Original Article

Computer simulation of site saturation and constant nucleation rate transformations on a network of Kelvin polyhedra

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ABSTRACT

A crucial step of transformations in solids is that of nucleation. To model nucleation, one must specify nuclei location in space as well as how nuclei appear as a function of time. In the classical theory of Johnson–Mehl–Avrami–Kolmogorov (JMAK), there are two essential nucleation modes. One is site-saturation in which all nucleation sites are exhausted early in the transformation. Another is the so-called constant nucleation rate. JMAK theory considers that nuclei are located uniform randomly within the matrix both in the case of site-saturation and constant nucleation rate. Nonetheless, it is usually common in polycrystals to observe nucleation taking place on the grain surfaces, edges, and vertices. Cahn proposed analytical expression for such situations. In this work, we conduct a computer simulation considering that grains can be represented by a network of Kelvin polyhedra. We restrict nucleation to the grain boundaries of the Kelvin network. Grain boundary nucleation can be either site-saturated or a constant nucleation rate. We compare the effect of these two nucleation modes. JMAK theory and Cahn’s theory are applied to the simulated results. The microstructures are characterized by several quantitative metallographic parameters. We observed that the two nucleation modes exhibited similar behavior.

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1. Introduction

Johnson–Mehl [1], Avrami [2], and Kolmogorov [3] (JMAK) employed uniform randomly nuclei. By contrast, Cahn supposed that nucleation took place on the grain faces, edges, and vertices [4,5].

Kelvin’s polyhedron has been used to represent a grain for quite some time. The advantage of using Kelvin’s polyhedron to represent a grain is that a polycrystal can be represented by a network of Kelvin’s polyhedra. In the present work, this representation is taken as the starting point of our simulation.

Two nucleation modes are exemplary to the transformation kinetics. One mode is the so-called site-saturated in which all nucleation sites are exhausted early in the transformations. In other words, all nuclei appear at $t = 0$, and no further nucleation takes place for $t > 0$. The other mode is the so-called constant nucleation rate. In this case, nuclei appear at a con-
stant rate. In other words, an equal number of nuclei appears per unit of volume per unit of time throughout the transformation.

In previous work [6], we examined the transformation nucleated by site-saturation on a network of Kelvin’s polyhedra. In this paper, we compare site-saturated and constant nucleation rate transformations on the same network. Moreover, we use microstructural descriptors proposed in Fonseca et al. [7] that worked very well to characterize transformations nucleated on a network of Kelvin polyhedra.

2. The theory of Johnson–Mehl, Avrami, and Kolmogorov, JMAK

Over 80 years old, their theory is still considered to be the basis of formal kinetics studies. Volume fraction, \( V_v \), against time of JMAK theory is given below. Eq. (1) is for site-saturated, the number of nuclei per unit of volume is represented by \( N_v \). Eq. (2) is for a constant nucleation rate per unit of volume per unit of time, \( I \). In both cases, the velocity, \( G \), remains a constant.

\[
V_v(t) = 1 - \exp \left( -\frac{4\pi}{3} N_v G^2 t^2 \right) \\
V_v(t) = 1 - \exp \left( -\frac{\pi}{3} G^2 t^4 \right)
\]

3. Cahn analytical model

The corresponding equations for constant nucleation rate, \( l_s \), Eq. (3), and site-saturated nucleation, \( \lambda_s \), Eq. (4), on the grain boundaries (grain faces) derived by Cahn [4,5] are given below.

\[
V_v(t) = 1 - \exp \left( -2 S_v G t \int_0^1 \left\{ 1 - e^{-\frac{2}{3} \lambda_s G^2 t^3 \left[ \frac{1}{2} z^2 \right]^2} \right\} dz \right)
\]

\[
V_v(t) = 1 - \exp \left( -2 S_v G t \int_0^1 \left\{ 1 - e^{\lambda_s G^2 t^3 \left[ 1 - \frac{1}{2} z^2 \right]} \right\} dz \right)
\]

\( S_v \) is the area per unity of volume of the grain boundaries. \( G \) is a constant velocity.

For a high nucleation rate or a high number of site-saturated nuclei, the new phase might form as a continuous “film” at the grain boundaries. When this happens only normal growth is possible, and both above formulas reduce to

\[
V_v(t) = 1 - \exp (-2 S_v G t)
\]

4. Microstructural descriptors

Previous work [7] established that two microstructural descriptors are especially useful when one has grain boundary nucleation. Here “\( \alpha \)” is the parent phase and “\( \beta \)” is the new phase.

