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Application of the cyclic phase transformation concept for determining the effective austenite/ferrite interface mobility

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ABSTRACT

A series of cyclic partial austenite–ferrite phase transformation computer simulation experiments have been performed to elucidate the rate controlling dissipative processes during austenite-to-ferrite and the ferrite-to-austenite transformation in lean C–Mn steels. The transformation kinetics is analyzed by comparing the results of two complementary sharp interface models – one is based on the assumption of local equilibrium at the migrating interface – in the other model diffusion in the interface and the interfacial reaction is implemented by an effective interface mobility but substitutional diffusion in the bulk phases is neglected.

Values for effective interface mobilities have been obtained for both the austenite-to-ferrite transformation and vice versa. By means of effective mobilities which depend only on initial composition and temperature, the transformation kinetics has been studied for other heat treatments than used to determine the effective interfacial mobility values. Although substitutional diffusion in the bulk is not taken into account, for the low Mn alloys it is possible to obtain similar trends by the effective mobility model as provided by the local equilibrium model. At modest to high interface velocities long range diffusion of the substitutional alloying elements can be ignored but then the effects of local diffusion processes near the interface need to be taken into account via an effective interface mobility. The effective mobility for the austenite-to-ferrite transformation differs from the effective mobility during the ferrite-to-austenite transformation in a rather essential manner.

1. Introduction

The properties of an alloy usually depend on its microstructure, which may result from the kinetics of diffusive phase transformations. According to Hillert [1] two extreme cases of the growth kinetics are to be distinguished, the transformation rate might be controlled by diffusion of the components in the bulk material of the phases or the interfacial reaction is the rate controlling process of the transformation. In the first extreme case local equilibrium can be assumed at the migrating interface. For simple lean alloys and non-extreme heating or cooling rates the local equilibrium condition at the migrating interface holds, and thus model predictions and experimental investigations have been found to be in good agreement, see e.g. Schneider and Inden [2]. The kinetics of the austenite-to-ferrite transformation in a binary Fe–C alloy may serve as another example. Béché et al. [3] showed that the growth of a planar ferrite front obtained from a decarburization experiment almost perfectly agrees with the results of a local equilibrium sharp interface model. However, by means of systematic decarburization experiments in ternary Fe–C–X alloys [3–6] (X being a substitutional component like Cr, Mn, and Ni) it has been demonstrated that component X influences the transformation kinetics in such a way that a simple sharp interface-local equilibrium model may fail to describe the transformation kinetics in a quantitative manner. It is assumed that diffusion processes of the substitutional alloying component in the migrating interface decelerate the kinetics [3]. In this context the reader is also referred to two review articles by Aaronson et al. [7,8] where numerous experimental data describing the influence of substitutional alloying component X on the nucleation and growth kinetics of proeutectoid ferrite are presented and the underlying mechanisms are studied and distinguished. The long-lasting and continuing efforts of the ALEMI (alloying elements effects on migrating interfaces) – community to better understand the effect of solute components on migrating interfaces are to be mentioned in this context and are documented in [9].

Deviation from local equilibrium at the migrating interface can be interpreted as a consequence of a slow interfacial reaction compared to bulk diffusion processes. During interfacial reaction or migration atoms have to dissolve and rearrange themselves in the new crystal lattice. Provided that certain conditions are fulfilled

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solute atoms are attracted to the migrating interface and retard the transformation kinetics by the so called solute drag process. This phenomenon cannot be measured directly and thus experimental results evaluated by a theoretical study comprising the underlying processes can help to understand solute drag. The influence of impurity segregation and drag on migrating grain boundaries has been investigated by Lücke and Detert [10], Cahn [11] and Lücke and Stüwe [12] in seminal theoretical studies. It has been tried to explain the experimental results, e.g. of Lücke et al. [13], Bolling and Winegard [14] and Rutter and Aust [15]. Purdy and Bréchet [16] further developed the theory to study the solute drag phenomenon during the proeutectoid transformation in Fe–C–X alloys and Enomoto [17] applied this theory to study solute drag during ferrite growth in Fe–C–Mn alloys. Hillert pointed out in a review article [18] that "it is not a trivial question how the definition of solute drag, as the net force of attraction between solute atoms and interface, can be generalized to the interface in a phase transformation". Hillert [19] introduced another modeling approach based on balancing the driving forces at a sharp interface. This approach has been further expanded by Hillert and Sundman [20]. The theory has been extended and it is now possible to describe the migration of an interfacial region of a certain width, see the papers of Odqvist et al. [21] and Svoboda et al. [22–24]. Recently, diffusion processes in the interface have also been investigated by a so called discrete jump model for substitutional diffusion and were compared to the results of decarburization experiments (see Qiu et al. [25]). A comparison between the sharp and the thick interface approach can be found in [26]. It turns out that the thick interface model can be replaced by a much simpler and more versatile sharp interface-finite mobility (SI-FM) model for describing the kinetics of the austenite-to-ferrite phase transformation in steels. Previously, the kinetics of the austenite-to-ferrite transformation in low alloyed steels has been simulated by means of different SI-FM or mixed-mode models [27–33]. Whereas it was only possible to simulate the kinetics in the binary Fe–C system based on the earlier models [27,28], the influence of substitutional alloying components on the kinetics can be considered by more recently developed models [29,30]. A further type of mixed mode models has been developed, where a mixed-mode variable S has been introduced [31,32], which helps to reduce the computational costs of the calculations and to open up the route of accurate transformation description in multi-level multi-scale models describing microstructure development for non-homogeneous starting conditions. The growth of ferrite spheres in a three-dimensional microstructure has been simulated [33].

