On the grain size distributions obtained from different grain growth simulation techniques

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Grain size distribution (GSD) is an important attribute of polycrystalline materials. For microstructure evolution processes such as grain growth, the evolution of grain size distribution can be predicted from both theoretical considerations [1] and computer simulations [2, 3].

Tikare *et al.* [2] compared two simulation models, i.e., the phase field model and the Potts model, and found that the GSDs obtained by these two models are very similar, but they did not provide the functional form of the GSDs.

In a recently published work, Wang *et al.* [3, 4] employed the Monte Carlo Potts method to study the grain growth process starting from initial microstructures with different grain size distributions. Their results show that the quasi-steady state grain size distribution has a Weibull function form, which is different from the Louat distribution form as reported by Fan and Chen [5] using a phase field method.

In this paper, the phase field model [5] was employed to investigate the quasi-steady state GSD in 2D in order to find reasons for the discrepancy mentioned above. A 512×512 square lattice was used for the simulation with periodic boundary conditions applied along both Cartesian coordinate axes. The grid size Δx was chosen to be 2.0 and the time step Δt to be 0.25. The number of field variables p was assumed to be 36.

The computer simulation started by assigning to all field variables a random value between -0.001 and 0.001, which corresponds to a super-cooled liquid state, and then allowing crystallization to occur, which generates a fine grain microstructure. Further microstructure evolution corresponds to the grain growth process. The microstructures at $t = 1000$ TS and $t = 5000$ TS is shown in Fig. 1.

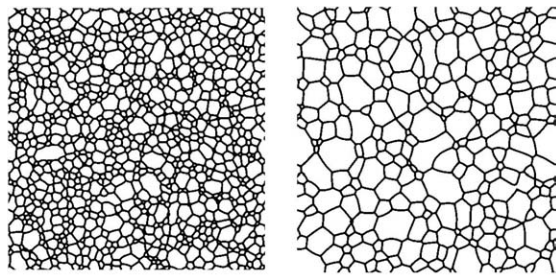

Figure 1 Microstructure evolution produced using the phase field method (TS = time step).

The grain size distribution obtained at time $t = 1000$ TS is shown in Fig. 2a. It can be seen that both Weibull function [6] and Louat function [7] give satisfactory fit to the simulated GSD, with their corresponding chi-square values better than 0.003 and the determination coefficients better than 0.98. It can also be clearly seen from the figure that the Weibull function agrees much better with the simulated GSD than the lognormal function [8]. The same is true over the whole simulation regime, as shown in Fig. 2b and c.

At $t = 3000$ TS, the Weibull function agrees a little better with the GSD than the Louat function. But when $t > 4000$ TS, both Weibull ($\beta = 2.1$) and Louat ($\alpha = 0.8$) functions give satisfactory fit to the GSDs again. So it is necessary to further compare these two functions.

The Weibull function can be written as:

$$\mathrm{Weibull}(r) = \frac{\beta}{\alpha^{\beta}} r^{\beta-1} \exp\left[-\left(\frac{r}{\alpha}\right)^{\beta}\right] \tag{2}$$

where β is an adjustable parameters and $\alpha = 1/\Gamma(1 + 1/\beta)$. The Louat function has a form:

$$\mathrm{Louat}(r) = 2\alpha r \exp(-\alpha r^2) \tag{1}$$

where α is an adjustable parameter.

Comparing the two functions above, it can be found that when β in Equation 2 equals to 2, the Weibull function actually reduces to the Louat function form with $\alpha = (\Gamma(1 + 1/\beta))^2$ in Equation 1. It can be easily verified in Fig. 3a where the two curves overlap. Fig. 3b shows further comparison between these two functions. It can be seen that Weibull function curves with parameter β ranging from 1.9–2.1 are very close to the Louat function curves with parameter α ranging from 0.7–0.9. This may indicate that the two functions can replace each other within this range, leading to the cases in Fig. 2a and c. Outside this range, however, the difference between these two functions becomes obvious, such as the case in Fig. 2b.