The first descriptor is the contiguous, \( C^{\alpha\beta} \), of the new phase

\[
C^{\alpha\beta} = \frac{2S_V^{\alpha\beta}}{S_V^{\alpha} + 2S_V^{\beta}}
\]

\( S_V^{\alpha\beta} \) is the interfacial area between the new phase and \( S_V^{\alpha} \) is the mobile interfacial area between the parent phase and the new phase. \( S_V \) used above is the same as \( S_V^{\alpha} \).

The second descriptor is the dispersion parameter, \( \delta \).

\[
\delta = \frac{S_V^{\alpha\beta}}{S_V^{\alpha}}
\]

5. Computer simulation methodology

Likewise, in previous work [7] the computer simulations of the nucleation and growth transformations were carried out using the causal cone method. The simulations employed a cubic matrix comprising 304 \( \times \) 304 \( \times \) 304 cubic cells with periodic boundary conditions. For normalization purposes, the matrix has a 1 mm \( \times \) 1 mm \( \times \) 1 mm; in other words, the matrix has a volume equal to the unit. Within this cubic matrix, one constructs a network of Kelvin polyhedra. The nucleation took place on the interfaces of these Kelvin polyhedra. In this work, one considered two kinds of nucleation: the constant rate nucleation, and the site-saturated nucleation. For the constant rate nucleation, one used rates between \( I = 27 \) and \( I = 500 \). The number of nuclei that were effectively nucleated throughout the constant rate transformation was employed for the site-saturated simulation. This means that the rate \( I = 27 \) generated 707 nuclei, these 707 nuclei were adopted for site-saturated simulation. In the same way, \( I = 500 \) generated 5195 nuclei. Then for the site-saturated, the number of nuclei, \( N_V \), was between 707 and 5195. In all simulations, the growth velocities were kept constant.

6. Microstructure

Fig. 1 shows the 3D microstructural evolution for a low value of a constant nucleation rate, \( I = 27 \). Fig. 1a displays the nuclei at an early nucleation stage. Fig. 1b displays the nuclei for \( V_V = 0.01 \). Fig. 1b clearly shows that the transformed grains have different volumes corresponding to the point in time in which they nucleated. Fig. 1c exhibits the microstructure for \( V_V = 0.5 \) fraction transformed. Fig. 1d depicts a fully transformed matrix.

Fig. 2 shows the 3D microstructural evolution for a small number of site-saturated nuclei, \( N_V = 707 \). Fig. 2a displays all nuclei already present at the beginning of the transformation. This contrasts to the nuclei generated by constant nucleation rate depicted in Fig. 1a. Fig. 2b compares with Fig. 1b. Owing to the site-saturation in Fig. 2b all regions have the same volume, and the number of grains is the same as the number of nuclei depicted in Fig. 2a. By contrast, in Fig. 1b, grains have varying sizes, and the number of grains is larger than the number of nuclei depicted in Fig. 1a. Fig. 2c shows the microstructure after \( V_V = 0.5 \) fraction transformed. Fig. 2d displays a fully transformed matrix.
For a more accurate analysis of the fully transformed microstructures, Fig. 3 compares a 2D section of Fig. 1d: Fig. 3a, with a 2D section of Fig. 2d: Fig. 3b. Fig. 3a clearly shows that for a constant nucleation rate, the final interfaces are curved.

Conversely, it is evident in Fig. 3b that site-saturated nucleation results in a final microstructure in which the grain boundaries are flat. This provides a useful metallographic feature that one can use when examining real transformations to distinguish between constant nucleation rate and site-saturated nucleation. It is important to stress that these fully transformed microstructures are obtained as soon as transformations end. If grain growth takes place after the transformation, these observations do not apply. It is well-known that in normal grain growth the triple junctions will tend to an internal dihedral angle equal to $2\pi/3$. Moreover, after grain growth, the interfaces are curved.

### 7. Transformation kinetics

Fig. 4a shows the transformation kinetics for a low constant nucleation rate of $I = 27$ and for a small number of site-saturated grains $N_V = 707$. Fig. 4b shows the transformation kinetics for a high constant nucleation rate of $I = 500$ and for a high number of site-saturated grains $N_V = 5195$.

Both in Fig. 4a and 4b the solid line represents the JMAK model, Eqs. (1) and (2) whereas the dashed line represents Cahn’s model Eqs. (3) and (4).

Examination of Fig. 4a reveals that both for a low constant nucleation rate and a small number of site-saturated nuclei, Eqs. (1) and (2) describe the transformations quite well.

By contrast, the examination of Fig. 4b reveals that both for a high constant nucleation rate and a high number of site-saturated nuclei, Eqs. (3) and (4) describe the transformations quite well.

In summary, JMAK describes the transformation well for a small number of nuclei, whereas Cahn’s model describes the transformation well for a high number of nuclei.

