LOW–CARBON STEELS: THE CALCULATION OF MIXED–MICROSTRUCTURES & THEIR MECHANICAL PROPERTIES

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Synopsis: Low carbon steels present special difficulties in the modelling of microstructure and mechanical properties. These are discussed briefly in the context of complicated microstructures which consist of mixtures of many phases.

Key words: phase transformations, kinetics, mechanisms, low–carbon steels, mixed microstructures, mechanical properties.

1. Introduction

Steels are being designed with ever decreasing interstitial contents. At the same time, processing technology allows accelerated cooling without excessive distortion or microstructural gradients [1–5]. Lean steels with lower 'carbon equivalents' can therefore be manufactured, making fabrication relatively easy. Alloys such as these give uniform microstructures in spite of solidfication–induced chemical segregation. Segregated microstructures are more susceptible to stress–corrosion and hydrogen–induced cracking. This paper has a discussion of some difficulties in dealing with transformations in low–carbon steels, and of aspects of the mechanical properties of mixed microstructures.

2. Sensitivity to Carbon

The solubility of carbon in ferrite is small and changes sharply with temperature and alloy composition (Fig. 1a, [6]). This has a major influence on austenite formation in almost pure iron (Fig. 1b, [7]). The effect illustrated is mostly thermodynamic in origin; kinetic factors are less important because both the diffusion coefficient and the driving force increase with temperature during austenite formation. Hence, the slope of the A_s line, and the interval $A_f - A_s$ can be explained by that of the Ae_1 line. The sensitivity of ferrite growth to carbon in dilute steels is discussed next.

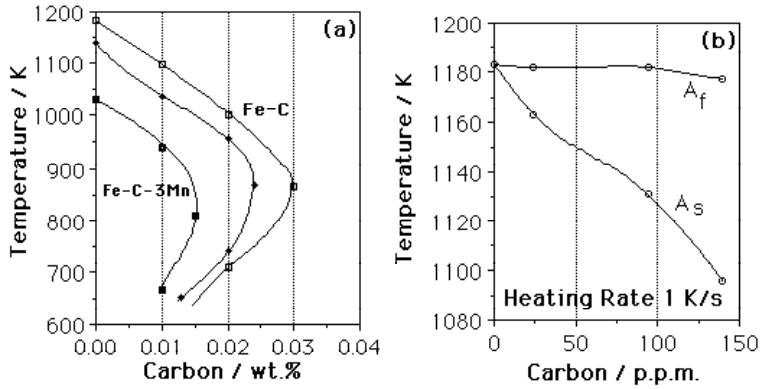

Fig. 1: (a) The $\alpha/(\alpha+\gamma)$ paraequilibrium (Ae_1') phase boundary for Fe–C, Fe–C–1Mn and Fe–C–3Mn wt.% steels [6]. (b) Austenite–start (A_s) and austenite–finish (A_f) temperatures for Fe–C low–carbon steels [7].

3. Ferrite Growth at Low Carbon Concentrations

With few exceptions [8], the growth of ferrite is treated using the theory of diffusion–controlled growth [9]. Diffusion–control is when the available free energy is dissipated mainly in the diffusion of solute ahead of the moving interface. Thus, the phases at the interface are approximately in local equilibrium [9] with their compositions at the interface fixed by tie–lines

of the phase diagram. The calculation of the growth rate then becomes simple since all the other processes that have to occur in order for ferrite to grow (such as the transfer of atoms across the boundary) can be 'neglected'. The growth rate is some function of the normalised supersaturation:

$$\Omega = (x^{\gamma\alpha} - \overline{x})/(x^{\gamma\alpha} - x^{\alpha\gamma})$$

where $x^{\gamma\alpha}$ and $x^{\alpha\gamma}$ are the equilibrium concentrations in austenite and ferrite respectively. The average concentration is designated $\overline{x}$. Ω is the term which appears in all kinetic equations for diffusion–controlled growth. As the carbon concentration $\overline{x}$ is reduced towards the solubility $x^{\alpha\gamma}$, $\Omega \to 1$ and the diffusion equations tend to predict infinite growth rates since there is no solute partitioned between the parent and product phases (Fig. 2a).

This is not realistic because transformation occurs in a series of steps of which solute diffusion is but one component; interface processes may become rate limiting (Fig. 2b). In any case, the assumption of diffusion–controlled growth, that local equilibrium exists at the transformation interface, must break down when the diffusion velocity (D/λ, where D is the solute diffusivity and λ is the smallest jump distance) becomes less than the interfacial velocity. The solute is then forced to enter the growing phase even though its free energy increases – this is called *solute trapping* (Fig. 2b).

