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Modelling grain growth with the generalized Kampmann-Wagner numerical model

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ABSTRACT

The multi-phase Kampmann-Wagner Numerical (KWN) model, which had been successfully applied for modeling particle precipitation (i.e. Ostwald ripening), is extended toward grain growth modeling. The extensions consist of adopting grain topology- and size-dependent growth rate equation obtained from either the reported parameterization of phase field simulations results or theoretical analysis. Global volume conservation equation is imposed in the extended model to reflect the spacing filling constraints that grains do not overlap and no voids appear. The extended model has been applied to simulate ideal grain growth, grain growth with the initial states of lognormal/normal/Weibull distributions, bi-modal grain size distribution and arbitrary Voronoi tessellations, and the simulation results have been verified by Hillert's asymptotic solution and phase field simulation results. The extension has enabled the KWN approach applicable to model grain growth thus reducing the threshold for the establishment of an efficient Integrated Computational Materials Engineering modeling framework.

1. Introduction

Computer simulations of grain growth has been an important topic of current grain growth research [1]. Upon the completion of recovery and recrystallisation, driven by the reduction of the total grain boundary area grains continue to grow resulting in the increase in average grain size. It is a research topic with practical applications and fundamental scientific interests. For example, grain growth is relevant to the thermal stability of nanocrystalline materials.

In his seminal work [2] Hillert demonstrated that the methodology of Lifshitz and Slyozov and Wagner, developed within the context of precipitate coarsening [3,4], is applicable to grain growth. Hillert's simple grain growth law is reproduced below:

$$\frac{dR}{dt} = \alpha M \gamma \left(\frac{1}{R_c} - \frac{1}{R} \right) \tag{1}$$

where R is the radius of an individual grain, t is time, α is a geometrical constant, M is the mobility of the grain boundary, γ is the grain boundary energy, and R_c is the critical grain size. This equation, in spite of being considered as over-simplified [5,6], has inspired many following researchers. Hillert's theoretical analysis for grain growth often serves as a benchmark for the numerical simulations of grain growth by the full field approaches such as phase field, cellular automaton and Lattice Boltzmann methods. One recent example is the ultra-large-scale phase field simulation of ideal grain growth reported in [7], in which the full field simulation results have been discussed in reference to Hillert's asymptotic analytical result.

Hillert's treatment and its extensions are more than providing asymptotic solution to ideal grain growth problem. They form the foundation for the numerical mean field grain growth modelling approach. The mean field approaches, which is the topic of this paper, differ from the full field approaches in that no spatial resolution of each grain is required. Instead a grain size continuity equation is numerically solved:

$$\frac{\partial \varphi(R,t)}{\partial t} + \frac{\partial (V\varphi)}{\partial r} = S. \tag{2}$$

φ is grains size distribution density function and V is grain growth rate representing grain exchange between different sizes. S is the source term due to nucleation or any other annulation events. This equation is the template for many existing mean filed microstructure models as to be discussed later in this section.

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Table 1
List of mean field microstructure models, all of which can be categorized as "Frequency Distribution Density Function method".

	φ	Growth Rate	Constrains	Existing models
As-cast grain size prediction	Frequency Distribution Density of particles or grains	Parabolic growth law	Heat and solute conservation	Hellawell-Maxwell model [18] Kampmann-Wagner model [19]
Precipitation kinetics			Solute conservation	Kampmann-Wagner model [13]
Grain Growth		Hillert's equation with additional stochastic contribution	Volume conservation	Pande model [8]

One good exemplified mean field grain growth modelling approach is the one proposed by Pande and his co-worker [8,9]. He employed the well-known second order partial differential equation in statistical mechanics, the so-called Fokker-Planck equation [10], as the governing equation to describe the temporal evolutions of grain size distribution. The Fokker-Planck equation is a generalized form of Eq.2 but with an additional diffusion term. Pande demonstrated that the solution obtained for Fokker-Planck equation is a modified form of Rayleigh distribution, which is like the log normal distribution seen in experimental measurements of grain size distributions. Pande's modelling methodology is closely related to the one used for precipitation modeling and as-cast grain size modelling, and in fact Pande indicated that his approach is extendable to the case of Oswald ripening. In [11] Lücke et al proposed a two-parameter statistical grain growth model. The model consists of numerical integration of the grain size continuity equation, the two "special linear (topological) relationships" between the average number of faces and grain size, and Neumann-Mullins growth law. They demonstrated that the normal or abnormal grain growth behaviour can be attributed to the differences in initial grain size distributions.

The mean field grain growth model in many aspects are in common to the Kampmann-Wagner Numerical (KWN) model developed primarily for modelling precipitation kinetics [12–17]. The original KWN model is a class-based model, and its essence is that the continuous Particle Size Distribution (PSD) curve is subdivided into multi-size classes to which growth equations are applied to. There are two different numerical scheme to track the temporal evolution of size distribution as described in [17]. The first one is "Euler-like" approach, in which the temporal evolution of particle size distribution is calculated by accounting the number of particles associated with each size class. The second is "Lagrange-like" approach, in which the temporal evolution of particle size distribution is calculated by accounting the size of particles associated with each class.

