grain topology both in 3D and 2D cross-sections was also intensively studied.

2. Computational methods

In our Monte Carlo simulation [13-15], a continuum microstructure was mapped onto a cubic lattice

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with full periodic boundary conditions. Each site in the lattice was assigned an index S_i(1-N) sequentially, corresponding to the orientation of the grain to which it belonged. Sites with the same index were considered to be part of the same grain and grain boundary only existed between neighbors with different orientations. The Potts model served as the grain boundary energy function:

$$E=-J\sum_{i=1}^{N}\sum_{j=1}^{N_N}(\delta_{S_iS_j}-1),\ \delta_{S_iS_j}=\begin{cases}1, & S_i=S_j\\ 0, & S_i\neq S_j\end{cases} \tag{1}$$

where J is the positive constant, which scales the boundary energy; N is the system size, N_N is the number of nearest neighbors j of site I; and δ is the Kronecher function. The simulation of grain growth involved the selection of a site S_i and its reorientation attempt. The reorientation attempt is restricted to the random site, adjacent to the selected site. Thus the net energy change associated with the reorientation trial can be expressed by

$$\Delta E_i=E_{i2}-E_{i1} \tag{2}$$

where E_{i1} and E_{i2} are the boundary energies of site i before and after the reorientation trial. The possibility of this reorientation is given by

$$W=\begin{cases}1, & \Delta E\le 0\\ \exp(-\Delta E/kT), & \Delta E>0\end{cases} \tag{3}$$

where k is the Boltzmann constant and T the absolute temperature; actually, they are thermal constants. The time is scaled by Monte Carlo step (MCS), which corresponds to the number of orientation trials equal to that of lattice sites.

The system contained N (300×300×300) sites on a cubic lattice with full periodic boundary conditions and the first, second, and third interactions were considered in the calculation of grain boundary energy. Now, the repeated procedure of Monte Carlo simulation was as follows.

(1) Each site was selected as a target at the same time.

(2) One of the sites in the range of the first, second, and third neighbors (*i.e.*, including 26 nearest neighbors) of the target was randomly selected and the orientation of the selected neighboring site was referred to a trial orientation of the target.

(3) The probability of the trial reorientation for the target was determined using Eq. (3) with the constant (kT/J)=0.5. 1 MCS corresponds to one reorientation trial for each site contemporaneously.

The grain volume V was determined by counting the lattice sites with the same index. The grain size R was defined as the sphere-equivalent radius. When the grain size distribution was referred, it was a function of the relative grain size r=R/<R>, where, <R> denotes the average grain size.

3. Simulation results and discussions

3.1. Microstructure and grain size, volume and boundary area distribution in 3D

Fig. 1 shows the simulated 3D microstructure in quasi-stationary state. It can be seen that a compact grain structure is developed. The grain boundaries are curved smoothly. The smaller convex grains will shrink with time, while the larger grains with concave faces will grow. This observation is consistent with the boundary motion by mean curvature.

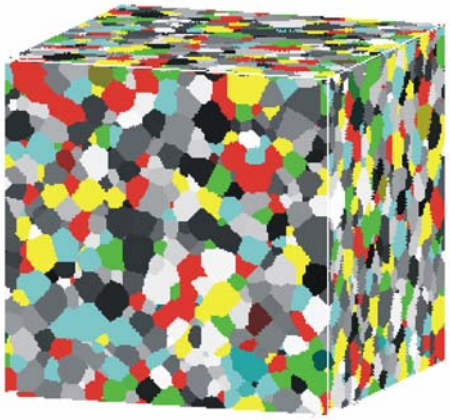

Fig. 1. Simulated microstructure in 3D.