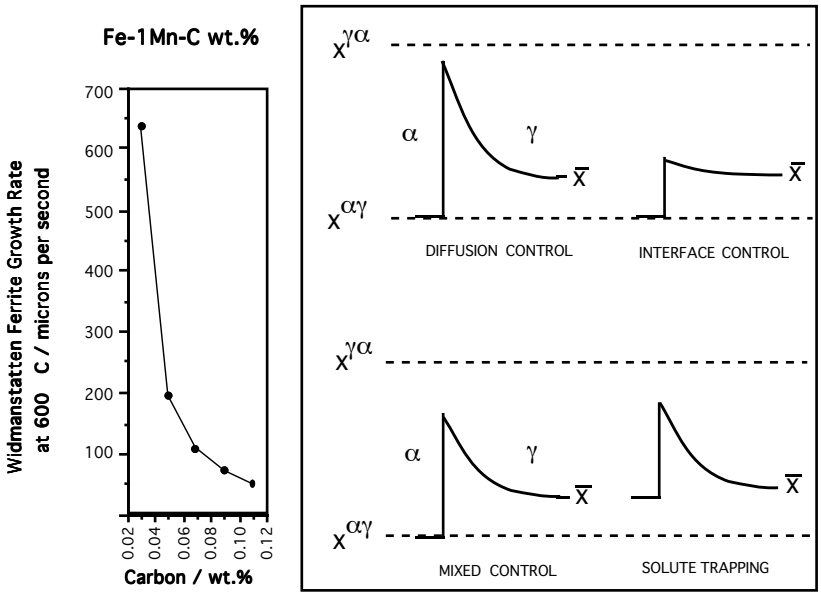

Fig. 2: (a) Rapidly increasing diffusion–controlled growth rate of Widmanstätten ferrite as the carbon concentration is reduced. (b) The concentration profiles at the α/γ interface for different kinetic control phenomena.

The point where interface processes become rate limiting must depend on the transformation mechanism (Fig. 3a). For Widmanstätten ferrite, which grows by a paraequilibrium displacive mechanism, all measured data can be predicted assuming carbon diffusion–controlled growth, because the interface associated with displacive transformations is glissile. This is not the case for reconstructive transformations (where all atoms diffuse). There are examples where the local equilibrium assumption gives growth rates which are incorrect by many orders of magnitude at low temperatures [10].

Solute trapping becomes important in the formation of the so–called massive ferrite in the two–phase $\alpha + \gamma$ field below the T_0 temperature [10]. The transformation is reconstructive in nature but the ferrite grows at a rate which does not allow the redistribution of solute. This is not to be confused with NPLE (negligible partitioning local equilibrium [9]) in which equilibrium exists at the interface.

4. Mechanisms and Nomenclature

A catalogue of names helps to communicate the form of a microstructure. An understanding of the mechanism of transformation can, however, be more revealing and useful in the calculation of microstructure. A mechanism consists of detailed information about interface structure, the state of equilibrium, the strain energy, the shape *etc.* The scheme illustrated in Fig. 3a categorizes all the ferritic transformation products via mechanism [10], and is used in the modelling of steels [11–14].

5. Mixed Microstructures: Impingement

An interesting problem in the calculation of mixed microstructures is the treatment of impingement between transformation products whose mechanisms of formation are different. One example of importance in industry is illustrated in Fig. 3b.

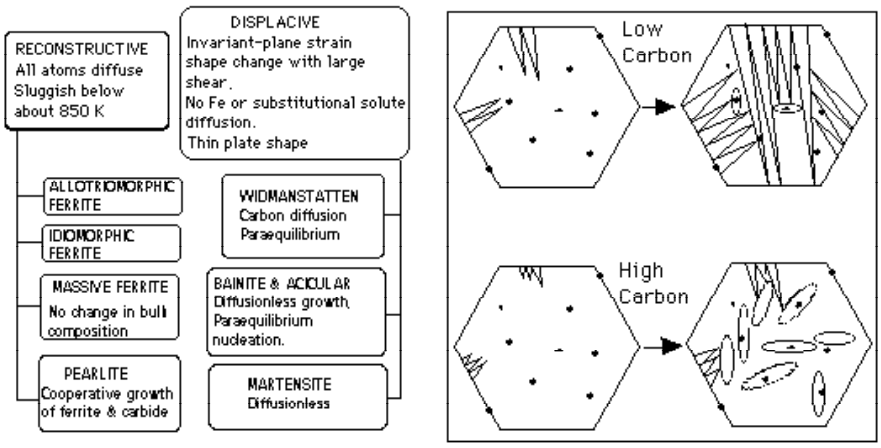

Fig. 3: (a) Classification of transformation mechanisms. (b) Hard impingement between γ grain surface nucleated Widmanstätten ferrite and acicular ferrite which is intragranularly nucleated on non–metallic inclusions.

Widmanstätten ferrite which occurs as packets of plates in identical crystallographic orientation is a highly organised microstructures (Fig. 3b). It can be harmful to mechanical properties because cleavage cracks, or deformation processes, can extend readily across the packets. The individual plates within these packets then have a minimal effect on the mechanical properties. Acicular ferrite on the other hand, is a more chaotic microstructure. Plates of acicular ferrite nucleate heterogeneously on small non–metallic inclusions and radiate in many different directions from these 'point' sites. Propagating cracks are therefore frequently deflected as they cross an acicular ferrite microstructure with its many different orientations, giving superior mechanical properties.

