Testing the potential of the phase field method for modeling Solid-Solid Phase Transformations in Aluminum Alloys

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Introduction

During the homogenization of aluminum alloys, several microstructural changes may occur. For example, grain growth, precipitate dissolution (Figure 1a) and phase transformation, and shape change of constituent particles (Figure 1b).

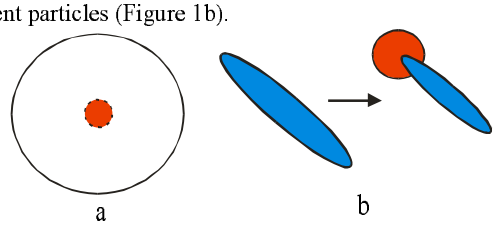

Figure 1 Microstructural changes.

All of these phenomena are now understood well enough to allow them to be modeled mathematically. For example, a model for dissolution of precipitating phases has been previously developed by *Vermolen et al* [1]. This model, based on the moving grid method, does not contain the required phase transformation and shape change of constituent particles.

Objective

To develop a mathematical model of the phase transformation and shape changes, which may occur during homogenization of constituent particles.

The Model

At the initial stage a test model must be developed to allow the accuracy of the methods to be assessed. We, therefore, assume a Si particle in an Al-Si matrix (Figure 1a).
The dissolution of a precipitate is modeled as a diffusion problem, where the equation for each alloying element is derived from Fick's second law

$$\frac{\partial c_i}{\partial t} = \nabla \cdot \left(D_i(T) \, \nabla c_i \right).$$

We assume no flux at the cell boundary and the concentration given at the moving boundary. A Stefan condition is used at the moving boundary to satisfy the balance between the diffusion and the volume decrease.
A numerical method to model this problem is the phase field method, which is able to capture the phase transformation and shape changes of the particles. To test this method, the method has to reproduce the results of precipitate dissolution obtained with the moving grid method (Vermolen).

Phase Field

The phase field method introduces an order parameter ϕ and an order equation. For a spherical geometry the diffusion equation becomes [2]

$$\frac{\partial c}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D(r,T) r^2 \frac{\partial c}{\partial r} \right) + \frac{M}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \phi}{\partial r} \right),$$

The order equation is given by

$$\tau \frac{\partial \phi}{\partial t} = \frac{\xi^2}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial \phi}{\partial r} \right) - w'(\phi) + DF,$$

Figure 2 shows the ideal situation of the order equation.

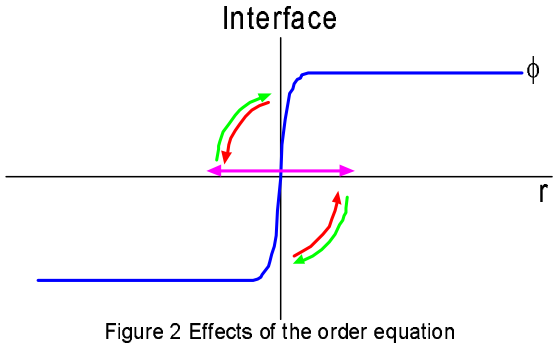

Figure 2 Effects of the order equation

Ideally, the time derivative should have no effect on the shape, while the space derivative flattens the function. This effect should be countered by the double well potential. Finally, the driving force only moves the function forward or backward horizontally.

Results

The results of the phase field method are compared with the results of the moving grid method in Figure 3.

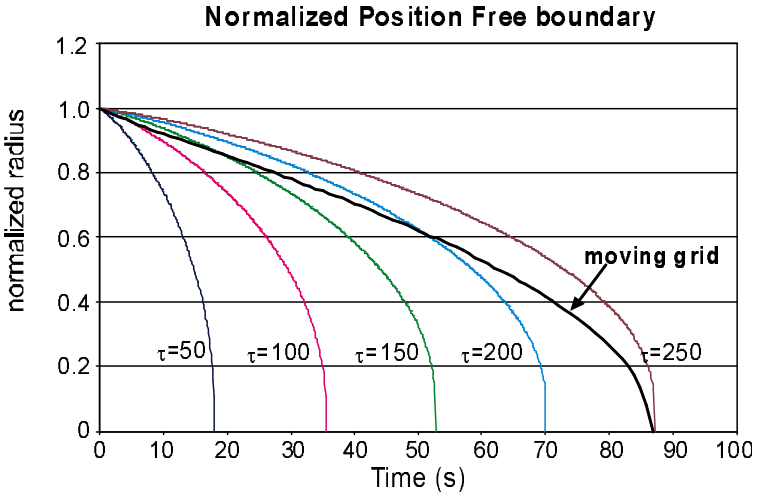

Figure 3 Dissolution path of spherical Si particle

Figure 3 shows that the shape of the dissolution paths of both methods is similar and that the final dissolution time with the phase field method depends on the relaxation time τ. At the moment we start to comprehend the meaning of τ.

Future Work

- Comparing the Phase Field method and the Level Set method with the Moving Grid method, using [3].
- Including the effects of the phase transformation, and shape change in the Phase Field method and the Level Set method.

References

[1] F.J. Vermolen, K. Vuik, S. van der Zwaag, Mat. Sci. Eng. A, 254:13-32, 1998.
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[3] W. van Til, C. Vuik, S. van der Zwaag, *An inventory of Numerical methods to model Solid-Solid Phase Transformations in Aluminum Alloys*, NIMR Report: P.00.4.001, 2000.

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