The simulated grain size distribution and the experiment result of pure iron [2] from Zhang are plotted in Fig. 2. Our simulated grain size distribution has a peak at R/<R>=0.9 and its left-skewed shape agrees very well with the experiment result of iron. The distributions are compared with Hillert's theoretical distribution function [16], the Yu-Liu theoretical distribution function [11-12], the Weibull function, and the lognormal function. Hillert [14] obtains the grain size distribution from the mean field theory,

$$f(u)=(2\mathrm{e})^{\beta}\frac{\beta u}{(2-u)^{2+\beta}}\exp(-\frac{2\beta}{2-u}) \tag{4}$$

where u=R/R_{cr}, R_{cr} is the critical grain size. β=3, R_{cr}=(9/8)<R> in 3D; β=2, R_{cr} =<R> in 2D. Unfortunately, Hillert's distribution in 3D has not been verified in practice. As seen in Fig. 2, Hillert's distribution has a peak at 1.1, which is larger than our simulation result and the experiment result of iron.

In 1997, based on Hillert's classical mean-field rate equation, Yu and Liu theoretically derived a set of analytical quasi-stationary grain size distributions [3].

Such grain size distributions were reconfirmed by Wang *et al*. [11]. Two years later, Rios independently obtained the same results [9]. The Yu-Liu distribution has the form:

$$f(r)=\frac{2H_0\xi_1{}^2 r\nu^{H_0}}{(\xi_1{}^2 r^2-\xi_1\nu r+\nu)^{1+H_0}}\exp\left\{\frac{-2H_0\nu}{\sqrt{4\nu-\nu^2}}\left[\arctan\left(\frac{2\xi_1 r-\nu}{\sqrt{4\nu-\nu^2}}\right)+\arctan\left(\frac{\nu}{\sqrt{4\nu-\nu^2}}\right)\right]\right\} \quad (5)$$

where, $\nu<4$, $\xi_1=\langle R\rangle^2/\langle R^2\rangle$, $H_0=(\nu/2)(f/r)_{r=0}$, and ν is the only parameter. As seen in Fig. 2, good agreement was obtained when the Yu-Liu distribution was compared with our computer simulation and experiment result. The correlation coefficient (R) is 0.975. The convergences of the experimental result, analytical theory, and computer simulation show the consistency of these three methods.

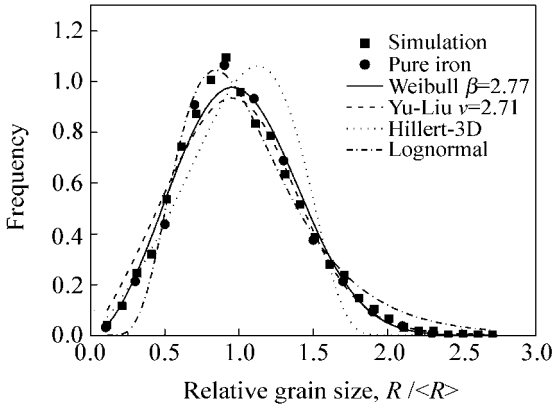

Fig. 2. Quasi-stationary grain size distribution in 3D.

The Weibull function was observed to describe well some 2D and 3D grain size distributions from the computer simulations and experiments [13]. However, it is only a cited function without specific physical meaning. The Weibull function has the form:

$$f(r)=\frac{\beta}{\alpha^{\beta}}r^{\beta-1}\exp[-(\frac{r}{\alpha})^{\beta}] \quad (6)$$

where α and β are the distribution parameters. $\alpha=1/\Gamma(1+1/\beta)$, where Γ is the gamma function. Therefore, Eq. (6) is a function of only one free parameter β. Our simulated grain size distribution and experiment result are compared with the Weibull function in Fig. 2. It can be seen that the Weibull function can describe very well our simulation and experiment. The correlation coefficient (R) is 0.985, which is slightly higher than that of Eq. (5). The lognormal function is also compared with the simulated grain size distribution and the experiment result in Fig. 2. However, it can be seen that both the Weibull function and the Yu-Liu distribution fit the data better than the lognormal function.

