# COMPARISON OF MULTI PHASE FIELD AND CONTINUUM FIELD MODELS FOR GRAIN GROWTH


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## Abstract

*The continuum field [1,2,3] and multi phase field [4,5] model are two alternative approaches following the 'phase field' methodology that can be applied for the simulation of grain growth. We derived relations between the parameters in both models and simulated the evolution of multi-grain structures with the two models using equivalent parameter values. The results are compared with analytical models.*


## Phase field models

| | Multi Phase Field (MPF)[5] | Continuum Field (CF)[3] |
|---|---|---|
| Variables | $\sum_\alpha \varphi_\alpha = 1$ | $\eta_\alpha$ : independent |
| Free energy | $F=\int_V \frac{1}{\varepsilon} w(\varphi) + \varepsilon a(\varphi,\nabla\varphi) dV$<br>$w(\varphi) = 9\sum_{\alpha<\beta}\gamma_{\alpha\beta}\varphi_\alpha^2\varphi_\beta^2$<br>$a(\varphi,\nabla\varphi) = \sum_{\alpha<\beta}\gamma_{\alpha\beta}\left(\varphi_\alpha\nabla\varphi_\beta - \varphi_\beta\nabla\varphi_\alpha\right)$ | $F=\int_V m f_0(\eta) + \frac{\kappa(\eta)}{2}\sum_\alpha (\nabla\eta_\alpha)^2 dV$<br>$f_0(\eta) = \sum_\alpha\left(\frac{\eta_\alpha^4}{4} - \frac{\eta_\alpha^2}{2}\right) + \sum_{\alpha<\beta}\gamma^*_{\alpha\beta}\eta_\alpha^2\eta_\beta^2$<br>$\kappa(\eta) = \frac{\sum_{\alpha<\beta}\kappa_{\alpha\beta}\eta_\alpha^2\eta_\beta^2}{\sum_{\alpha<\beta}\eta_\alpha^2\eta_\beta^2}$ |
| Kinetics | $\tau\varepsilon\frac{\partial\varphi_\alpha}{\partial t} = -\frac{\partial F}{\partial\varphi_\alpha} + \lambda$<br>$\lambda$ : lagrange multiplier | $\frac{\partial\eta_\alpha}{\partial t} = -L\frac{\partial F}{\partial\eta_\alpha}$ |

## Equivalent parameters

Equal interfacial energy ($\sigma_{\alpha\beta}$)

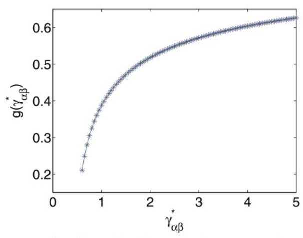
$$\gamma_{\alpha\beta} = g(\gamma^*_{\alpha\beta})\sqrt{\kappa_{\alpha\beta} m}$$

Equal interface velocity ($\mu_{\alpha\beta}$)

$$\frac{\gamma_{\alpha\beta}}{\tau} = L\kappa_{\alpha\beta}$$

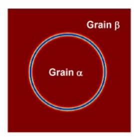
Comparable interface width ($\varepsilon$)

$$\varepsilon\gamma_{\alpha\beta} = \kappa_{\alpha\beta}$$




$g(\gamma_{\alpha\beta}^*)$ calculated via numerical integration

## Shrinking circle



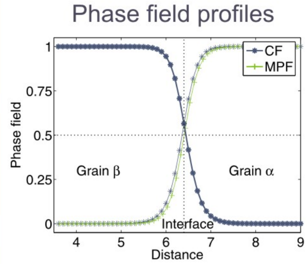

Grain area:

$$A_\alpha(t) = A_{\alpha,0} - 2\pi\mu_{\alpha\beta}\sigma_{\alpha\beta}t$$

Total grain boundary

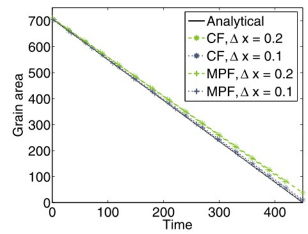
$$E_{gb}(t) = 2\sqrt{\pi}\sigma_{\alpha\beta}\sqrt{A_{\alpha,0} - 2\pi\mu_{\alpha\beta}\sigma_{\alpha\beta}t}$$

Phase field profiles



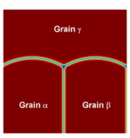

for $\sigma_{\alpha\beta}$=0.25, $\mu_{\alpha\beta}$=1, ε=0.5,

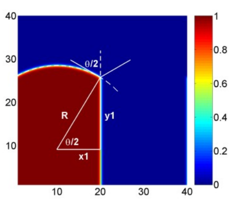
Temporal evolution grain area




for $\sigma_{\alpha\beta}$=0.25, $\mu_{\alpha\beta}$=1, ε=0.5

## Three-grain structures




Constant triple-junction angle

$$\frac{\theta}{2} = \arccos\left(\frac{\sigma_{\alpha\beta}}{2\sigma_{\alpha\gamma}}\right)$$

Constant velocity $v_{\alpha\gamma} = v_{\beta\gamma} = -\mu_{\alpha\gamma}\sigma_{\alpha\gamma}\frac{1}{R}$

and $R = \frac{x_1}{\cos\left(\theta/2\right)}$

$$\Rightarrow \frac{dA_\alpha}{dt} = -\mu_{\alpha\beta}\sigma_{\alpha\beta}$$

| | MPF | CF |
|---|---|---|
| $\sigma_{\alpha\beta} = \sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.25$<br>θ=120°, dA/dt=0.25 | θ=122.06°<br>d A/dt=0.247 | θ=117.7°<br>d A/dt=0.250 |
| $\sigma_{\alpha\beta} = 0.25$, $\sigma_{\alpha\gamma} = \sigma_{\beta\gamma} = 0.2$<br>θ=102,6°, dA/dt=0.25 | θ=104.8°<br>d A/dt=0.248 | θ=102,0°<br>d A/dt=0.255 |

for Δx=0.2, ε=0.5, $\mu_{\alpha\beta}$=1

## Conclusions

Although the mathematical formulation is very different, both models give nearly the same simulation results. Small differences are probably due to the use of different numerical techniques. In the multi phase field model, the parameters equal measurable quantities, such as interfacial energy, mobility and width, whereas parameter determination in the continuum field model is more laborious. On the other hand, the continuum field model is more straightforward to implement and simulations are faster. However, so far, there is no decisive indication that one model is preferable for grain growth simulations.

## Further research

Comparison of grain size distribution and triple junction angles for polycrystalline structures. Comparison for systems with bulk driving force.


***References***

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