Acicular ferrite is intragranularly nucleated bainite; it therefore forms at a lower temperature when compared with Widmanstätten ferrite. During continuous cooling transformations, excessive preemptive formation of Widmanstätten ferrite prevents the formation of acicular ferrite as illustrated in Fig. 3b. In particular, the growth rate of Widmanstätten ferrite increases drastically as the carbon concentration is reduced (Fig. 2a). At low carbon concentrations, Widmanstätten ferrite plates can grow across austenite grains in a fraction of a second, and stifle the subsequent formation of acicular ferrite. This problem has been modelled quantitatively and the methodology developed is used extensively in alloy design [14].

6. Microalloying of Low Carbon Steels

A reduction in the carbon concentration can lead to an increase in the strength of microalloyed steels [15]. Small concentrations of titanium in HSLA steels can lead to quite large increases in their strength, if enough titanium can be retained in solid solution to temperatures where ferrite formation occurs (Fig. 4). The titanium can then precipitate on a fine scale via an interphase precipitation mechanism. A high carbon concentration prevents this by precipitating most of the Ti in the austenite prior to ferrite formation.

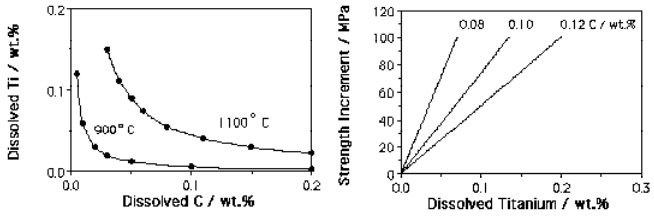

Fig. 4: (a) Soluble Ti as a function of C. (b) Increase in strength due to interphase precipitation of TiC.

7. Mechanical Properties

The properties of mixed microstructures do not scale with the fractions of the variety of phases. Recent data [16] show that the strength of a mixture of tempered bainite and martensite can peak at an intermediate fraction of martensite (Fig. 5a). This can be modelled quantitatively [17]; the peak is due to two factors. When the bainite forms it enriches the residual austenite with carbon, so that the strength of the subsequent martensite increases. A second significant contribution is that the bainite is plastically constrained in its deformation by the surrounding stronger martensite. Fig. 5b shows how the ratio

of the strength of bainite in a mixed microstructure (σ_b) to that of pure bainite (σ_{b0}) varies with the fraction of bainite, due to a constraint effect alone.

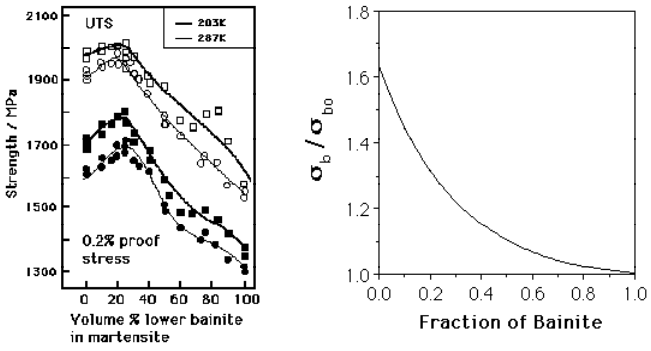

Fig. 5: (a) Peak in strength as a function of fraction of bainite in a mixed microstructure of bainite + martensite [16] (b) How the yield strength of bainite increases as it is constrained by hard martensite [17].

8. Low C steels - Grain boundary embrittlement

In the absence of carbon, iron fails by intergranular decohesion at very low temperatures [18], although the actual temperature below which there is a transition to intergranular fracture is sensitive to the impurity content and to the character of grain boundaries†. Indeed, it has been suggested [19] that body–centered cubic metals in general need carbon to maintain their integrity at high stresses; nitrogen is believed to have a similar effect [20]. Of course, low–carbon steels tend to have a low yield strength so the problem of interfacial decohesion may not be revealed in ordinary applications. However, interstitial–free steels can embrittle after cold work, the fracture initiating in an intergranular manner but propagating by cleavage.

Maehara *et al.* [21] have shown that the critical temperature below which the steel embrittles is raised by phosphorus and reduced by boron. This is consistent with the known influence of phosphorus on the mechanical properties of steels, but the effect is exaggerated in interstitial–free steels by the fact that the phosphorus can segregate without interference (site competition) from carbon which also prefers grain boundary sites. The beneficial effects of boron in interstitial–free steels containing traces of phosphorus are also attributed to site competition effects.

9. References

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† Grain boundaries parallel to $\{1\ 0\ 0\}_\alpha$ and $\{1\ 1\ 0\}_\alpha$ are more sensitive to intergranular fracture, particularly when the stress axis is normal to the boundary plane [18]. Many low carbon steels are used in applications where formability is important. Formability is frequently achieved by controlling the crystallographic texture. It would be interesting to discover whether the textures achieved are such that the tendency to intergranular fracture is reduced

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