The distributions of grain volumes and boundary area are plotted in Fig. 3. The grain volume distribution is a function that decreased exponentially with increasing grain volume. The distribution of boundary area of grains had a peak at $S/\langle S\rangle=0.5$. These results are consistent with the experiment data of iron [2] and other computer simulation [5].

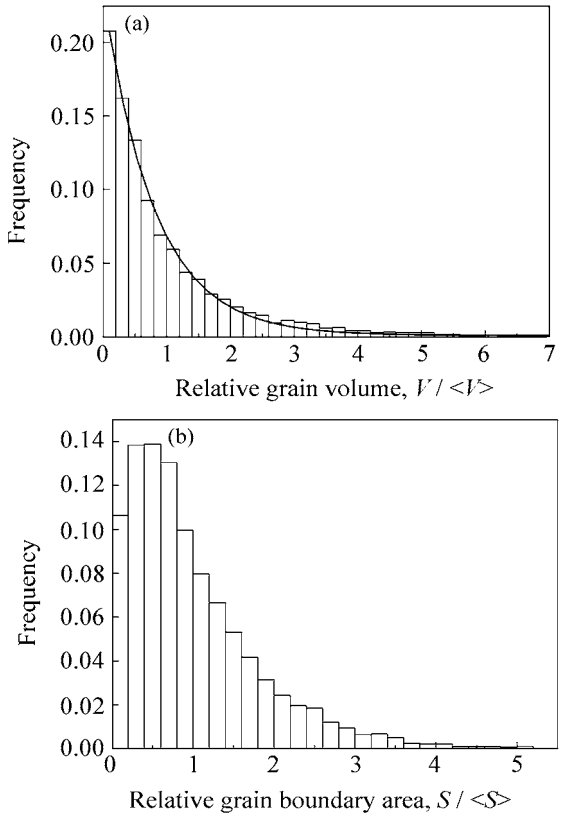

Fig. 3. Grain volume distribution (a) and grain boundary area distribution (b) during three-dimensional grain growth simulation.

3.2. Distribution of the number of grain faces in 3D

Fig. 4 shows the distribution of grain face numbers, or the number of nearest neighbor grains. The peak of the distribution is seen to be $f=10$. The lognormal function with parameters $\sigma=0.36$ and $\mu=11.38$ can describe the grain face distribution very well. The shape of distribution reported by other computer simulation [5] and experiment results [2-3] in 3D agreed with our result very well. The average number of faces per grain fluctuated around 12.95 in the quasi-stationary grain growth.

3.3. Microstructure in 2D cross-section

The microstructure and the distribution of the number of edges per grain in 2D cross-section are shown in Figs. 5 and 6, respectively. Various microstructural features of normal grain growth commonly observed in real materials are also seen in the simula-

tion microstructure. For example, the grains with faces more than 6 have concave grain boundaries and grains with faces less than 5 have convex grain boundaries, and 120° angles are found at most grain corners. The peak of the distribution is n=6 and the number of edges per grain in 2D cross-section is between 3 and 8.

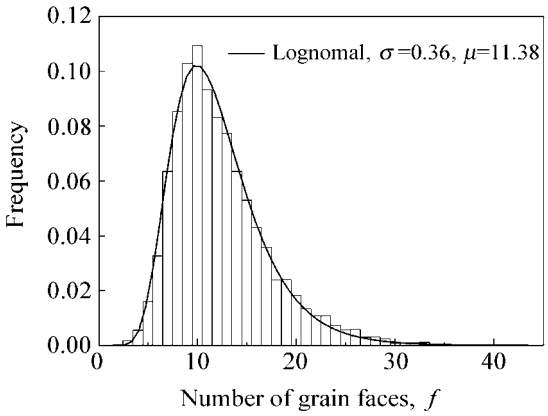

Fig. 4. Grain face number distribution.

Fig. 5. Microstructure in 2D cross-section.

