

Kinetic models for austenite to ferrite transformation in Fe-C-X

Introduction

There are at least three kinds of models of moving 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. That will give the boundary conditions for diffusion inside the volumes of the phases in the system. In reality, there may be important cases where there is an appreciable deviation from local equilibrium at the moving interfaces in phase transformations. It may be described as an effect of some friction in the interface acting against the motion, which is usually assumed to be proportional to the rate of motion. It may be visualized as a difficulty of the atoms to rearrange themselves into the structure of the new lattice. Another kind of model is based on a description of the interface as a layer of appreciable thickness, which makes it possible to consider the composition profile inside the interface. It is then possible to describe the friction as a requirement of driving force for the diffusion inside the interface. This is closely related to the phenomenon of solute drag occurring in grain growth in single phase materials. A third kind of model is based on assuming that there is a diffuse region of gradual transition of the properties from one phase to the other. The first approach (1) was one-dimensional and was made on the atomic level but has now developed into the very powerful Phase Field Method where one considers mesh points in a three-dimensional network. It will be treated in another section.

Sharp interface models

a) *Modelling of friction term.* One may accept that there is some friction acting against the motion of the phase interface and requiring some driving force. It is usually assumed that the velocity should be proportional to the driving force and the constant of proportionality is regarded as the mobility. Its value under various circumstances is not well established but a new attempt has recently been made to evaluate the mobility of “random” ferrite/austenite interfaces by analyzing experimental data on the massive transformation from the literature (2).

The driving force for overcoming the friction has to come from some deviation from local equilibrium at the moving interface. Thus, one must evaluate the deviation and that gives the necessary boundary conditions at the interface and, in turn, that makes it possible to treat the diffusion inside the volumes of the phases. It is thus necessary to analyze the relation between the fluxes across the interface and the fluxes in the two phases simultaneously. This has now been attempted in a special case (3).

b) *Modelling of diffusion across interface.* Another method of predicting the rate of motion is to assume that the atoms cross the interface by individual jumps and to evaluate the net flux of atoms. That process will dissipate Gibbs energy, i.e., consume driving force. The effect could be experienced as a friction although it originates from a different physical process. The rate of motion of the interface would 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, which is not allowed by the ordinary diffusion equation. Such an equation has now been found and it could be derived using an absolute reaction rate approach (4).

c) *Finding the proper tie-line for a moving interface.* The conditions at the phase interface, which will be used as boundary conditions for diffusion within the phases, 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-lines and it is not self-evident how to find the operating tie-line and that tie-line will normally change during diffusional phase transformations. The problem increases with each increase of the number of components in the alloy. Advanced programs for simulating diffusional transformations must be provided with an automatic procedure for finding the “relevant tie-line”. It seems that such a procedure may turn very time-consuming for higher-order systems and may even have difficulties converging. A new approach has now been attempted where those boundary conditions are not required but the local conditions at the interface are made to approach the relevant tie-line gradually during the ordinary iteration procedure for diffusion by considering the diffusion across the interface and inside the phases simultaneously. Since local equilibrium between the two phases is not used as a prerequisite but will be the result of the process itself, it seems possible to apply the method also to cases where there is some deviation from local equilibrium (5).

d) *Modelling trapping and diffusionless growth.* The equation mentioned above cannot describe the phenomenon of trapping and even less the diffusionless growth of the new phase that may happen in a massive transformation, i.e., a partitionless transformation where there is not even a pile-up of solutes in front of the moving interface. 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 (6) system and a first version of the revised equation has been applied to analyze the new information (7). A method that has been used before is based on adding cross terms to the diffusion equations of individual alloy elements (8).

Wide interface model

The simplest version this model was applied to an interface of fixed width and uniform properties and an analytical expression was used to describe the composition profile inside the interface. The dissipation of Gibbs energy due to the diffusion was treated as a friction (9). In the next version (10) the properties were allowed to vary across the interface and the diffusion process was solved numerically. Then one can describe a composition profile within the interface and work with some special thermodynamic model for a solution phase within the interface. It was then possible to simulate the transition from diffusion controlled to diffusionless solidification (11).

Solute drag

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 moves. That causes a dissipation of Gibbs energy which has to be subtracted from the driving force for the motion. This is related to the phenomenon called solute drag which was modelled in a similar way for grain boundaries in homogeneous, single-phase systems (12). It got its name because the treatment was not based on the dissipation of Gibbs energy but considered the actual attraction between the solute atoms and the centre of the interface. It turned out that when the solute drag treatment was applied to a phase transformation in an alloy, it did not give the same result as the treatment based on the dissipation of Gibbs energy. Finally a unified treatment was found (13).

Today the term 'solute drag' is commonly applied to both grain growth and phase transformations. The application of the mathematically formulated treatments are few but it is common to propose that various discrepancies from expected results are caused by solute drag or even by a 'solute drag like effect'. It is interesting that it was found (12) that the same treatment does not always give a drag but a driving force. That is always the case when applied to the phenomenon called CIGM (Chemically Induced Grain boundary Migration) (14), a name that was later changed to DIGM (Diffusion induced grain boundary Migration) when it was incorrectly proposed that it was the diffusion process itself that caused the phenomenon (15).

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