One point that is crucial when transformation nucleates at grain boundaries or here in a network of Kelvin polyhedra take place when there is a high number of nuclei on the boundaries. In these circumstances, it might happen that at a certain point of the transformation, the boundaries are entirely covered with transformed areas. In other words, impingement takes place on the grain boundary plane. Owing to this, the new regions can only grow in the direction normal to the boundary plane. Such a situation may happen both for a constant nucleation rate and site-saturated nucleation. When this situation takes place, one must use Eq. (5). Therefore, the time exponent is now low and equal to one, see Eq. (5).

The classical double log plot is useful to understand the difference in the behavior of Fig. 4a and 4b. Fig. 5a and 5b, corresponding to Fig. 4a and 4b. Likewise Figs. 4a and 5a shows good agreement between JMAK and simulation. The slopes are 4 for constant nucleation rate and 3 for site-saturation. See Eqs. (1) and (2). Fig. 5b also behaves according to Cahn’s

![Fig. 1 - Constant nucleation rate microstructure: (a) Early nucleation stage, (b) $V_V = 0.01$, (c) $V_V = 0.5$, (d) fully transformed matrix.](image-url)
model, Eqs. (3) and (4), up to a point. For high volume fractions, both the constant nucleation rate and the site-saturated nucleation decrease their exponent to one and follow Eq. (5). For the reader’s convenience, $\ln(\ln(1/(1 - V_V))) = 0$, corresponds to $V_V \approx 0.63$. The lines start to converge more rapidly for $V_V > 0.63$.

8. Microstructural descriptors

Fig. 6a and 6b show the contiguity as a function of fraction transformed for constant nucleation rate and site-saturated nucleation. For a low constant nucleation rate and a small
Fig. 4 – Transformation kinetics for the transformation nucleated on the network of Kelvin’s polyhedra for the two nucleation modes. (a) $I = 27$, $N_V = 707$; (b) $I = 500$, $N_V = 5195$.

Fig. 5 – Double log plot of the transformation kinetics shown in Fig. 4. (a) $I = 27$, $N_V = 707$; (b) $I = 500$, $N_V = 5195$, the full line represents the situation in which the time exponent is equal to one, see Eq. (5).

Fig. 6 – Contiguity of the new phase as a function of volume fraction transformed. (a) Contiguity of the constant nucleation rate, (b) contiguity of the site-saturated nucleation.

number of site-saturated nuclei, the simulation follows the solid line that corresponds to the contiguity of a transformation that follows JMAK kinetics. This agrees with Fig. 4a. As the nucleation rate $I$ and the number of nuclei $N_V$ increase the contiguity curve lies increasingly higher than the JMAK curve. Vandermeer [8] states that when the contiguity lies above JMAK, the nuclei tends to clustering. This has been corroborated by both by experimental evidence and computer simulation [6]. In the present case, the cluster means the high number of nuclei on the grain boundaries. This is a type of clustering. Both Fig. 6a and 6b exhibit a similar behavior. It is difficult to distinguish constant nucleation rate from site-saturation for the examination of the contiguity against fraction transformed curve. The reason for that is as follows. All nuclei appear at $t = 0$ for site-saturated nucleation and appear as time passes for a constant nucleation rate. Nonetheless, in both cases, nuclei are uniform randomly located in space in other words, nuclei are located in space according to a homogeneous Poisson point process. The fact that nuclei are similarly arranged in space causes the contiguity to be similar. The dispersion parameter, not plotted here, behaves in an analogous way to the contiguity. It is not possible to distinguish the nucleation mode from the dispersion parameter alone.
9. Conclusions

We compared transformations nucleated on the faces of a network of Kelvin’s polyhedra by a constant nucleation rate and site-saturated nucleation.

- For a low constant nucleation rate and a small number of site-saturated nuclei, JMAK theory, Eqs. (1) and (2), describes the transformations quite well. See Figs. 4a and 5a.
- By contrast, for a high constant nucleation rate and a high number of site-saturated nuclei, Cahn’s theory, Eqs. (3) and (4) describe the transformations quite well up to a point. See Figs. 4b and 5b.
- This point corresponds to the situation in which the grain boundaries, or in this case, the faces of the polyhedra are covered by a continuous film of the transformed region. Beyond this point, the kinetics still follows Cahn’s theory but now a form of Cahn’s equations, Eq. (5), is obeyed. See Fig. 5b.
- The contiguity indicates that in both cases, the higher the number of nuclei, the higher is the contiguity curve relative to the contiguity of transformations following JMAK. See Fig. 6a and 6b.
- The dispersion parameter also behaves similarly for both constant nucleation rate and site-saturated nucleation.
- The fact that can explain the similarity in the contiguity for both kinds of nucleation is that in both cases the nuclei are uniform randomly located in space or, in other words, according to a homogeneous Poisson point process.

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