As shown in Table 1, all the governing equations of the existing mean field approaches are in the form of Eq.2 with φ being essentially a frequency distribution density function. Table 1 shows that the existing mean field models are nothing else but the numerical solution of the frequency distribution density function in the size space with the constrains of different conservation laws. Considering the long tradition, initiated by Hillert [2], of building a single mathematical/physical foundation for grain growth and precipitation kinetics, the similarities seen here is not a coincidence. There are many benefits of explicitly exploring the connections between the modelling approaches used in grain growth and precipitation kinetics research fronts as evidenced by Hillert's seminal work [2] including sharing the numerical solutions, theoretical foundations and promoting the models applications.

To highlight the similarities in the existing mean field models we have grouped the models listed in Table 1 into the category called "Frequency Distribution density Function (FDF) method". FDF methods contrast with the direct detailed approaches represented by phase field in which spatial resolutions of "fields" are mandatory. Of course, the full field simulations are insightful and irreplaceable. They are complementary to the FDF methods, and often used as computational experiments to verify the latter. On the other hand, when it comes to the applications to industrial problems and direct comparison with the experimental measurements, the FDF methods are superior due to their ability to *efficiently* and *statistically* address the multi-scale and multi-parameter problem. It is worthy of mentioning that phase field method, which was initially used for diffusive phase transformation [20,21], has been becoming versatile and applied to grain growth, recrystallization, displacive phase transformation, texture evolution, etc [22–24].

With these observations in mind, in this paper we extend the Kampmann-Wagner numerical model, which had been successfully applied for modeling particle precipitation and as-scast grain size prediction [12,14–16,19], toward grain growth modeling. The extensions consist of adopting a size and grain-topology dependent growth rate equation obtained either from the parameterizations of phase field simulation results [25,26] or theoretical analysis [2]. Global volume conservation equation is imposed to replace solute balance equation in the original KWN approach reflecting the spacing filling constraints that grains do not overlap and no voids appear. Extending the KWN approach towards grain growth are valuable. It would enable the treatment of the multi-modal grain size distributions and even the one with singularities in the distribution curve (i.e. the co-existence of few ultra-large particles with many small particles). This extension is also beneficial for the further development of the KWN model for precipitation modelling. One of the benefits is to make a bridge between the two research communities and learn from the reported mean field grain models on how to obtain the log-normal distributions for achieving the same goal in precipitation modelling. In addition, the extension would enable the KWN precipitation modeling approach applicable to model grain growth thus reducing the threshold for the establishment of an efficient Integrated Computational Materials Engineering modeling framework.

A challenge in making this extension is how to parameterize grain growth rate equation as function of grain radius or topological features. We would start with the original Hillert's analytical equation for grain growth rate. Then the topology-dependent growth rate equations parameterized from phase field simulation results [7], are adopted in the extended model.

The paper is organized as following: the extended model is described in *Model* Section. Then in *Results and Discussions* section the extended model is applied to ideal grain growth, grain growth with the initial states of lognormal/normal/Weibull distributions, bi-modal grain size distribution and arbitrary Voronoi tessellations, and the simulation results are discussed in reference to the asymptotic solution and phase field simulation results.

2. Model

The grain growth model is developed on the base of the Kampmann-Wagner Numerical model [15,16]. It is multi-size class "Lagrange-like" mean field precipitation modelling approach, in which the temporal evolution of particle size distribution is calculated by accounting the size of particles associated with each class. To address the differences between precipitation and grain growth, two adaptations of the original KWN model have been made. The first adaption is for growth rate equation, the second for conservation equation. In addition, the main assumptions adopted in our extended model include:

I. Grains are of spherical shape and their growths/dissolutions are solely controlled by grain boundary curvature.
II. Explicit relation exists between grains radius and their topological features.

Below is the description of the extended KWN model with the two adaptions.

2.1. Grain growth rate equation and topological effects

One of the key components in the extended KWN model is size and grain-topology dependent growth rate equation. As mentioned earlier, they can be obtained with either direct numerical phase field simulation results or theoretical analysis. Below the two adopted equations, namely Hiller's equation and the ones validated by direct numerical simulation results, are described respectively.

2.1.1. Hillert's growth rate equation

The first equation adopted is Eq.1 presented in *Introduction* section. This analytical equation was derived by Hillert. Being consistent with topological requirements as demonstrated in [2], it is the equation which acts as the starting point of any statistics-based grain growth modelling approach.

Hillert also discussed the explicit relation between grains radius and their topological features. For grain growth in two-dimensional domain, by combining with the results from Neumann [27] and Mullins [28] on grain topology, Hillert has demonstrated that there is a simple relation between the number of sides (or the number of neighbors per grain), n, and grain size.

$$n = 6 + 6\alpha\left(\frac{R}{R_c} - 1\right) \quad (3)$$

in which α is a geometrical constant and estimated to be ½. R_c, the critical grain size, can be worked out from the space filling constraint (volume conservation law) as discussed in Section 2.2.

