Available online at www.sciencedirect.com

jmr&t
Journal of Materials Research and Technology
www.jmrt.com.br

Original Article

Microstructural descriptors to characterize computer simulated microstructures generated by nucleation on a Kelvin polyhedra network☆

Guilherme Dias da Fonseca*, Felipe da Silva Siqueira, André Luiz Moraes Alves, Weslley Luiz da Silva Assis, Paulo Rangel Rios

Universidade Federal Fluminense, Escola de Engenharia Industrial Metalúrgica de Volta Redonda, Av. dos Trabalhadores, 420, Volta Redonda, RJ 27255-125, Brazil

ARTICLE INFO

ABSTRACT

Computer simulation is used to generate microstructures by nucleation on a 3D network of Kelvin polyhedra. The Kelvin polyhedra network was used as a model for a polycrystalline network. Information provided by usual descriptors of microstructural evolution: the volume fraction and mean interfacial area density are perhaps insufficient to fully characterize those microstructures. Therefore, microstructural descriptors that are less often used such as the contiguity, the contiguity ratio, the dispersion parameter and the duplex parameter were tested. These parameters showed to be able to increase the understanding of the microstructural changes for Kelvin polyhedra/grain boundary nucleated transformations. The contiguity and the dispersion parameter were particular useful to provide better understanding of the microstructural evolution studied here.

© 2018 Brazilian Metallurgical, Materials and Mining Association. Published by Elsevier Editora Ltda. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

1. Introduction

Nucleation and growth transformations are often described by two main stereological parameters: the volume fraction, V_V, of the new phase, here denoted the β phase and the mean interfacial area density between the new and the parent phase, S_V or $S_V^{\alpha\beta}$, where the parent phase is here denoted the α phase. Using these parameters, one may describe the micro-structural evolution by plotting the transformation kinetics, i.e. V_V as a function of time and the microstructural path (MP) [1], that is, S_V as a function of V_V. This methodology describes microstructural evolution well when the nucleation sites are uniform randomly distributed in space. The location of the nuclei is clearly very important to phase transformations and it is the subject of study of several researchers [2–4]. In fact, in many cases the nuclei might not be uniform randomly distributed in space. For example, nucleation sites may be located within spherical clusters [5] or on the grain boundaries or grain edges [2]. Under those circumstances the characterization of microstructural evolution using stereological parameters becomes more complex. In those cases, the volume fraction and the microstructural path are not perhaps enough on their own to fully describe the characteristics of the microstructural

evolution. For those more complex cases, the usage of additional parameters that are defined below were proposed. It is thought that some of those additional parameters might be helpful to understand microstructural evolution better in those complex situations. One advantage of those parameters is that they are still defined in terms of two easily measurable stereological quantities. The first quantity is the mean interfacial area density between the parent phase, $S_V^{\alpha\alpha}$, that expresses how much of the grain boundaries are consumed by the new phase over transformation time. The second is the mean interfacial area density between the new phase, $S_V^{\beta\beta}$, that expresses how much new interface is created. Notice that for, $V_V \to 1$, $S_V^{\alpha\alpha} \to 0$, and $S_V^{\beta\beta} \to$ constant.

These two interfacial parameters may be combined with volume fraction and mean interfacial area density between the new and the parent phase so that new useful parameters may be defined [1,6]. First one can define the contiguity, which is a parameter that quantifies the amount of contact between the grains of the same phase, or the degree of adjacency of each phase. The contiguity of either the parent, $C^{\alpha\alpha}$, or the new phase, $C^{\beta\beta}$ can be estimated by Eqs. (1) and (2), respectively.

$$C^{\alpha\alpha} = \frac{2S_V^{\alpha\alpha}}{S_V^{\alpha\beta} + 2S_V^{\alpha\alpha}} \tag{1}$$

$$C^{\beta\beta} = \frac{2S_V^{\beta\beta}}{S_V^{\alpha\beta} + 2S_V^{\beta\beta}} \tag{2}$$

The advantage of using the contiguities is that when $V_V \to 1$, $C^{\alpha\alpha} \to 0$, and $C^{\beta\beta} \to 1$. Another possible parameter is simply the ratio of the contiguities: $C^{\alpha\alpha}/C^{\beta\beta}$.

