EFFECT OF MICROSTRUCTURE AND TRAP TYPOLOGY ON HYDROGEN REDISTRIBUTION IN STEEL

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Abstract:

Hydrogen trapping plays an important role in the embrittlement of some high performance alloys. A correct understanding of hydrogen redistribution from the onset of the manufacturing process would allow the prediction and prevention of severe material degradation.

Hydrogen presents high solubility at high temperatures in many alloys, but not so at room temperature. As the solubility of hydrogen drops with lowering temperature or microstructure change, excess hydrogen becomes stored in various microstructural features (traps) including dislocations, grain boundaries or precipitate interfaces.

Traps are often categorised in two wide groups: shallow or reversible traps and deep or irreversible ones. A physically more accurate model describes each trap as potential energy pits and considers the characteristic energy barrier to release an hydrogen atom from it. Using that description, a physical model accounting for the redistribution of interstitial atoms in ferrous alloys has been implemented.

The model permits the study of the effect of different microstructure characteristics on the trapping, detrapping and general redistribution of hydrogen, taking into account the thermal cycle and the separate contribution of deformation level, dislocation distribution, grain size, carbide presence and distribution, *et c.* and their interaction.

To illustrate the predictions of the model, a comparison between two idealised low alloy steels is finally presented. Both alloys are rapidly cooled and in each austenite transforms into a different microstructure. Steel A transforms at high temperature to become large grained, undeformed allotriomorphic ferrite while Steel B transforms at lower temperature becoming a stressed mixture of bainite and martensite..

Keywords:

Hydrogen, trapping, steel, microstructure, physical model.

1 Introduction

The risk of severe degradation caused by hydrogen on some high strength alloys has long been acknowledged [1-2], and due to their technological and economic relevance, it is a phenomenon that has attracted intense research for decades [1-6] although it has not been physically modelled until recently [7-10].

However, as important as understanding the flux of hydrogen atoms within the metal matrix, is understanding the influence of microstructure and the distribution and physical characteristics of different types of traps in such flux and redistribution [11-14]. In the same way that the early stages of this work did permit to propose method to reduce hydrogen content in ferrous alloys [15], the work presented here contributes toward the acquisition of a better understanding of the interaction between trap type and trap

distribution, alloy microstructure and temperature history on the hydrogen redistribution, and therefore, on its effects on the physical properties of the alloy.

2 Description of the Model

2.1 Intersticial diffusion model

A physical model describing the diffusion of interstitial atoms has been constructed and applied to the redistribution of hydrogen [16]. This model incorporates previously developed work of temperature evolution and phase transformations in steel so that is able to contemplate the thermal and microstructure evolution during a simple heat treatment [17-18].

The evolution of hydrogen distribution is determined as a function of thermal agitation and atom mobility by relating it to a random walk process, taking into account diffusivity and saturation of hydrogen through each of the different metallic phases, as extensively described elsewhere [7, 9-10, 16, 19].

2.2 Microstructure and traps

The enhanced model presented here incorporates the effect of various trap types to the redistribution of hydrogen. Hydrogen contained in the metal either stays in solution up to the matrix phase's solubility limit or is expelled from the matrix and becomes *trapped* into various types of lattice defects available.

The nature of trapping sites range from the distortion field surrounding a dislocation to the surfaces of certain precipitates and microcracks in the material, but they can all be modelled as a potential well. In many respects, this description makes an analogy between the energy barrier for the release of an atom from a lattice site at each difusion jump and the release from a trap site. This process is suitably described by a characteristic activation energy, as shown in Figure 1.
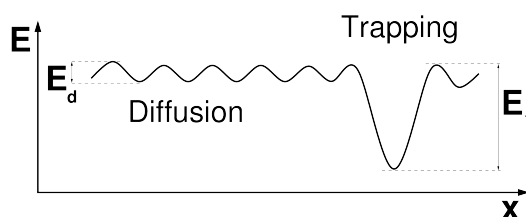

Figure 1: Diagram comparing the lattice position energy well (diffusion) and a generic trap site energy well.