Due to the extension of the 2D topology dependent growth rate equation by MacPherson and Srolovitz in [29], it is possible to establish the relation between the number of sides and grain size and the critical size for grain growth in 3D domain. Following the derivation of Okita and Schibuta [30],

$$\frac{dR}{dt} = \frac{\pi M\sigma}{6R}\left(\sqrt{n} - \frac{12}{\pi}\right) \quad (4)$$

Comparing with Eq. (1), the following relation can be obtained.

$$n = 36\left(\frac{\alpha\left(\frac{R}{R_c} - 1\right) + 2}{\pi}\right)^2. \quad (5)$$

Hillert's growth rate equation has been used in the simulations presented in Section 3.1 and 3.3.

2.1.2. Growth equations verified with the direct numerical simulation method

The growth rate equation proposed by Miyaoshi and his co-works in [7] is adopted in the extended model. They have parameterized the volumetric growth rate of individual grains as a function of their radius.

$$\frac{dR}{dt} = \frac{\pi M\gamma}{6R} g_1(n)\left(\sqrt{n} - \frac{12}{\pi} g_2(n)\right). \quad (6.1)$$

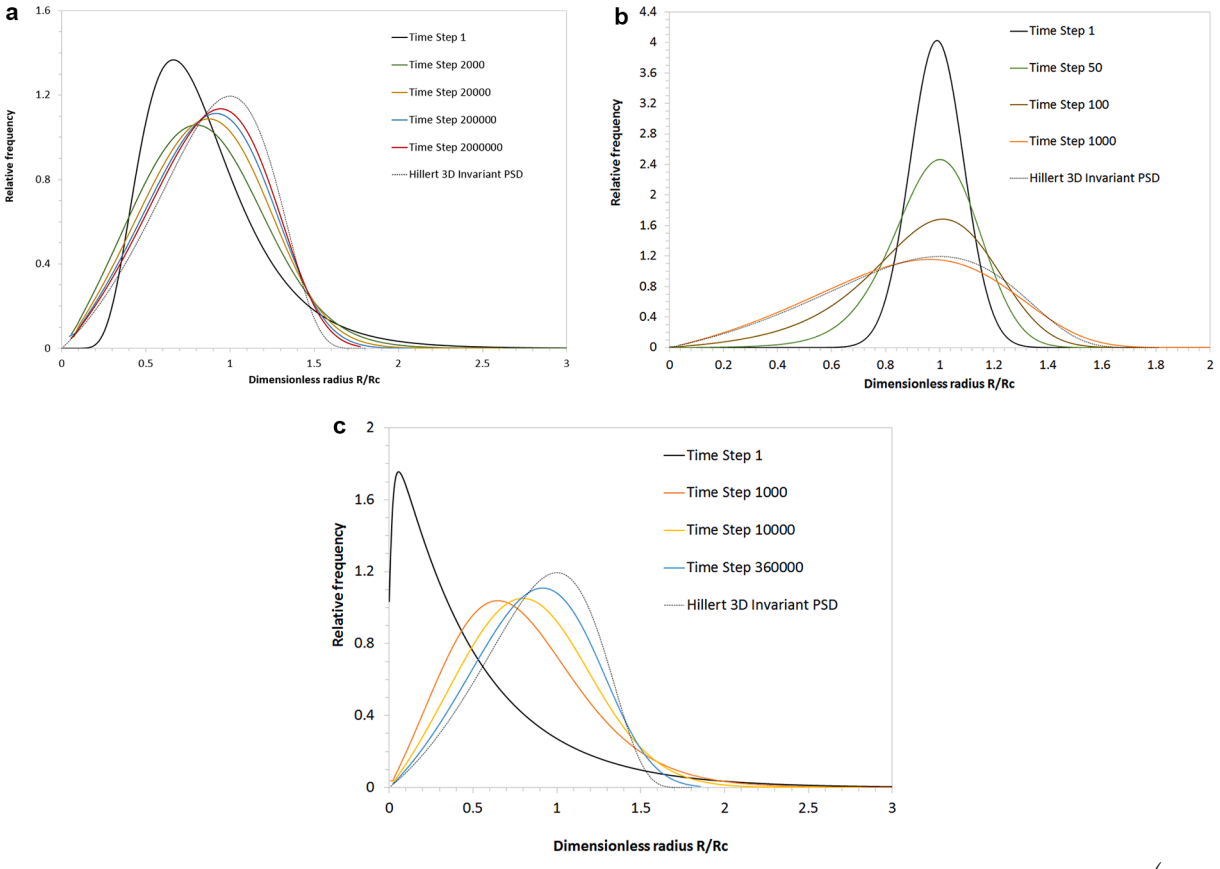

Fig. 1. Evolutions of grain size distribution density functions with the initial distributions of (a) lognormal described by $\varphi(R,0) = \frac{N_0}{R\sigma\sqrt{2\pi}}\exp\left(-\frac{(\ln R-\mu)^2}{2\sigma^2}\right)$, $\mu = 10.0\mu m$, $\sigma = 0.40535$, $N_0 = 1.14\times10^6/mm^3$ (b) normal described by $\varphi(R,0) = \frac{N_0}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(R-\mu)^2}{2\sigma^2}\right)$, $\mu = 10.0\mu m$, $\sigma = 2.0$, $N_0 = 0.23\times10^6/mm^3$, and (c) Weibull described by $\varphi(R,0) = \frac{N_0 k}{\lambda}\left(\frac{R}{\lambda}\right)^{k-1}\exp\left(-\left(\frac{R}{\lambda}\right)^k\right)$, $k = 10.0\mu m$, $\lambda = 1.0$, $N_0 = 0.23\times10^6/mm^3$.