From the discussions above, there exists no significant discrepancy between Wang and Liu's Weibull-type GSD [3, 4] obtained from Monte Carlo Potts simulation, shown in Fig. 4a, with Fan and Chen's Louat-type GSD [5] from phase field simulation. It can also be deduced that Weibull function fits the GSDs well

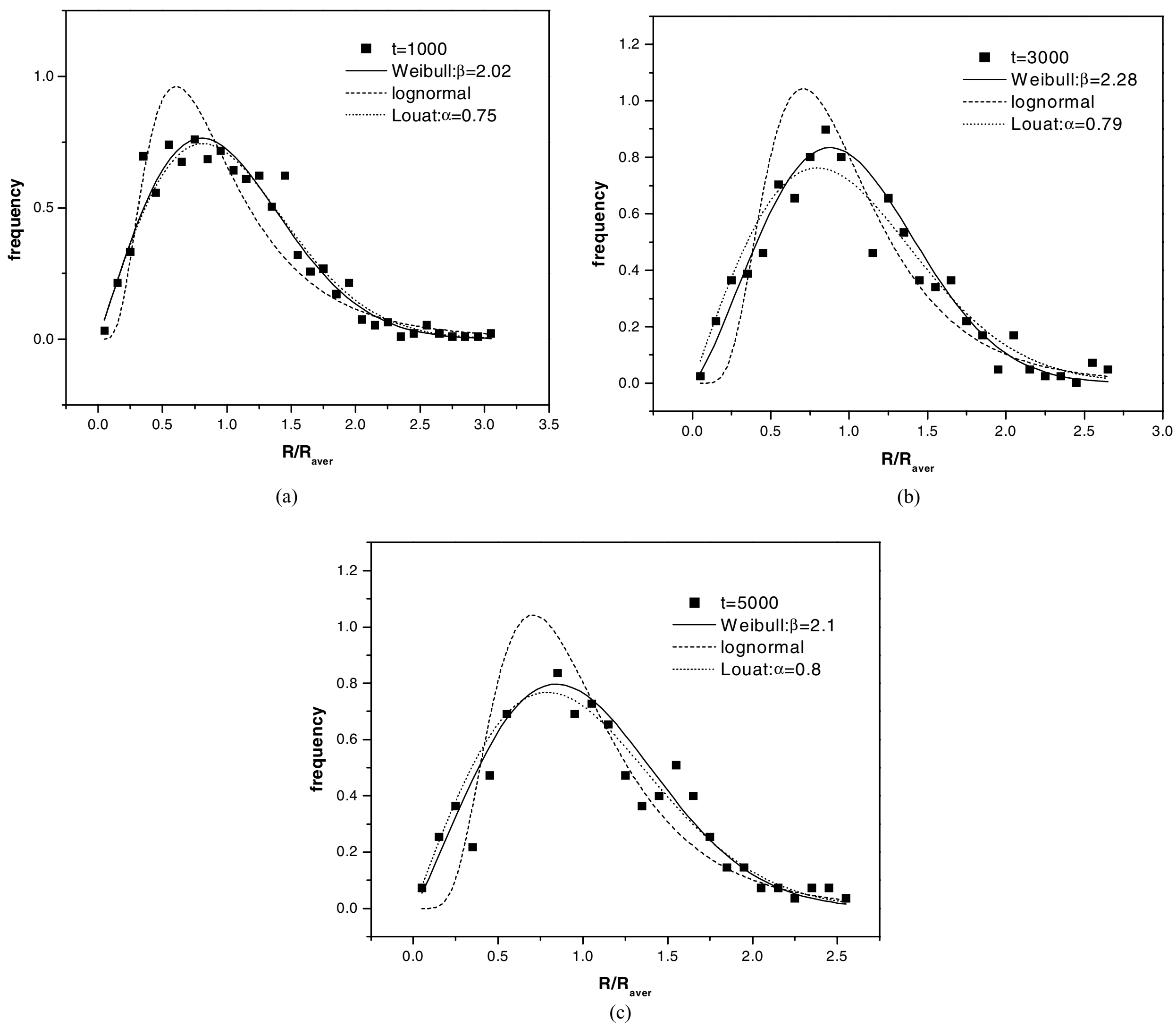

Figure 2 GSDs at different time steps, comparing with the lognormal [16], Weibulll and Louat functions.