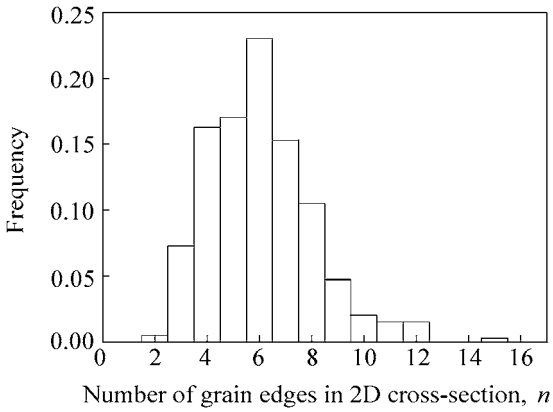

Fig. 6. Grain edge distribution in 2D cross-section.

3.4. Aboav-Weaire law in 2D cross-section

The Aboav-Weaire law in 2D [15] is the relation between the number of sides n of a grain and the mean number M_n of the sides of neighboring cells surrounding it. It has the form,

$$M_n = a + \frac{b+\mu}{n} \tag{7}$$

where, μ is the variance of n, a=5, and b=6. The mean value $<nM_n>$ against n is plotted in Fig. 7. The relation of $<nM_n>$=4.84 n+8.86 is obtained by a linear fit. Although the coefficient is different from Eq. (7), the linear relation is excellent.

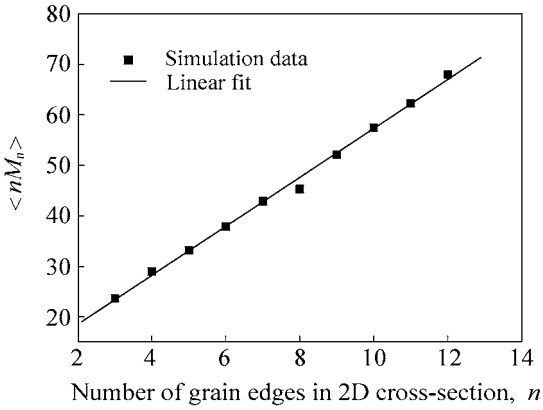

Fig. 7. Relationship between the number of edges n and $<nM_n>$ in 2D cross-section.

3.5. Perimeter law in 2D cross-section and 3D

Lewis proposed the relation between the size and the coordination number of cellular random networks in 2D [16]; the average area of cells was proportional to the number of sides. Polycrystals are not "ideal" random structures. Rivier [19] found the most probable distributions of cell sizes and shapes, which maximized entropy. The energy constraint in grain growth gives a 2D-perimeter law,

$$< R(n) >= \beta(n - n_0) \tag{8}$$

where, $<R(n)>$ is the mean radius of n-sided cells. In order to obtain the perimeter law, $<R(n)>$ is plotted as a function of the number of edges per grain in 2D cross-section in Fig. 8. It is seen that the fit of the perimeter law to the simulation results was very good. The relative average area of grains $<A(n)>/<A>$ is also plotted as a function of the number of edges per grain in 2D cross-section in Fig. 9. Where $<A(n)>$ is the mean area of n-sided cells and $<A>$ the mean area of all cells in 2D cross-section. The relationship between $<A(n)>/<A>$ and n is expressed by a curve. Lewis's suggestion is not observed to hold in 2D cross-section of grain structure.

Fig. 10 illustrates the size distribution of f-faced grains for various f values. As expected, the peak of the distribution is located at a larger grain radius with increasing f values. In three dimensions, the grain radius may be related linearly to the face number ac-

cording to the perimeter law. The mean radius of f-faced grains $\langle R_f \rangle$ is plotted against f in Fig. 11. It is seen that the mean radius is related to the face number by a curve convex upward. This curve agrees with the experimental observation for Al and pure iron [2, 20]. Thus, the perimeter law in three dimensions is unlikely to hold. The relation indicates that the larger grains are surrounded by the larger number of neighbors.