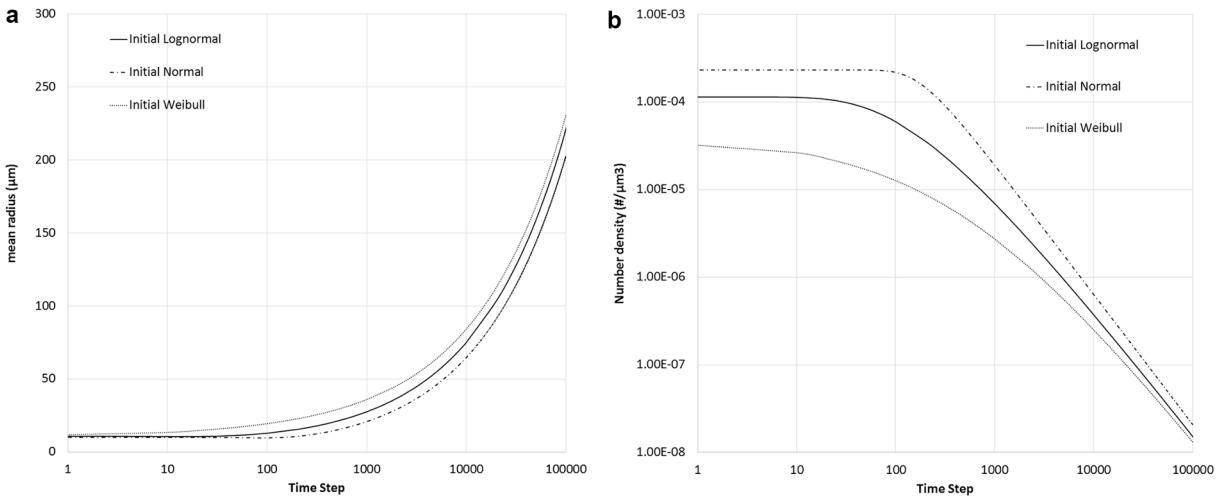

Fig. 2. the evolutions of mean radius (a) and number densities (b) in the three simulations starting with Normal, Lognormal and Weibull distributions.

$$g_1(n) = (\frac{\sqrt{n(n-1)}}{n-2})^{1/3}. \tag{6.2}$$

$$g_2(n) = 0.52504\sqrt{n}\arctan\sqrt{1-2\cos(\frac{\pi n}{3(n-2)})}. \tag{6.3}$$

$$n = 3.944\alpha^2\rho^2(\frac{R}{R_{ave}})^2 + (13.91 - 7.887\alpha)\alpha\rho\frac{R}{R_{ave}} + 14.76 - 13.91\alpha + 3.944\alpha^2. \tag{6.4}$$

ρ is defined as the square of the mean radius over the average of the radius square. The validity of the above equations has been discussed in [7], and the equations is to be tested further in Section 3.2.

2.2. Volume conservation equation

Instead of solute conservation equation, it is the total volumes of grains that is conserved during grain growth. Volume conservation results from the space filling constrains that no grains overlap, and no pores appear during grain growth. Considering the growth of spherical grains within a 3d domain with its total volume denoted by V_{domain}, or a 2d domain with its total area denoted by $S_{domain}$the following volume conservation equation can be written for 3D and 2D respectively:

$$\sum_{i=1}^{NOG} n_i \frac{4}{3}\pi R_i^3 = V_{domain}. \tag{7.1}$$

$$\sum_{i=1}^{NOG} n_i 4\pi R_i^2 = S_{domain}. \tag{7.2}$$

where R_i and n_i are the radius and the number of the grains associated with size class i, NOG is the total number of grain size classes.