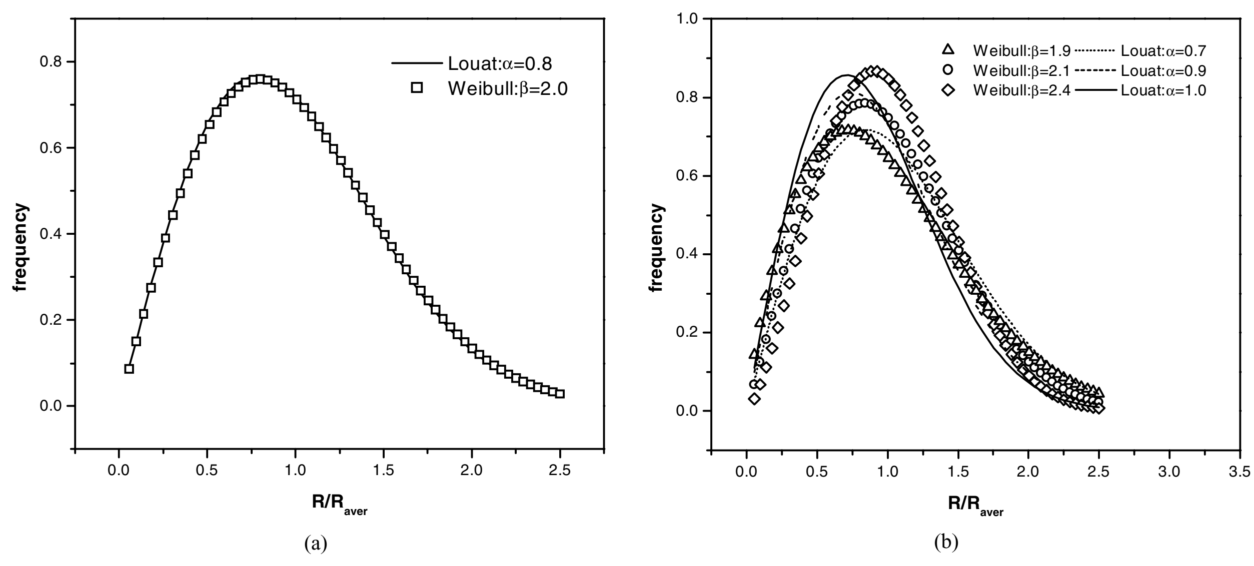

Figure 3 Comparison between Weibulll and Louat functions.

over the whole simulation regime using both simulation methods.

For more evidence, the quasi-steady state GSDs obtained from three other different simulation techniques are also shown in Fig. 4.

Battail and Holm [9] produced initial microstructures with GSDs of Hillert distribution form through two different approaches, and then let them evolve by performing the Monte Carlo algorithm. The GSD obtained is plotted in Fig. 4b. We fitted the data with the Weibull

