Investigation on the existence of a ‘Hillert regime’ in normal grain growth

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Abstract

The existence of a ‘Hillert regime’ in 3D normal grain growth, where the grain size distributions (GSDs) at different time-steps match the Hillert distribution during parabolic grain growth, is investigated for different initial GSDs using large-scale phase-field simulations. The short-lived ‘Hillert regime’ was present in the early-stage only in few cases. The GSDs obtained at a later-stage for all cases are: self-similar over long period; independent of the initial GSDs; and wider than the Hillert distribution. Also, the topological properties in the ‘Hillert regime’ were different from that in the later-stage self-similar regime.

Keywords: Grain growth, Hillert distribution, Simulation and modeling

The commonly accepted characteristics of steady-state normal grain growth (NGG) in an isotropic single-phase system [1–3] after a transient regime are: parabolic growth rate and unique self-similar grain size distribution (GSD) and grain topology distribution (GTD) (also known as distribution of number of faces). In 1965, Hillert [4] proposed an analytical expression for the steady-state GSD based on a mean-field treatment of the evolution of the individual grains. Battaile and Holm [5] observed, based on 2D Monte Carlo Potts simulations, that the self-similar steady-state GSD deviates from the Hillert distribution. Recent large scale 3D simulations [6–8] using the multi-phase field model [9] have shown inconsistent results during NGG. In a first study, Kim et al. [6] found that the steady-state GSDs at different time-steps were independent of the initial GSDs and in excellent agreement with the Hillert distribution. They concluded

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that the Hillert theory can be regarded as an accurate description of 3D steady-state NGG. In a second study, Suwa et al. [7] noted that the steady-state GSDs were wider than the Hillert distribution. In a third study, Kamachali and Steinbach [8] observed ‘Hillert regime’ during parabolic grain growth, where the GSDs in the early-stage match the Hillert distribution for some time-steps. Later, as simulation progressed, the GSDs evolved towards a wider distribution, which were considered as the self-similar GSDs. They also claimed that ‘the same behaviour has been observed from simulation boxes of different sizes and initial distributions’, but, unlike Kim et al. [6], no supporting material was given. Furthermore, Kamachali and Steinbach [8] observed that the GTDs, unlike the GSDs, were invariant throughout the Hillert and later-stage regimes. Other large-scale computer simulations using various numerical schemes [10–13] did not observe a ‘Hillert regime’ during NGG. The mean number of faces in Kim et al. [6] study was $\langle F \rangle = 13.4$ whereas others have reported $\langle F \rangle \approx 13.7$ [7, 10–13]. Kamachali and Steinbach [8] did not report on the $\langle F \rangle$ value. The goal of this paper is to understand the discrepancies between previously published different 3D multi-phase field simulation results and to study the effect of the initial grain size distribution on the existence of a Hillert regime in NGG.

In the present study, simulations are carried out using a continuum phase-field model [14]. The details of the model [15], numerical scheme [16], model parameters (like, Δt -time-step, etc), initial GSDs, calculation of grain radius R and mean grain size $\langle R \rangle$ are given in the ‘Supplementary material’. The system size and other simulation parameters in this paper are identical to the Kamachali and Steinbach [8] study. Six different initial grain size distributions are considered here. The initial shape of the GSDs after $100\Delta t$ time-step (where $\Delta t = 0.1\text{sec}$) is shown in Fig. 1. For Cases 1-4 and 6, 30,000 grains (N) were present at the start of the simulation. For Case 5, the initial grain structure contained 50,000 grains. In all cases, grains were initialized as spherical grains and distributed randomly over the 3D system. The initial grain radii were selected to obtain the desired initial GSDs (further details in ‘Supplementary material’). For Case 3, the shape of the GSD is similar to the Hillert distribution at $100\Delta t$ (Fig. 1). For Cases 4-6, the tail of the initial GSD is longer than the Hillert distribution.