Other two interesting parameters proposed by Hornbogen [6] are the dispersion, δ, and the duplex, Δ, Eqs. (3) and (4), respectively. The dispersion parameter seeks to quantify the scattering of particles of a new phase, which are isolated from each other by the parent phase. On the other hand, the duplex parameter presents a relationship between the interfacial area density of the parent phase and the new phase.

$$\delta = \frac{S_V^{\alpha\beta}}{S_V^{\alpha\alpha}} \tag{3}$$

$$\Delta = \frac{S_V^{\beta\beta}}{S_V^{\alpha\alpha}} \tag{4}$$

All the above parameters attempt to describe the position of the transformed regions relative to one another. Some of them are especially useful here, as will be seen in what follows.

In this work computer simulation is carried out with the intention of studying the effect of nucleation on the grain boundaries on the microstructural evolution. Specifically, we wish to find out which of the stereological parameters defined above better characterize the evolving microstructures. In the present simulations, the polycrystal is represented by a space-filling network of Kelvin polyhedra [7]. We compare transformations in which nuclei are uniform randomly located within space with transformations in which nuclei are located on the Kelvin polyhedra network interfaces.

2. Computer simulation methodology

Computer simulation of the 3D nucleation and growth transformation was carried out using the causal cone method [8–10]. The matrix comprised $304 \times 304 \times 304$ cubic cells. To assign physical dimensions to the simulation we regard each cubic cell edge length to be equal to $1\,\mu m$. Therefore, our "sample" was a cube with a total edge length of $304\,\mu m$. Of course, periodic boundary conditions used here ensured that the simulation space was "infinite". Within this cubic matrix a network of Kelvin polyhedra was constructed. Nucleation took place on the interfaces of this network. The absolute number of nuclei, N, used were $N = 28$, $N = 438$, $N = 1040$ and $N = 3511$. These number of nuclei were adopted to obtain final grain sizes between 10 and $150\,\mu m$, approximately. Site-saturated nucleation was used in all simulations. That is, all nucleation takes place at the start of the transformation so that the number of nuclei remains the same and only growth takes place over time. All growth velocities were kept constant.

3. Nucleation and growth kinetics

Fig. 1 shows two examples of nucleation on the boundaries of the Kelvin polyhedra network. Fig. 2 shows the transformation kinetics, volume fraction against time, for a varying number of nuclei. The solid curves are calculated from Johnson-Mehl, Avrami and Kolmogorov [11–13], the so-called JMAK theory, for homogeneous nucleation and provide a frame of reference to evaluate the effect of nucleation on the boundaries. The kinetic curves fall fairly close to the JMAK theory and significant deviation only starts to be visible when one has $N = 3511$ nuclei on the boundaries. Thus, the kinetics is not very sensitive to the nucleation site except for a large number of nuclei.
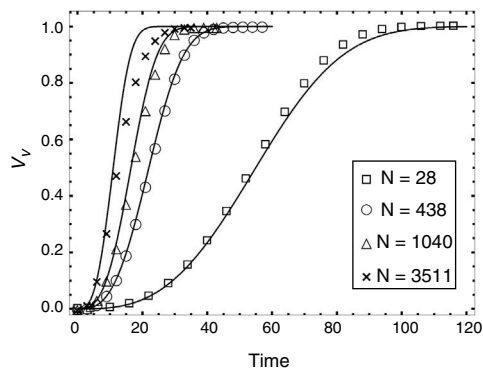
4. Microstructural path (MP)

Fig. 3 depicts the microstructural path (MP) of the transformations. The solid curves correspond to the MP for homogeneous site-saturated nucleation [8]:

$$S_V = (36\pi N_V)^{1/3} (1 - V_V) \left(\ln \left(\frac{1}{1 - V_V} \right) \right)^{2/3} \tag{5}$$