Each trap type is then characterised by a speciffic activation energy, E_t, necessary for the release of an hydrogen atom contained in it [4, 20]. The types of trapping sites considered in this work, and their characteristic energies are listed in Table 1.

Trap site type	E [kJ·mol^{-1}]
Dislocation distortion	20.6
Grain boundary	58.6
Precipitate surface	84.0
(Diffusion in ferrite)	*13.4*

Table 1: Characteristic release energy for each trap site type considered in this work, as well as lattice diffusion activation energy for comparison [4, 7].

3 Results and discussion

3.1 Modelling conditions

The model described in Section 2 has been used to calculate the evolution of the hydrogen distribution during the cooling process of two different low alloy steels.

The process studied consists in continuous cooling of an alloy piece of 25 cm in thickness, from 1600ºC to approximately 200ºC. Heat extraction by radiation and intense convection. The convection severity has been set as and kept constant during the whole process. With these conditions, the alloy cools from 1600ºC to roughly 200ºC in aproximately 45 minutes (2740 s).

The material modelled consists of two idealised low alloy steels with slightly different composition so that their microstructure evolves differently when cooled to room temperature. Austenite in Steel A transforms at higher temperature (725°C) to become allotriomorphic ferrite presenting large grain and a very low deformation and stress profile [17-18, 21]. In the case of Steel B austenite starts to transforms at a lower temperature (450°C) ending up forming bainitic ferrite and martensite [17-18]. The structure of Steel B has characteristically smaller grain structure and a high dislocation density due to the transformation residual stresses [21]. The detailed microstructure parameters for Steels A and B are summarised in Table 2.

	Steel A	Steel B
Transf. temp:	725°C	450°C
Austenite Transforms to:	Allotriomorphic Ferrite	Bainite & Martensite
Grain size:	Large 0.1 mm	Small 10μm
Dislocation density:	Low 10^{10} m/m^3	High 10^{15} m/m^3
Ppt. trap site density:	$5 \cdot 10^{20}$ site/m^3	$5 \cdot 10^{24}$ site/m^3

Table 2: Austenite transformation temperature and microstructure for Steel A and Steel B [18, 21].

The different evolution of hydrogen distribution as function of microstructure is described in the Section 2.1. Additionally, it has been considered to be of interest to add a consideration on the effect of carbides as well. In a structure like the one of Steel A cementite distribution would take the form of either lamellar pearlite bi-crystals or spheroidised perlite. In an alloy like Steel B however, the carbide volume fraction would form a much finer distribution. For this to be taken into account, a different carbide distribution has been considered in each case and the results obtained are discussed in Section 3.3.

3.2 Effect of microstructure

According to the calculations, the overall redistribution of hydrogen is influenced by the microstructure evolution during cooling. As hydrogen diffuses in the metal and solubility in the matrix lowers, some hydrogen content seeks containment in lattice defects like dislocation distortion sites and grain boundaries.

The characteristics of Steel A and Steel B have been chosen so that the difference in their microstructures is large and therefore the effect on hydrogen redistribution clearly noticeable. As shown in Figure 2, as temperature in the metal drops, there is partitioning from the matrix towards dislocations and grain boundary trap sites. In both cases, the influence of grain boundary sites is of a small relevance compared to that of dislocation sites.

Additionally, at the end of the treatment, virtually all the hydrogen content in Steel B becomes stored at microstructure defects, while Steel A still retains some hydrogen in the matrix. The final hydrogen content for each site type and steel is detailed in Table 3.