The evolution of the square of the $\langle R \rangle$ with time for all cases is shown in Fig. 2a. The inset figure in Fig. 2a shows the evolution of the $\langle R \rangle$ from $100\Delta t - 4000\Delta t$. The evolution of the GSDs for Cases 1-5 are shown in Figs. 3a-3c, 3g and 3h. We distinguished two regimes during the parabolic grain growth: 1) Regime I, part of an early-stage regime ($100\Delta t - 4000\Delta t$), where quasi-steady-state (QSS) is observed. In the QSS, GSDs are constant for some time before they change shape. For all cases, the duration of this regime was different; and 2) Regime II, the later-stage regime ($4000\Delta t - 20000\Delta t$), where the GSDs remained invariant (self-similar) over this period, and are the same for Cases 1-5. In the same way, the evolution of the GTDs for Cases 1-5 is presented in Figs. 3d-3f, 3j and 3k. The standard deviation (σ) of the normalized grain sizes ($R/\langle R \rangle$), mean number of faces $\langle F \rangle$ and second moment (μ) of number of faces F of all grains are shown in Figs. 2b-2d for all cases. Further details are presented in Table 1. For Case 6, the steady-state was achieved later than in Cases 1-5. Finally, the GSD and GTD, obtained for Case 1, are compared with previously published results in Fig. 4.

The linear relation between the square of the $\langle R \rangle$ and time (t) in Regime I and Regime II for all cases (see Fig. 2a) indicates that parabolic growth kinetics, $\langle R \rangle^2 - \langle R_o \rangle^2 = Kt$, are followed for both regimes, where $\langle R_o \rangle$ is the mean grain radius at the start of parabolic growth and K is a kinetic coefficient. The GSDs for Regime I (see Fig. 3) suggest that QSS GSDs are observed for Cases 1-5, but the Hillert Regime is observed only for Cases 1-3. The K_I , σ_I , $\langle F_I \rangle$ and μ_I in this Hillert Regime have similar values for Cases 1-3 (see Table 1a). However, the GTDs in the Hillert regime behaved differently in the different Cases. For Cases 1-2, the GTDs are constant in Regime I, while this is not the case for Case 3. For Cases 4-5, where the QSS GSDs do not match the Hillert distribution, the K_I and σ_I are different, whereas the $\langle F_I \rangle$ and μ_I are similar to those in the Hillert regime in Cases 1-3. For Case 4, the GTD in Regime I is constant, while this is not the case for Case 5. Suwa et al. [7] reported that the $\langle F \rangle = 14$ in the early-stage of their simulation, which is similar to the $\langle F_I \rangle$ value in the present study. However, Kim et al. [6] found that the $\langle F \rangle = 13.4$ in the Hillert regime. Our results from Regime I for the different Cases show thus large variation in GSDs, GTDs, K_I , σ_I , $\langle F_I \rangle$ and μ_I despite showing

parabolic grain growth. This indicates that the Hillert regime cannot be considered as a unique regime in the early-stage of parabolic grain growth.

On the other hand, the GSDs, GTDs, K_{II} , σ_{II} , $\langle F_{II} \rangle$ and μ_{II} of Regime II for all cases are similar and invariant despite having different initial GSDs (see Table 1b). The K_{II} obtained in this study is also close to the kinetic coefficient $K = 5.1 \times 10^{-15} \text{ m}^2/\text{s}$ obtained in [8]. The $\langle F_{II} \rangle$ for all cases also agrees with the $\langle F \rangle$ value published in previous results [7, 10–13]. The averaged GSDs and GTDs over Regime II are similar to the steady-state GSD and GTD reported by Elsey et al. [10] (see Figs. 3a-3h, 3j and 3k). In Figs. 3i and 3l, the GSDs and GTDs for Regime II are compared for Cases 1-6 and with the results of Kamachali and Steinbach [8]. The GSD from [8] at $8200\Delta t$ looks similar to our GSDs, however, the peak is shifted towards lower grain sizes and a few large grain sizes are also present in their simulations (see Fig. 3i). The peak position of the GTD from [8] at $1800\Delta t$ matches with the present results, but the match at the ‘ear’ and ‘tail’ of the distributions is poor (see Fig. 3l). The GTD from the later-stage ($9400\Delta t$ [8]) matched the peak position and tail end but the ear position showed the existence of more grains belonging to $F \leq 6$ topological class than the present study. Different from our findings, Kamachali and Steinbach [8] observed that the GTDs remained invariant over Regime I and Regime II. They suggested that the possible reason behind invariant GTD and different GSD shapes during parabolic grain growth may be due to a non-linear relation between the $\sqrt{F}$ and grain sizes R . However, in our study, the GTDs from Regime I and Regime II are different for different initial GSDs, showing that their observation of an invariant GTD over the two regimes is not generally true. In Fig. 4, the GSD and GTD for Regime II from our simulations agree well with the previous simulation results [7, 12, 13, 17] corresponding to the steady-state regime. The Rios distribution [18] (with $\nu = 3.2$) also matches our GSD results, whereas, the log-normal distribution fit [19] (with $\mu = 0.0529$ and $\sigma = 0.4125$) showed a poor match. Krill and Chen [20] observed parabolic grain growth with $\langle F \rangle = 13.7$. However, their GSD and GTD show a poor match with our results. It was, however, already suggested [6] that the simulations in the Krill and Chen [20] study may not represent a steady-state NGG. The GTD shape in the Kim