where N_V is the number of nuclei per unit of volume and V_V was calculated by JMAK theory. The curves generated by Eq. (5) are used as a reference in Fig. 3. The MP is more sensitive to the nucleation site than the kinetics. The total interface area of a certain new phase region is the sum of two components: the interface area between parent phase/new phase, $S_V^{\alpha\beta}$, and the interface area between new phase/new phase, $S_V^{\beta\beta}$. We think that the position of nuclei in space affects more significantly the magnitude of each component thus affecting any interface area-based indicator more strongly than the volume fraction. One can see that, already for $N = 1040$ nuclei a significant discrepancy between Eq. (5) and the transformation nucleated at the boundaries can be seen. For $N = 3511$ nuclei the MP of Eq.
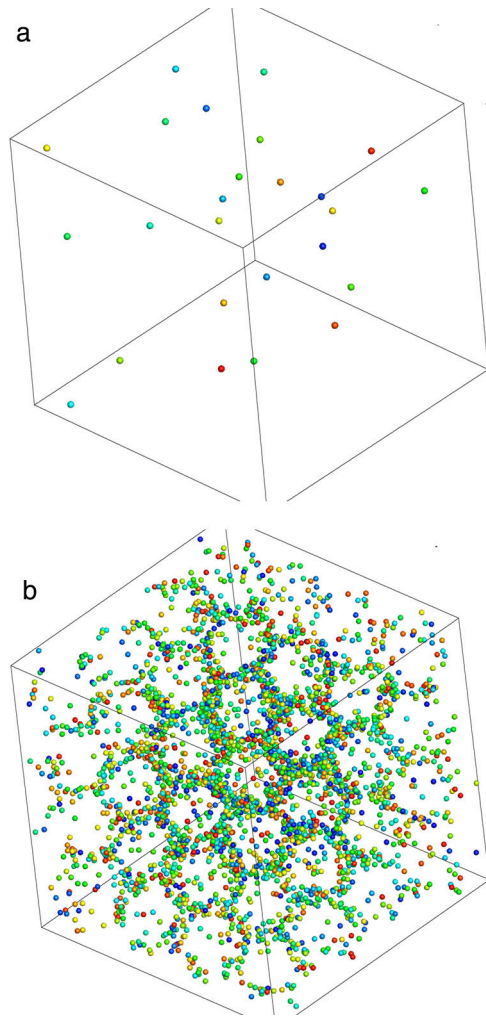
Fig. 1 – **Computer simulated microstructures of the early stage of the transformations nucleated on the Kelvin polyhedra network. (a) Low number of nuclei showing that the nuclei behavior approaches the behavior of the uniform nucleation. (b) High number of nuclei showing the Kelvin polyhedra network saturated by nuclei.**

Fig. 2 – **Transformation kinetics for the transformation nucleated on the Kelvin polyhedra network. The solid lines serve as a reference and were calculated from JMAK [11–13] theory.**
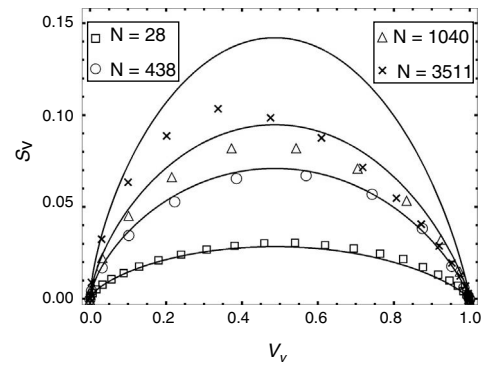

Fig. 3 – **Microstructural path for the transformation nucleated on the Kelvin polyhedra network. The solid lines serve as a reference and were calculated from Eq. (5).**

(5) is far from that produced by the simulation. The discrepancies in the kinetics and in the MP increase as the number of nuclei increases. The higher is the number of nuclei on the grain boundary the higher is the "clustering" effect meaning a less homogeneous nuclei dispersion. Strictly speaking, the kinetic curves deviate from JMAK as soon as the underlying point process is not a Poisson Point Process anymore. Thus, for any N the kinetic curve deviates from JMAK. The fact is that the deviation, although mathematically present, is initially small for visual detection. Obvious visual discrepancy only takes place for large N. Therefore, the sensitivity is more a matter of whether one can visually distinguish the curves rather than a mathematical issue. Of course, if this were only a mathematical issue we could perhaps use the kinetic curves. But the point of the study is to determine which indicator is more appropriated to be used in real microstructures. In those cases, one must consider experimental errors. So, a higher sensitivity is extremely important as it permits the detection of specific characteristics even in the presence of experimental errors. If the sensitivity is too small, say well below the experimental errors then the indicator is not going to be able to show any difference between two situations.