The volume conservation equation is used to compute R_c, the key parameter for calculating grain growth rate in Eq. (1) and Eq. (6). For the 2D case, by demanding the changing rate of the total area occupied by grain is zero and combining with Eq. (1), one could derive:

$$\sum_{i=1}^{NOG} n_i R_i \dot{R}_i = \sum_{i=1}^{NOG} n_i \alpha M\sigma\left(\frac{R_i}{R_c} - 1\right) = 0. \tag{8.1}$$

$$R_c = \frac{\sum_{i=1}^{NOG} n_i R_i}{\sum_{i=1}^{NOG} n_i} = R_{ave}. \tag{8.2}$$

For 3D case

$$\sum_{i=1}^{NOG} n_i R_i^2 \dot{R}_i = \sum_{i=1}^{NOG} n_i \alpha M\sigma\left(\frac{R_i^2}{R_c} - R_i\right) = 0. \tag{8.3}$$

$$R_c = \frac{\sum_{i=1}^{NOG} n_i R_i^2}{\sum_{i=1}^{NOG} n_i R_i}. \tag{8.4}$$

It should be noted that Miyoshi's growth rate equation, as described in Section 2.1.2, results from the parameterization of phase field simulation results. It is by itself in consistence with the volume conservation equation and does not contain any parameters to be determined by volume conservation equation.

3. Results and discussions

This section is devoted to demonstrating the validity of the extended KWN model and identify the needs for further improvement. The model is applied to simulate grain growth with various initial grain size distributions. The model predictions are compared with the analytical asymptotic solutions and phase field simulation results. The case studies

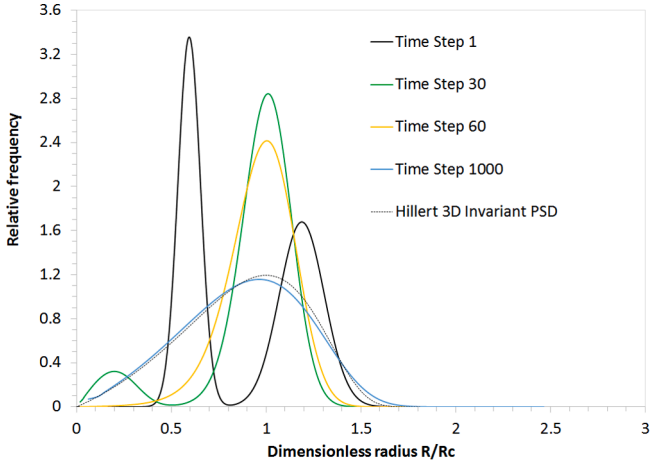

Fig. 3. Evolutions of grain size distribution density functions with an initial bimodal distribution described by $\varphi(R,0) = N_0(\frac{1}{\sqrt{2\pi\sigma_1{}^2}}\exp\left(-\frac{(R-\mu_1)^2}{2\sigma_1{}^2}\right) + \frac{1}{\sqrt{2\pi\sigma_2{}^2}}\exp\left(-\frac{(R-\mu_2)^2}{2\sigma_2{}^2}\right))$, $\mu_1 = 5.0\mu m$, $\sigma_1 = 1.0$,$\mu_2 = 10.0\mu m$, $\sigma_2 = 2.0$,$N_0 = 0.21 \times 10^6/mm^3$