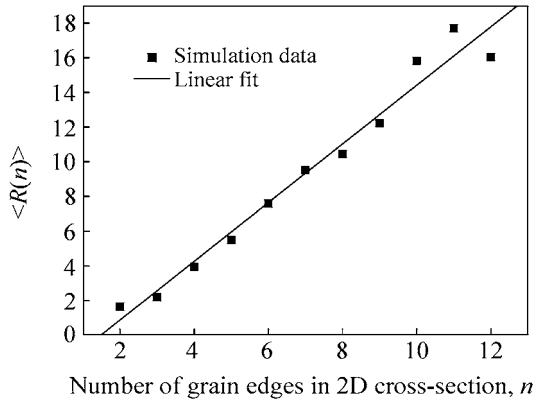

Fig. 8. Relationship between the number of grain edges n and grain radius $\langle R(n) \rangle$ in 2D cross-section.

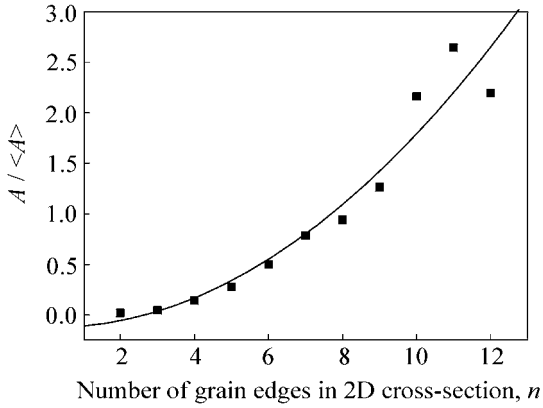

Fig. 9. Relationship between the number of grain edges n and relative grain area in 2D cross-section.

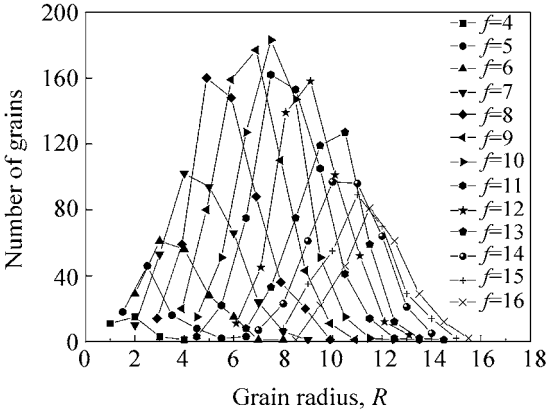

Fig. 10. Distribution of radius of f-faced grains.

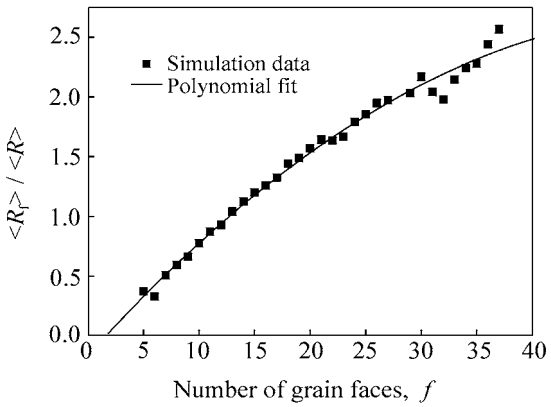

Fig. 11. Relationship between the number of grain faces and the relative radius.

4. Conclusions

(1) The quasi-stationary grain size distribution obtained from simulation agrees well with the experiment result of pure iron. The Weibull function with a parameter β=2.77 and the Yu-Liu function with a parameter ν =2.71 fit the quasi-stationary grain size distribution well.

(2) The lognormal function fits the face number distribution well and the peak of the face number distribution is f=10. The grain volume distribution is a function that decreased exponentially with increasing grain volume. The distribution of boundary area of grains has a peak at $S/\langle S \rangle$=0.5.

(3) The mean radius of f-faced grains is not proportional to the face number, but appears to be related by a curve convex upward.