5. Contiguity

Fig. 4 depicts the contiguity of the new phase, Eq. (2). Fig. 5 shows the contiguity ratio: $C^{\alpha\alpha}/C^{\beta\beta}$. In Fig. 4 the solid line corresponds to the contiguity of homogeneous nucleation. It is interesting to compare Fig. 4 with Fig. 5 of Rios et al. [14]. In their work, Rios et al. [14] used cellular automata to simulate transformations with nuclei location ranging from periodic to clusters. A periodic nucleation resulted in a contiguity curve *below* the solid curve that represents uniform nucleation. This suggests that for a small number of nuclei, $N = 28$, the periodic nature of the Kelvin polyhedra network predominated, and one can see in Fig. 4 that the simulated results for $N = 28$ nuclei are located below the curve for uniform nucleation, consistent with the result from Rios et al. [14]. In contrast, the curves for higher number of nuclei are located *above* the solid curve for uniform nucleation, suggesting that the clustering effect represented by nucleation on the boundaries
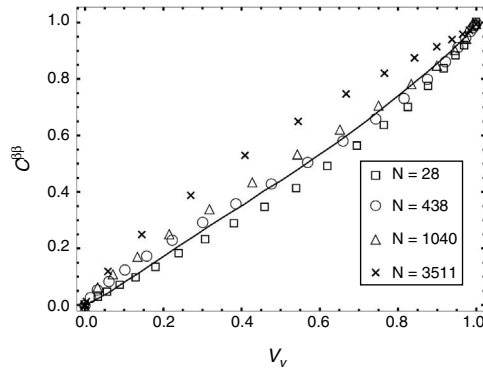
Fig. 4 – Contiguity of the new phase as a function of volume fraction transformed. The solid line represents the situation in which nucleation takes place uniform randomly throughout the matrix.
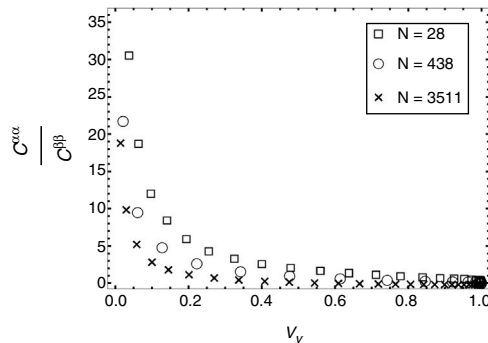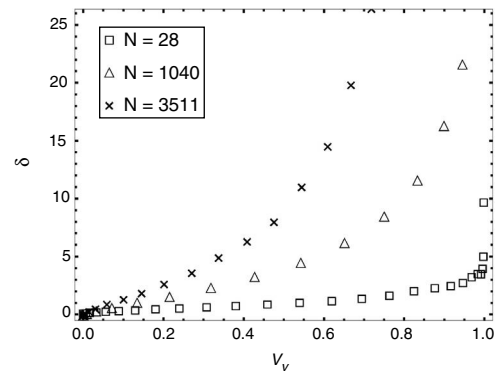

Fig. 5 – Contiguity ratio, $C^{\alpha\alpha}/C^{\beta\beta}$, as a function of volume fraction transformed.

Fig. 6 – Dispersion parameter, δ, as a function of volume fraction transformed.

Fig. 7 – Duplex parameter, Δ, as a function of volume fraction transformed.

predominates for higher number of nuclei. Again this is similar to what was observed by Rios et al. [14] for nucleation within clusters. Vandermeer [1] has already remarked this tendency of the behavior of the contiguity for nucleation in clusters.

The contiguity ratio shown in Fig. 5 does not seem to add new information to what was already obtained from the behavior of the contiguity of the new phase shown in Fig. 4. Of course, the contiguity ratio curves are asymptotic to the vertical and horizontal axes. This is so because when $V_V \to 0$, $C^{\alpha\alpha} \to 1$, and $C^{\beta\beta} \to 0$ and when $V_V \to 1$, $C^{\alpha\alpha} \to 0$, and $C^{\beta\beta} \to 1$.

