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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.

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 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 $\Delta t = 0.1$ s) 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 the ‘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

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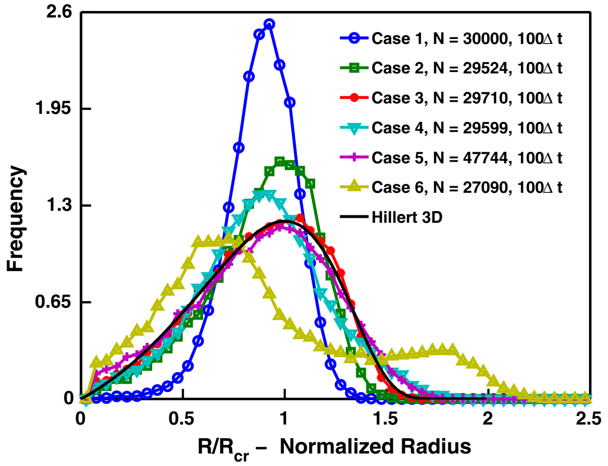

Fig. 1. Initial grain size distributions (GSDs) for all 6 cases considered in this paper. The GSDs of all 6 cases are normalized with R_{cr} where $R_{cr} = 9/8 \cdot \langle R\rangle$. The total number of grains present at 100Δ*t* are shown in the legend. The Hillert 3D distribution is added for comparison.

are shown in Fig. 3a–c, g and h. We distinguished two regimes during the parabolic grain growth: 1) Regime I, part of an early-stage regime (100Δ*t*–4000Δ*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 (4000Δ*t*–20, 000Δ*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 Fig. 3d–f, j and k. 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–d 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

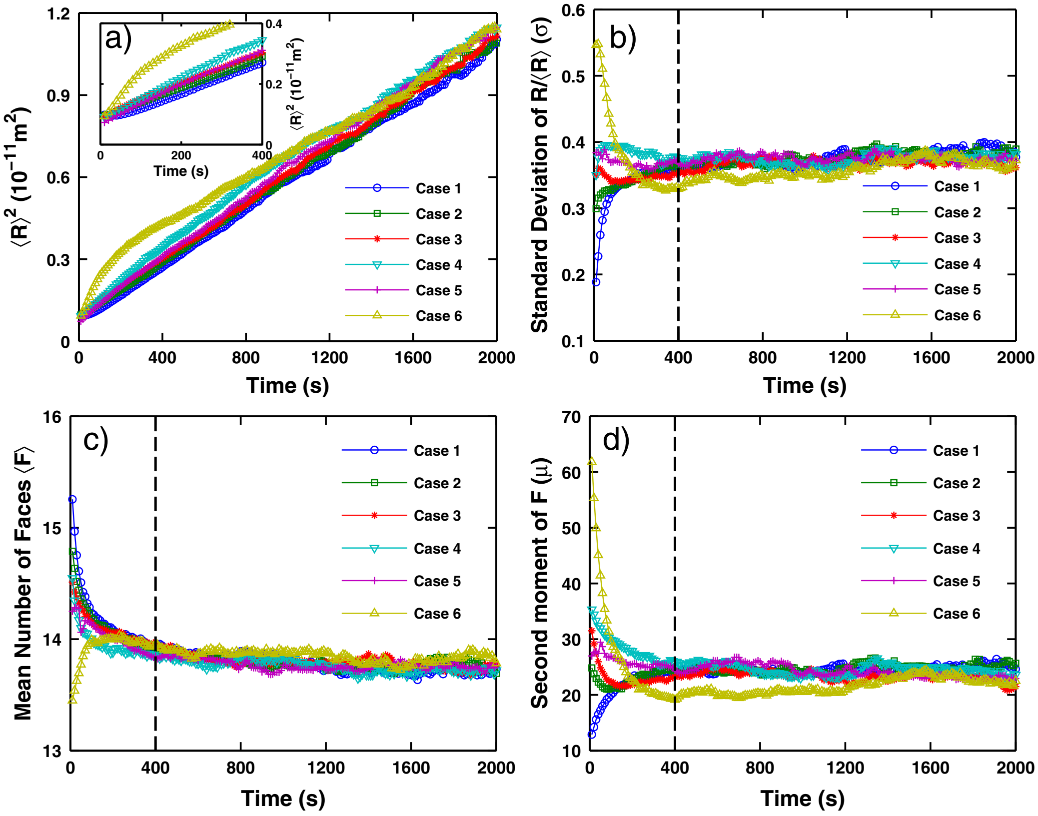

Fig. 2. Evolution of the square of the mean grain radius $\langle R\rangle$, standard deviations σ of all normalized grain sizes, mean number of faces $\langle F\rangle$ and second moment μ of the number of faces with time for the 6 Cases. The inset figure in Fig. 2a shows the evolution of the mean grain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