Models for diffusion control of migrating phase interfaces

a) *Sharp Interface Model*. There are at least three kinds of models of migrating interfaces. The simplest one is the sharp interface model and it is very widely used for the treatment of diffusion controlled phase transformations. Basically, it simply assumes that there is full chemical equilibrium between the two phases locally at the interface. In addition, one may accept that there is some friction acting against the migration, which is usually assumed to be proportional to the rate of migration. That migration will then require some driving force that has to come from some deviation from local equilibrium at the interface. In order to evaluate that driving force it is necessary to analyze the relation between the fluxes across the interface the fluxes in the two phases. This has now been analyzed in detail (1). An attempt has also been made to evaluate the mobility of "random" ferrite/austenite interfaces by analyzing experimental data on the massive transformation from the literature (2).

Another method of predicting the rate of migration is to assume that the atoms cross the interface by individual jumps. The rate will then depend on the individual diffusivities of the components across the interface. The diffusion equation for this process must take into account that there is a considerable difference in composition between the two sides of the interface. Such an equation has now been derived using an absolute reaction rate approach (3).

This equation cannot describe the phenomenon of trapping and even less the diffusionless growth of the new phase in a massive transformation. To handle such cases work has started to include cooperative transfer of groups of atoms across the interface. Experimental study of the critical solute content above which massive transformation cannot occur has been performed on the Fe-Ni (4) systems and a first version of the revised equation has been applied to analyze the new information (5).

As an attempt to improve the sharp interface model further we have tried to make it find the correct boundary conditions for diffusion in a phase at the interface to an adjacent phase automatically. They are directly obtainable by calculation from a thermodynamic database if one can assume local equilibrium and if one works with binary systems. In ternary systems there is a two-phase field with a series of tie-line and it is not self evident how to find the operating tie-line and that tie-line will normally change during diffusional phase transformation. Advanced programs for simulating diffusional transformations must be provided with automatic procedures but they may turn very time-consuming for higher order systems and may even have difficulties converging. A completely new approach (6) is now attempted where those boundary conditions are not required but the local conditions are made to gradually approach the relevant "tie-line" during the ordinary iteration procedure for diffusion. Since local equilibrium between the two phases is not used as a prerequisite but will be the result of the process itself, it should be possible to apply the method also to cases where there is some deviation from local equilibrium.

b) *Wide interface model.* In the simplest version this model is applied to an interface of fixed width. Then one can describe a composition profile within the interface and work with some special thermodynamic model for a solution phase within the interface. If that model is made to attract the solute atoms to the central part of the interface, they tend to diffuse with the interface if it migrates. That causes a dissipation of Gibbs energy which has to be subtracted from the driving force for the migration. This is called solute drag and was first modelled for grain boundaries in homogeneous, single-phase systems. Another model was developed for phase transformations and there seemed to be a conflict between the two approaches. That conflict has now been resolved by a treatment that applies to both cases (7).

c) *Interface with undefined width*. This case will be discussed under the heading "Phase-Field Model".

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