6.   Dispersion and duplex parameters

Figs. 6 and 7 depict the dispersion and duplex parameters, Eqs. (3) and (4) respectively. Both parameters have a similar behavior in this case. The reason for this is that at some point during the transformation the interfaces of the parent phase, $S_V^{\alpha\alpha}$, are consumed by the growing new phase. When the number of nuclei is small, say 28, the nuclei behavior approaches the behavior of the uniform nucleation and the interfaces of the parent phase, $S_V^{\alpha\alpha}$, are fully consumed only toward the very end of the transformation, when $V_V \to 1$, $S_V^{\alpha\alpha} \to 0$ so that both δ and $\Delta \to \infty$. Alternatively, for a large number of nuclei at the
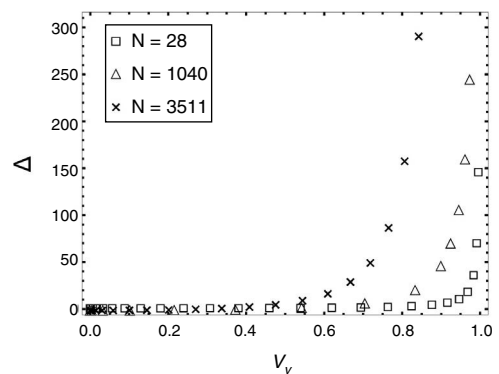
boundaries, the boundaries are fully consumed quickly so that $S_V^{\alpha\alpha} \to 0$ before V_V reaches one. In Fig. 6, $\delta \to \infty$ for V_V between 0.6 and 0.7. Fig. 6 shows that in the case of grain boundary nucleated reactions the dispersion parameters are very sensitive to nuclei density on the boundaries. Fig. 7 essentially shows the same information, but the asymptotic behavior appears to take place for higher volume fractions for the same number of nuclei. Therefore, it seems that the dispersion parameter, Eq. (3), is the most useful parameter.

7.   Summary and conclusions

In this work, several stereological parameters were tested to see which ones were more useful to describe microstructural evolution of grain boundary nucleated transformations. The main conclusions are:

- The kinetics, volume fraction against time curve, is the least sensitive to nuclei location.
- The microstructural path was revealed significant more sensitive to nuclei location than the kinetics.
- The contiguity of the parent phase was revealed to be quite a useful parameter and exhibited trends that were consistent with those observed in previous work [14]. In contrast,

the contiguity ratio did not seem to add new significant information.

- The dispersion parameter was strongly sensitive to nuclei location. In the present case both the dispersion and the duplex parameter behaved similarly but the dispersion parameter appears to be the best choice.
- The contiguity of the new phase, Eq. (2), and the dispersion parameter Eq. (3), showed to be useful parameters to measure in addition to the usual volume fraction and mean interfacial area density between the parent and the new phase.
- In summary, both the dispersion and the contiguity supplied information about microstructural evolution that would be hard to infer without their use.

Conflicts of interest

The authors declare no conflicts of interest.

Acknowledgements

REFERENCES

[1] Vandermeer RA. Microstructural descriptors and the effects of nuclei clustering on recrystallization path kinetics. Acta Mater 2005;53:1449–57.

[2] Cahn JW. The kinetics of grain boundary nucleated reactions. Acta Metall 1956;4:449–59.

[3] Rios PR, Honeycombe RWK. Effect of niobium on decomposition of austenite in 0.2C–10Cr steel. Mater Sci Technol 1992;8:1057–62.

[4] Rickman JM, Barmak K. Kinetics of first-order phase transitions with correlated nuclei. Phys Rev E 2017;22121: 1–5.

[5] Villa E, Rios PR. Transformation kinetics for nucleus clusters. Acta Mater 2009;57:3714–24.

[6] Hornbogen E. On the microstructure of alloys. Acta Metall 1984;32:615–27.

[7] Da Fonseca GD, Alves ALM, Da Costa MB, Lyrio MS, Assis WLDS, Rios PR. Modeling and simulation of nucleation and growth transformations with nucleation on interfaces of Kelvin polyhedra network. Mater. Sci. Forum 2018 [in press].

[8] Rios PR, Villa E. Transformation kinetics for inhomogeneous nucleation. Acta Mater 2009;57:1199–208.

[9] Alves ALM, Assis WLS, Rios PR. Computer simulation of sequential transformations. Acta Mater 2017;126: 451–68.

[10] Alves ALM, Villa E, Rios PR. Transformation kinetics for nucleation on second-phase particles: analytical solution and computer simulation. Acta Mater 2017;131:523–33.

[11] Johnson WA, Mehl RF. Reaction kinetics in processes of nucleation and growth. Trans Metall Soc AIME 1939;135:416–41.

[12] Avrami M. Kinetics of phase change. I. General theory. J Chem Phys 1939;7:1103.

[13] Kolmogorov AN. On the statistical theory of metal crystallization. Isvetiia Acad Nauk SSSR-Seriia Mat 1937;1:335–59.

[14] Rios PR, Pereira LO, Oliveira FF, Assis WLDS, Castro JA. Impingement function for nucleation on non-random sites. Acta Mater 2007;55:4339–48.