(4) In the 2D cross-section, the perimeter law and the Aboav-Weaire law are observed to hold.

References

[1] F.C. Hull, Plane section and spatial chacteristics of equiaxed β-brass grains, *Mater. Sci. Technol.*, 4(1988), p.778.

[2] C. Zhang, A Suzuki, T. Ishimaru, and M. Enomoto, Characterization of three-dimensional grain structure in polycrystalline iron by serial sectioning, *Metall. Mater. Trans. A*, 35(2004), p.1927.

[3] H.B. Yu, *Quantitative Geometrical Characterization, Grain Growth Theories and Computer Simulation in Single-Phase Materials* [Dissertation], University of Science and Technology Beijing, Beijing, 1997, p.116.

[4] D. Weygand, Y. Brechet, J. Lepinoux, and W. Gust, Three-dimensional grain growth: a vertex dynamics simulation, *Philos. Mag. B*, 79(1999), p.703.

[5] F. Wakai, N. Enomoto, and H. Ogawa, Three-dimensional microstructural evolution in ideal grain growth-general statistics, *Acta Mater.*, 48(2000), p.1297.

[6] C.E. Krill and L.Q. Chen, Computer simulation of 3-D grain growth using a phase-field model, *Acta Mater.*, 50(2002), p.3057.

[7] H. Wang, G.Q. Liu, and X.G. Qin, Simulation study of evolution from an initial grain structure with Weibull grain size distribution, *J. Univ. Sci. Techno.l Beijing* (in Chinese), 30(2008), p.848.

[8] C. Wang and G.Q. Liu, Verification of topological relationship in 2-D grain growth process by simulation, *J. Univ. Sci. Technol. Beijing*, 11(2004), No.2, p.138.

[9] X.Y. Song and G.Q. Liu, Three-dimensional and cross-sectional characteristics of normal grain growth based on Monte Carlo simulation, *J. Univ. Sci. Technol. Beijing*, 5(1998), No.3, p.129.

[10] X.Y. Song and G.Q. Liu, Discussion on the Hillert theory of normal grain growth with a modified Monte Carlo simulation, *J. Univ. Sci. Technol. Beijing*, 4(1997), No.1, p.24.

[11] C. Wang and G.Q. Liu, Reanalysis of the 3D quasi-stationary grain size distribution based on Hillert's grain growth rate equation, *Sci. China Ser. E*, 47(2004), p.112.

[12] P.R. Rios, Comparison between a computer simulated and an analytical grain size distribution, *Scripta Mater.*, 40(1999), p.665.

[13] X.G. Qin, *Study on Potts Models for Grain Growth with Different Algorithms and Parameters* [Dissertation], University of Science and Technology Beijing, Beijing, 2003, p.39.

[14] H. Wang, G.Q. Liu, and X.G. Qin, Verification of 3D grain growth rate equations with large-scale Potts model Monte Carlo simulation, *Acta Metall. Sin.* (in Chinese), 44(2008), p.13.

[15] H. Wang and G.Q. Liu, Evaluation of growth rate equations of three-dimensional grains using large-scale Monte Carlo simulation, *Appl. Phys. Lett.*, 93(2008), p.131902-1.

[16] M. Hillert, On the theory of normal and abnormal grain growth, *Acta Metall.*, 13(1965), p.227.

[17] D. Weaire, Some remarks on the arrangement of grains in a polycrystal, *Metallography*, 7(1974), p.157.

[18] F.T. Lewis, The correlation between cell division and the shapes and sizes of prismatic cells in the epidermis of cucumis, *Anat. Rec*., 38(1928), p.341.

[19] N. Rivier, Statistical crystallography structure of random cellular networks, *Phil. Mag. B*, 52(1985), p.795.

[20] F.N. Rhines and B.R. Patterson, Effect of the degree of prior cold work on the grain volume distribution and the rate of grain growth of recrystallized aluminum, *Metall. Trans. A*, 13(1982), p.985.