There is no doubt that solute drag plays a rate-controlling role during the austenite-to-ferrite transformation in low alloyed steels. That is why the finite interface mobility of a sharp interface is often one or more orders below the estimated intrinsic mobility [34] for these transformation processes and represents thus an effective mobility. In addition it has been found out that the kinetics of diffusive phase transformations is controlled by the interfacial reaction in the initial stages of transformation and becomes more and more bulk diffusion controlled before equilibration, see the papers [31,35,37,38].

An important experimental complication in the determination of the transformation rate (and from this the speed of motion of the actual austenite–ferrite interfaces) from bulk transformation experiments such as conducted in a dilatometer or differential scanning calorimetry is the simultaneous occurrence of nucleation and growth. To overcome this problem recently the concept of cyclic partial transformation has been introduced [38]. In such an experiment the temperature is cycled in various modes between an upper and lower temperature both located in the two phase regime. This mode of operation results in the absence of the complicating factors related to nucleation as the number of moving interfaces in the sample remains more or less constant [42]. The absence of nucleation also has as a results that the geometry of the transformation model can be simplified and a simple 1-D model is sufficient. Notwithstanding the absence of nucleation effects the features of such cyclic partial austenite–ferrite transformation are rather complex and far from linear against changes of temperature. Chen et al. [39–42] have shown for various Fe–C–Mn–X alloys that the rather complicated features of the transformation kinetics during such cyclic partial transformation experiments can all be described very accurately by means of a LE/LENP (local equilibrium/local equilibrium no partitioning) – model. Furthermore, the cyclic partial transformation concept was shown to be able to discriminate the predictive power of the various phase transformation models for binary and lean (total mass fraction of alloying components typically below 5%) ternary and even quaternary alloys far better than the conventional experiments imposing isothermal or isochronal transformation conditions. Hence, cyclic partial transformation data seem rather appropriate to be used to determine the effective interface mobility of the austenite–ferrite and the ferrite–austenite transformation.

While there is now quite some experimental data available to determine the effective mobility directly from the experimental data, we have chosen to use as the reference data for the determination of the effective mobility values the results of the LE/LENP model calculations as such a model-to-model comparison allows imposing exactly the same (1-D) model conditions, alloy compositions and imposed thermal conditions (heating and cooling rates and lower and higher transformation temperatures within the two phase region). Hence, the model-to-model comparison approach followed in this work makes it easier to properly address the implications of the underlying physics behind the effective mobility. For the alloy compositions and thermal conditions explored in this study, the LE/LENP model describes the experimental (quantitative dilatometry) data very accurately, more or less within the level of experimental uncertainty.

2. Theory

A diffusional phase transformation with n components in each phase is a problem that comprises $(2n-1)$ independent variables at the interface, $(n-1)$ independent mole fractions in the parent phase at the interface $(n-1)$, independent mole fractions in the product phase at the interface and the interface velocity. Two different concepts can be followed to formulate the according $(2n-1)$ equations assuming either equilibrium or off-equilibrium conditions at the migrating interface. Based on these complementary concepts two models are used to investigate the cyclic phase transformation of the austenite-to-ferrite and ferrite-to-austenite transformation in the Fe–C–Mn system.

2.1. Model 1 (sharp interface with LE/LENP contact conditions)

The software DICTRA [43] contains model 1 and has been used for the according calculations. The theoretical background of model 1 is formulated in the papers [43–48]. The phases are separated by a sharp interface and local equilibrium with respect to all components is assumed to prevail at the interface in model 1. Thus, the jump of the chemical potentials of each component i at the interface is zero, yielding n equations:

$$[\![\mu_i]\!] = 0, \quad i = 1, \ldots, n \tag{1}$$

According to Eq. (1) the driving force Δf acting at the migrating interface must be zero. As the interface is assumed to migrate with a finite velocity, the interface mobility M has to be infinite.