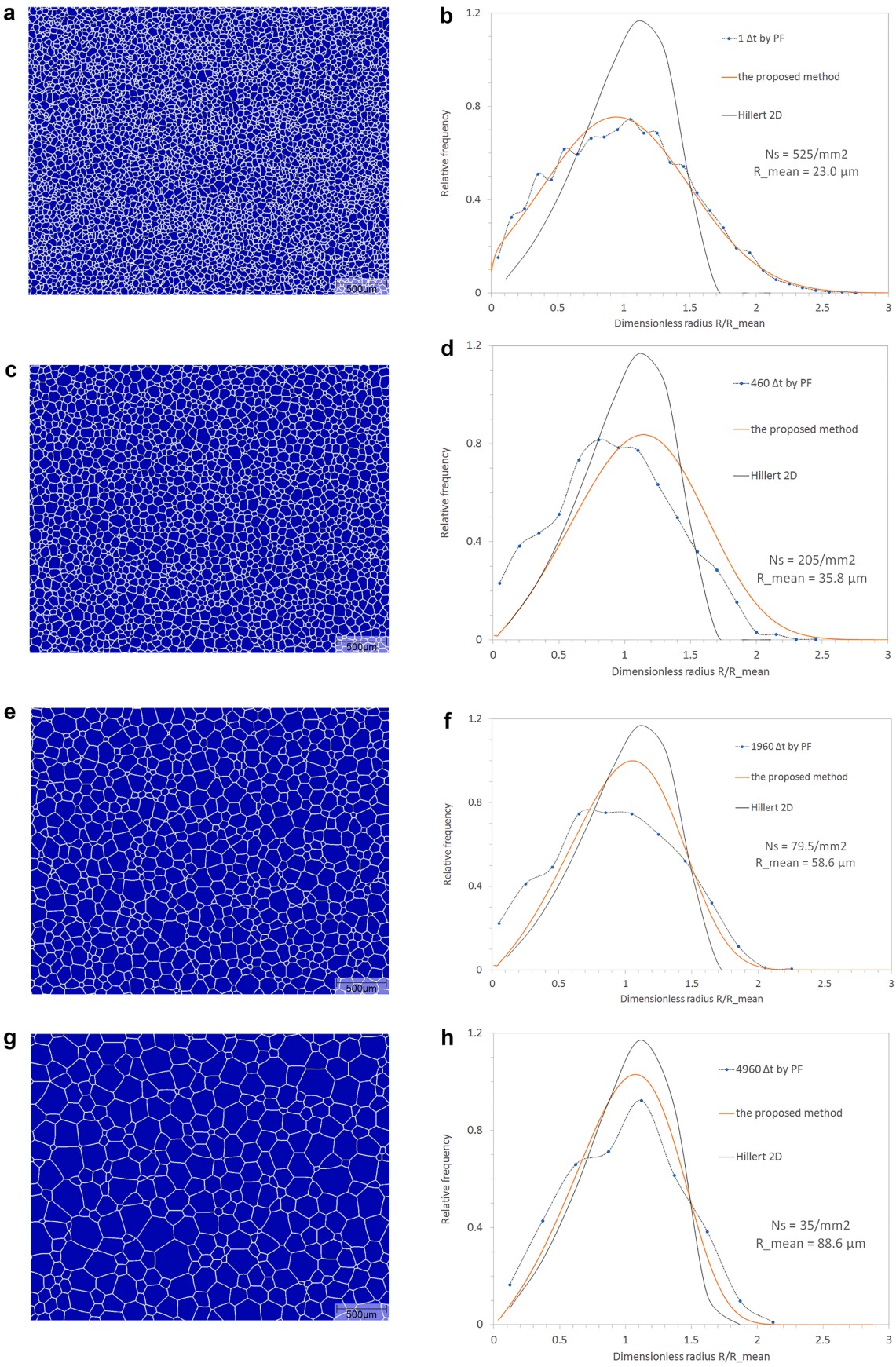

Fig. 4. Evolutions of grain size distribution density functions with the initial distributions of a random Voronoi polygon tessellation. The KWN simulation results starts with the initial distribution function generated by Voronoi tessellations with the phase filed simulation, $\varphi(R,0) = \frac{N_0}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(R-\mu)^2}{2\sigma^2}\right)$, $\mu = 18\mu m$, $\sigma = 21\mu m$,

$N_0 = 700/mm^2$. (a) Grain structure by PF at time step 1 (b) Normalized Grain Size Distribution (GSD) by Phase Field (PF) and the proposed model at time step 1 (c) Grain structure by PF at time step 460 (d) Normalized GSD by PF and the proposed model at time step 460 (e) Grain structure by PF at time step 1960 (f) Normalized GSD by PF and the proposed model at time step 1960 (g) Grain structure by PF at time step 4960 (h) Normalized GSD by PF and the proposed model at time step 4960 (i) Grain structure by PF at time step 9960 (j) Normalized GSD by PF and the proposed model at time step 9960 (k) Grain structure by PF at time step 14,960 (l) Normalized GSD by PF and the proposed model at time step 14,960.