3.3 Effect of carbides

When a distribution of precipitate (*i.e.* cementite) related trap sites is considered, an extra effect is described in the results of the model. For the sake physical plausibility the distribution of trapping sites related to carbide surface has been described in very different terms. In short, in an alloy like Steel B, with a final microstructure described as a mixture of bainitic ferrite and martensite the carbide distribution would be expected to be very finely distributed when compared with the one in an aloy like Steel A that has transformed at higher temperature to mixture of allotriomorphic ferrite and coarse cementite. This difference is reflected in the different precipitate trap site distribution used as input paramenters in the model, shown in Table 2.
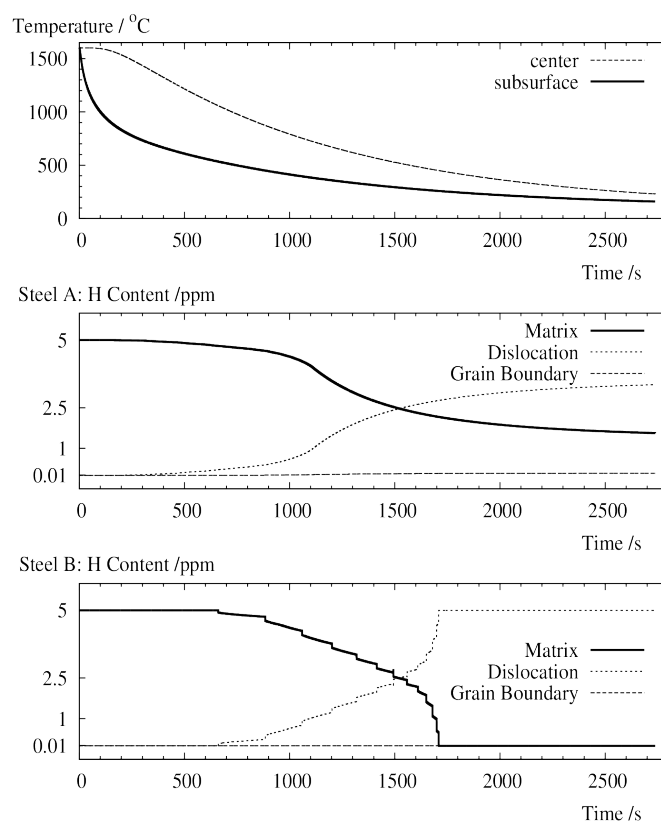
Figure 2: Temperature evolution and hydrogen redistribution into different trap sites for Steel A and Steel B.

	Steel A	Steel B
H content	5.0 ppm	5.0 ppm
No Ppt.		
Matrix	1.564	$5 \cdot 10^{-6}$
Dislocation	3.352	4.998
Grain boundary	0.084	$1.250 \cdot 10^{-3}$
With Ppt.		
Matrix	0.427	$5 \cdot 10^{-6}$
Dislocation	2.010	4.998
Grain boundary	0.050	$1.250 \cdot 10^{-3}$
Ppt. surf.	2.513	$6 \cdot 10^{-6}$

Table 3: Final hydrogen distribution (/ppm) for Steel A and Steel B considering a microstructure without and with, a precipitate distribution.

Nevertheless, as the predictions of the model show (Table 3) the influence of the distribution of carbide surface trapping sites is very different in Steel A and Steel B. In the case of Steel A, the inclusion of precipitate trap sites induces the redistribution of hydrogen among all 3 possible trapping sites, reducing the content in the matrix. In the case of Steel B however, the inclusion or not of precipitate trapping sites does not affect the final distribution of hydrogen, even though the number of potential trap sites is four orders of magnitude higher with respect to Steel A.

4 Conclusion

A model describing the hydrogen diffusion in ferrous alloys and its redistribution into various types of lattice defects or traps has been presented. The model provides a description of the effect of microstructural details in hydrogen behaviour.

When trapping in precipitates is disregarded, and for both steels investigated, the influence of grain boundary sites is of small relevance compared to that of dislocation sites. On the other hand, at the end of the treatment, virtually all the hydrogen content in bainitic Steel B becomes stored at microstructure defects, while allotriomorfic ferrite Steel A still retains some hydrogen in the matrix.

When the carbide distribution is accounted for, its influence is very different in Steel A and Steel B. For Steel A, the inclusion of precipitate trap sites induces the redistribution of hydrogen among all 3 possible trapping sites, reducing the content in the matrix. For Steel B however, the inclusion or not of precipitate trapping sites does not affect the final distribution of hydrogen, even though the number of potential trap sites is four orders of magnitude higher with respect to Steel A.

This description could help improve our understanding of such phenomena and to reduce the incidence of hydrogen embrittlement in the future.

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