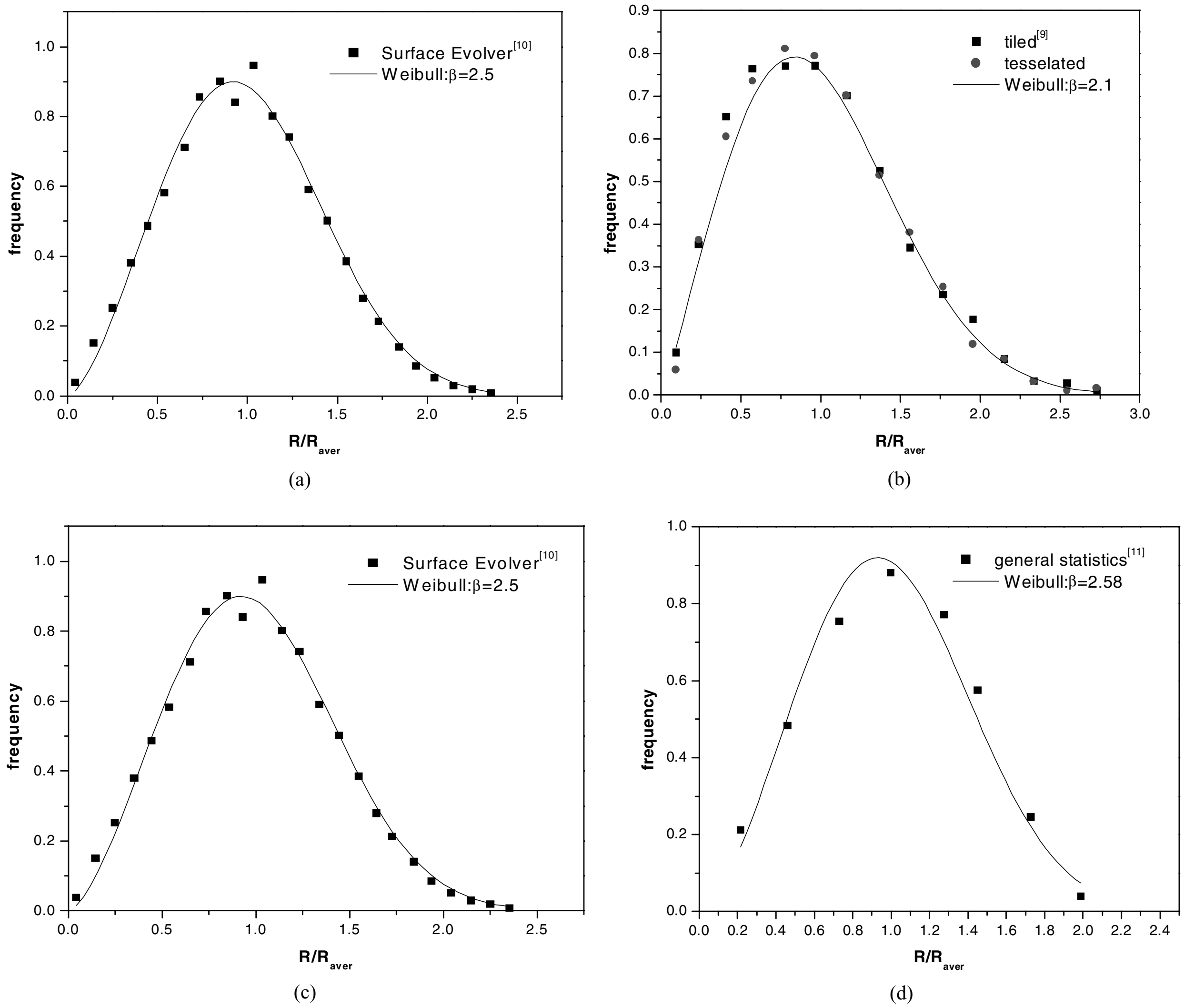

Figure 4 GSDs obtained from different simulation techniques.

function and found that the chi-square value is better than 0.002 and the determination coefficient better than 0.99. This fact further suggests that the Weibull function is at least one of suitable forms to describe the quasi-steady state GSD in 2D grain growth process.

Marthinsen *et al.* [10] used Surface Evolver[1] to simulate the normal grain growth in 2D. Their result, shown in Fig. 4c, also can be well described by the Weibull function with the chi-square value close to zero and the determination coefficient better than 0.99.

Fig. 4d shows the GSD acquired using the general statistics method [11]. Again the Weibull function fits it well with the chi-squares value better than 0.003 and the determination coefficient better than 0.98, which further demonstrates that Weibull function is suitable to describe the quasi-steady state GSD in 2D.

In conclusion, the grain size distributions obtained using the phase field method is not only very similar to the GSDs obtained by the Monte Carlo Potts model [3, 4, 9], but also quite similar to those obtained by both the Surface Evolver method [10] and the general statistics method [11] as demonstrated in Fig. 4.

[1]Surface Evolver is a computer program first developed by K. A. Brakke (See: *Exp. Math.* **1** (1992) 141).

It is further concluded that the Weibull function is at least one of the mathematical expressions suitable to describe the quasi-steady state grain size distribution in 2D normal grain growth resulting from all the four different simulation techniques mentioned above. No essential difference exists among the basic forms of grain size distributions obtained in References [3–5, 9–11] and this work, though different simulation techniques were employed.

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