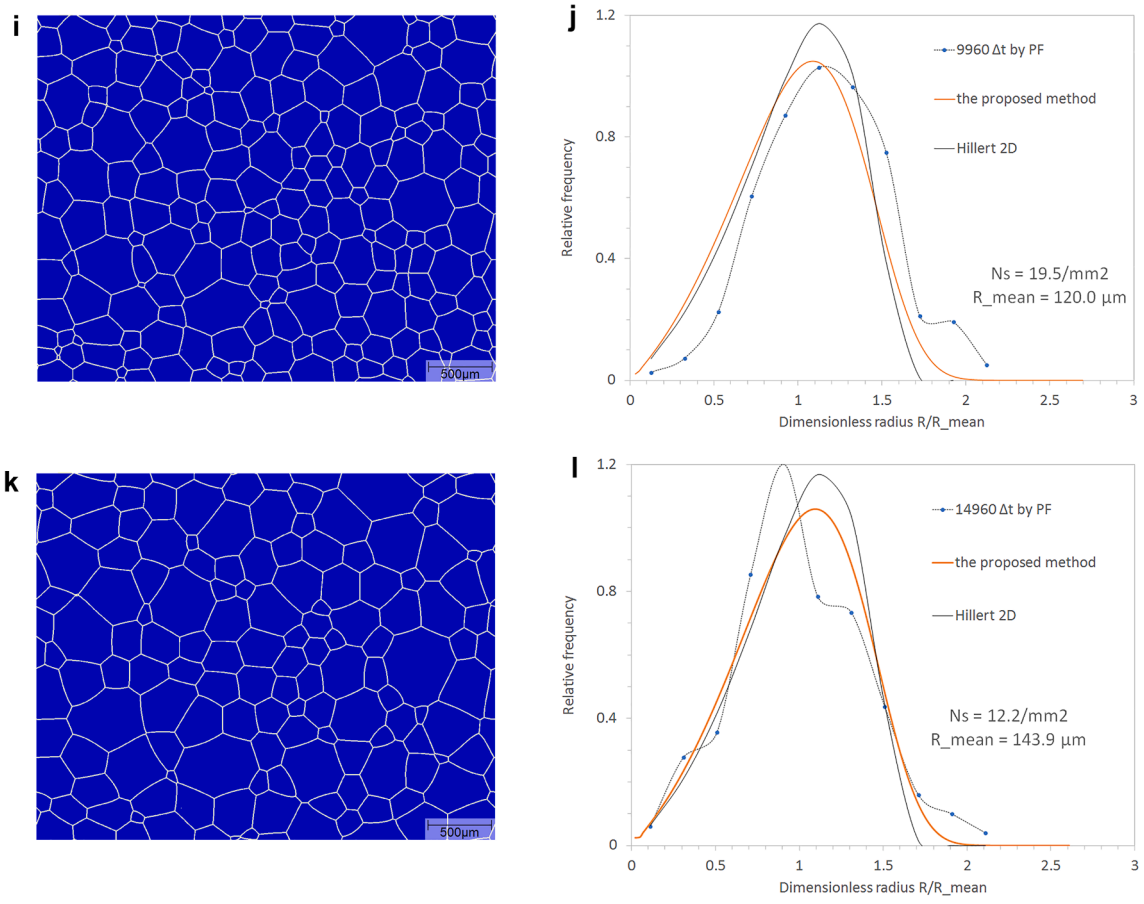

Fig. 4. (*continued*).

reported here range from simple ideal grain growth to the one with a random placement of grains in space to verify the wide breadth of its applications.

3.1. Lognormal distribution, normal distribution and Weibull distribution

In this subsection the results of three simulations are reported. The three simulations start with different initial conditions, which are described respectively by the lognormal, normal and Weibull distribution functions as given in the Fig. 1 caption. The 3D Hillert's growth rate equation, i.,e. Eq.1, have been employed. The predicted evolutions of grain size distribution density functions by the proposed model are shown in Fig. 1a, b and c, and mean radius and grain number density in Fig. 2.

As shown in Fig. 1, although initially the normalized size distributions for the three simulations are different, they gradually approach to Hillert's invariant distribution represented in each figure by the dotted curve. The attainment of this stable distribution in the simulation results provides the first validation of the model implementation. It is worthy of noting that to reach stable distribution state it takes only 1000 time steps in the simulation with the initial normal Grain Size Distribution (GSD) while it takes more than 360,000 time steps in the simulation with the initial of lognormal. It indicates that size distributions have a great influence grain growth process, a statement raised earlier by other researchers [11]. This is more evident in Fig. 2 (a) in which the evolutions of mean radius in the three simulations are presented. Starting with the same mean radius value of 10 μm, the three simulations predict different coarsening rate. The one with the Weibull initial has been leading in the race to the invariant distribution although its initial grains number density is lowest as shown in Fig. 2b. These simulation results highlight the importance of addressing initial size distributions when analyzing grain growth process. It also indicates that one could tune grain growth by customizing initial grain size distribution.

3.2. Bi-modal initial grain size distribution

In this section, the proposed model is applied to predict grain growth from an initial grain structure with a bimodal distribution. This case study is relevant to abnormal grain growth in which multi-modal grain size distributions usually exist. Due to the Lagrangian scheme used in solving the proposed model, there is no numerical difficulties to handle this case as to be demonstrated below. Miyoshi equation, i.e. Eq. (6), have been selected in this simulation for growth rate calculation. One of the reasons we have used Miyoshi growth rate equation in this simulation is to demonstrate the equation, which is derived from the parameterization of phase field simulation results, is as valuable as the analytical Hillert equation. We also want to demonstrate the proposed model can take different forms of growth rate equations, which is a valuable feature when the model is applied to a scenario with a growth rate equation not described in this paper.

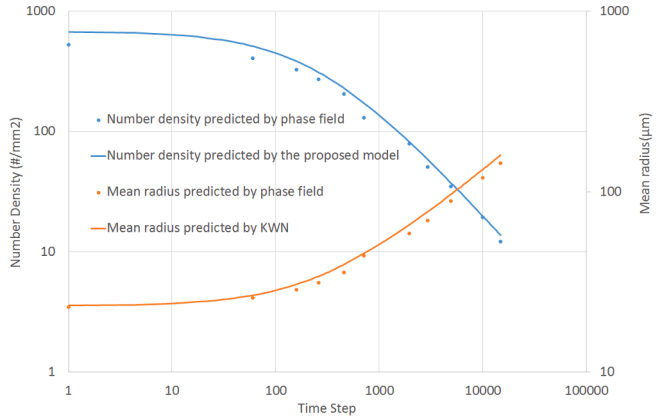

Fig. 5. The predicted evolution of grains number density and mean radius by phase field method and the proposed model. In this paper, we have extended the Kampmann-Wagner numerical model, which had been successfully applied for modeling particle precipitation (i.e. Ostwald ripening), toward grain growth modelling. The model has been applied to simulate grain growth with different initial grain size distributions. The figure above shows the results from the case study with the initial distribution of arbitrary Voronoi tessellations. The predictions on the evolutions of grains number density and mean radius by the proposed model and phase field have been presented with solid lines and markers in the figure. Good agreement can be observed. We also have made an animation for demonstrate the good agreements of the two models' predictions on the evolutions of grain size distributions. The animation file (2D_grain_growth_PF_KWN_Distribution_Curves.mp4) is enclosed to this paper. We conclude that the extension has enabled the KWN approach, which had been employed successfully for precipitation modeling and as-cast grain size prediction, applicable to model grain growth thus reducing the threshold for the establishment of an efficient Integrated Computational Materials Engineering modeling framework.