et al. [6] study is similar to our steady-state GTD but their GSD is similar to the Hillert distribution. The simulations in this study are carried out with the continuum phase-field model and Moelans et al. [21] confirmed that the continuum phase-field model and the multi-phase field model should give similar grain growth results. However, unlike the findings of Kamachali and Steinbach [8], we find that the topological properties in the Hillert regime are different from those in the later-stage self-similar regime and that the Hillert regime is dependent on the initial GSD.

It is important to note that the analytical solutions for parabolic grain growth and the Hillert distribution do not contain topological information, while microstructure evolution is also constrained by the presence of grain topology. Our results show the importance of verifying not only the self-similar GSDs but also the invariant topological properties during parabolic grain growth when determining the steady-state regime.

In summary, based on large-scale grain growth simulations starting from six different initial GSDs, we conclude that only the later-stage microstructure evolution (Regime II) is a self-similar regime and independent of the initial GSD. Thus, the Hillert regime, whose existence is dependent on the initial GSD during parabolic grain growth, does not represent a steady-state regime in normal grain growth.

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Appendix A. Supplementary material

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Fig. 1. Initial grain size distributions (GSDs) for all 6 cases considered in this paper. The GSDs of all 6 cases are normalized with R_{cr} where $R_{cr} = 9/8 \cdot \langle R \rangle$. The total number of grains present at $100\Delta t$ are shown in the legend. The Hillert 3D distribution is added for comparison.

Table 1. Comparison of growth kinetics $K(10^{-15}m^2/s)$, standard deviation of normalized grain sizes σ , mean number of faces $\langle F \rangle$ and second moment μ of number of faces F in Regime I and Regime II.

(a) Regime I

GSD	K_I	σ_I	$\langle F_I \rangle$	μ_I
Case 1	5.27	0.35 ± 0.0030	14.04 ± 0.024	23.29 ± 0.31
Case 2	4.85	0.35 ± 0.0045	14.01 ± 0.032	23.34 ± 0.54
Case 3	5.00	0.35 ± 0.0053	14.03 ± 0.029	22.89 ± 1.54
Case 4	6.45	0.37 ± 0.0024	13.89 ± 0.018	27.02 ± 0.41
Case 5	5.73	0.38 ± 0.0072	13.97 ± 0.038	26.65 ± 1.11
Case 6	5.27	0.35 ± 0.0058	13.89 ± 0.026	20.19 ± 0.45

(b) Regime II

GSD	K_{II}	σ_{II}	$\langle F_{II} \rangle$	μ_{II}
Case 1	4.98	0.38 ± 0.010	13.78 ± 0.077	24.53 ± 0.60
Case 2	5.06	0.38 ± 0.009	13.78 ± 0.049	24.76 ± 0.70
Case 3	5.04	0.37 ± 0.006	13.79 ± 0.054	23.36 ± 0.82
Case 4	4.98	0.38 ± 0.007	13.76 ± 0.051	24.58 ± 0.91
Case 5	5.27	0.38 ± 0.006	13.77 ± 0.042	24.23 ± 1.09
Case 6	5.06	0.37 ± 0.007	13.79 ± 0.029	23.21 ± 0.71

Fig. 2. Evolution of the square of the mean grain radius $\langle R \rangle$, standard deviations σ of all normalized grain sizes, mean number of faces $\langle F \rangle$ and second moment μ of the number of faces with time for the 6 Cases. The inset figure in Fig. 2a shows the evolution of the mean grain radius in the early-stage regime I ($100\Delta t - 4000\Delta t$). The vertical broken line in these figures indicates start of the Regime II for Cases 1-5.

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