The simulation starts with two peaks in the size distribution function as shown by the black curve in Fig. 3. After an initial transient period of growth, the first peak quickly become smaller as seen in the green curve and disappear after 60 time steps as seen in the yellow curve. The distribution attains the invariant state after about 1000 time step as shown by the dotted curve in Fig. 3. This simulation demonstrates the model's ability of treating grain growth with a multi-modal size distribution. The simulation results indicate that the bimodal distribution is not a good candidate if one wants to design a material that requires slow precipitate coarsening rate.

3.3. Modelling the transient grain growth from the initial grain structure of Voronoi tessellations

In this section, the extended model is applied to predict grain growth from the initial grain structure of a random placement of grains in space. This initial grain structure is called Voronoi polygon tessellation, and often used as the starting point for modelling grain growth [31]. It has been accepted that when the initial distribution is not self-similar such as that of a Voronoi tessellation the transitions take place in such a way that they 'transform' the random spatial arrangement of Voronoi polyhedral into the correlated spatial arrangement of the self-similar state [1]. This observation is to be used for the verification of the simulation results. We also performed the phase field simulation by the commercial phase field modelling software Micress [32] with the same initial conditions to validate the proposed model ability to capture the transformation stages before reaching the self-similar state.

The phase field simulation starts with the initial grain structure of a random placement of 5440 grains in a 3600 μm × 2880 μm 2D space. The predicted grain structure images, presented in Fig. 4 (a) (c) (e) (g) (i) (k), clearly show all the aspects of grain growth process including grain metrics and topology for this given assembly of grains. It should be emphasized again this unique ability of phase field method is insightful and predictive so that the method is often considered "computer experiment" to verify other less-detailed methods such as the proposed model in this paper.

The phase field simulation results are also presented in the form of grain size distribution function, which are readily used to verify the predictions from the proposed model. The temporal evolution of the normalized grain size distributions together with the predicted results from the proposed model with the same initial distribution are presented in Fig. 4 (b) (d) (f) (h) (j) (l). Good agreements are achieved between the phase field and the proposed model predictions in both the transient growth stages (up to Time Step 1960) toward self-similarity and the final self-similarity stage (from Time Step 4960 upwards).

The good agreement is also observed in Fig. 5, which shows the the grains number density and mean radius by phase field method and the proposed model. Both two models predicted the same paths along which the number density has been reduced to about 2% of the initial value and mean radius increased by 6 times. The transient growth stage, i.e. the ones before the asymptotic solution has been reached, are clearly quantitatively reproduced by the the proposed model.

It is safe to conclude that in spite of lacking the ability of presenting visual images for grain growth process the proposed statistical model can capture the evolutions of grain size distribution reasonably well at a tiny fraction of the computational time spent by phase field simulation.

4. Conclusions and future work

We have demonstrated that the extension of the multi-phase Kampmann-Wagner Numerical (KWN) model, which had been successfully applied for modeling particle precipitation (i.e. Ostwald ripening) toward grain growth, is successful. The extended model has been applied to simulate ideal grain growth, grain growth with the initial states of lognormal/normal/Weibull distributions, bi-modal grain size distribution and arbitrary Voronoi tessellations, and the simulation results have been verified by asymptotic solution and by phase field simulation results. The extension has enabled the KWN approach, which had been employed successfully for precipitation modeling and as-cast grain size prediction, applicable to model grain growth thus reducing the threshold for the establishment of an efficient Integrated Computational Materials Engineering modeling framework.

There are three directions the proposed model can be further extended. The first is to adopt solely the 3D topology dependent growth rate proposed by MacPherson and Srolovitz in [29] and solve the frequency distribution density function in both size space and topology space (e.g. the number of sides) while still imposing the volumetric constrains. This extension would enable the derivation of the relation between grain topological feature and size. The second is to address the mismatch on the invariant grain size distribution between the model predictions and the experimental results, which is an open question remained to be solved for modelling both grain growth and particle coarsening. The proposed model opens the possibility to address this mismatch by the joint efforts in the two research communities, and hopefully good synergies will lead to a break-through in the near future. The third is to extend the model to handle real materials including a range of more complicating aspects such as orientation dependent boundary properties as well as possible solute/particles drag effects.

5. Data availability

Data will be made available on request.

Author contribution

Q. Du and J.X. Xie planned the study. Q. Du and M.M. Chen extended the KWN model, and performed the simulations. M.M. Chen and Q. Du conducted the phase field simulations. All authors discussed the results and were involved in the writing of the manuscript.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.commatsci.2020.110066.

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