

# Determining hydrogen saturation degree at trap sites and evaluation of a novel hydrogen removal treatment

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## Abstract

A physical model, where diffusion is driven by the reduction of the Gibbs energy of the system and describing traps as potential energy pits with a characteristic release energy barriers has been used to describe redistribution of hydrogen in ferrous alloys.

The effect on redistribution of hydrogen between matrix phases and trap sites, accounting for thermal cycle, microstructure, grain size, dislocation and carbide distributions, *et c*, on the degree and distribution of saturation during a standard heat treatment, is determined and compared with a novel hydrogen removal treatment developed during this work, based on the application of customised temperature gradients.

**Keywords:** Hydrogen redistribution. Embrittlement. Hydrogen reduction treatment.

## Description of the model and results

A simple but physically robust model is used to describe the redistribution of hydrogen in steel[1]. As this model incorporates a description of thermal and microstructure evolution it can be applied to the study of real heat treatments[2].

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[1, 3].

The effect of various trap types to the redistribution of hydrogen is incorporated into the model by providing that hydrogen contained in the metal either stays in solution in the matrix or is expelled from the matrix and becomes *trapped* into various types of lattice defects available[4].

The nature of trapping sites vary, but they can all be modelled as a potential well[4, 5]. In many respects, this description makes the analogy between the energy barrier for the release of an atom from a lattice site at each diffusion jump and the release from a trap site.

This process is suitably described by a characteristic activation energy. Each trap type is then characterised by a specific activation energy,  $E_t$ , necessary for the release of an hydrogen atom contained in them[4, 5].

Although several embrittlement mechanisms have been characterised, often they share a local supersaturation in hydrogen as a start. By considering the fluxes between phases and trap sites and their respective partial saturation, it is possible to determine the risk of hydrogen supersaturation, and therefore, to estimate the effective risk of embrittlement as well as to devise new strategies to avoid it[3, 6].

Determining hydrogen redistribution fluxes and the final hydrogen content distribution at the different microstructure sites during a simple heat treatment (cooling from solidification) is used as an example. Being able to predict the regions or microscopy sites where supersaturation is likely to occur (with the increased risk of hydrogen embrittlement that implies), permits the prediction of embrittlement phenomena and therefore enables its prevention.

In particular, during the course of this research, a novel method to reduce hydrogen content and supersaturation peaks has been developed based on these results[6]. The difference in hydrogen loss and subsequent local supersaturation, between a standard process and one where this patented modified treatment is applied, consisting in the deliberate imposition of severe thermal gradients to the cooling solid, are evident and show how the final supersaturation in trapping sites can be effectively reduced[1, 6].

	Ave. Content /ppm	Super-Saturation
<b>Start H cont.</b>	3.0	—
<b>Standard</b>		
<b>Matrix</b>	2.75	—
<b>Dislocation</b>	$9.6 \cdot 10^{-3}$	$\approx 1.13$
<b>Grain boundary</b>	$2.5 \cdot 10^{-5}$	$\approx 11.5$
<b>Precipitate</b>	$1.4 \cdot 10^{-2}$	$\approx 136$
<b>Desorption</b>	0.22	<b>H Reduction: 7%</b>
<b>with Treatment</b>		
<b>Matrix</b>	2.36	—
<b>Dislocation</b>	$9.7 \cdot 10^{-3}$	$\approx 1.14$
<b>Grain boundary</b>	$2.3 \cdot 10^{-5}$	$\approx 11.0$
<b>Precipitate</b>	$0.9 \cdot 10^{-2}$	$\approx 88$
<b>Desorption</b>	0.62	<b>H Reduction: 21%</b>

Table 1: Final hydrogen distribution (/ppm) for standard cooling process and applying the patented hydrogen removal treatment[6].

## References

- [1] D. Gaude-Fugarolas. Understanding hydrogen redistribution during steel casting, and its effective extraction by thermally induced up-hill diffusion. *Journal of Iron and Steel Research International*, 18 suppl.1.1:159–163, 2011.
- [2] D. Gaude-Fugarolas. *Modelling Induction Hardening*. VDM Verlag Dr. Muller, Saarbrüchen, 2008. ISBN-10: 3639062965.
- [3] D. Gaude-Fugarolas. Application of a physical model on interstitial diffusion to the issue of hydrogen damage during casting and forming of ferrous alloys. In *Proceedings of METAL2011, 18-20 May, Brno, Czech Republic*. Tanger Ltd., 2011.
- [4] D. Gaude-Fugarolas. Effect of microstructure and trap typology on hydrogen redistribution in steel. In *Proceedings of METAL2013, Brno, Czech Republic, 15-17 May 2013*, 2013.
- [5] J. P. Hirth. Effects of hydrogen on the properties of iron and steel. *Metallurgical Transactions A*, 11A:861–890, 1980.
- [6] D. Gaude-Fugarolas. Method for the reduction of interstitial elements in cast alloys and system for performing said method. Patent: US 8,286,692 B2. Awarded in US and Spain. In process Europe and elsewhere.

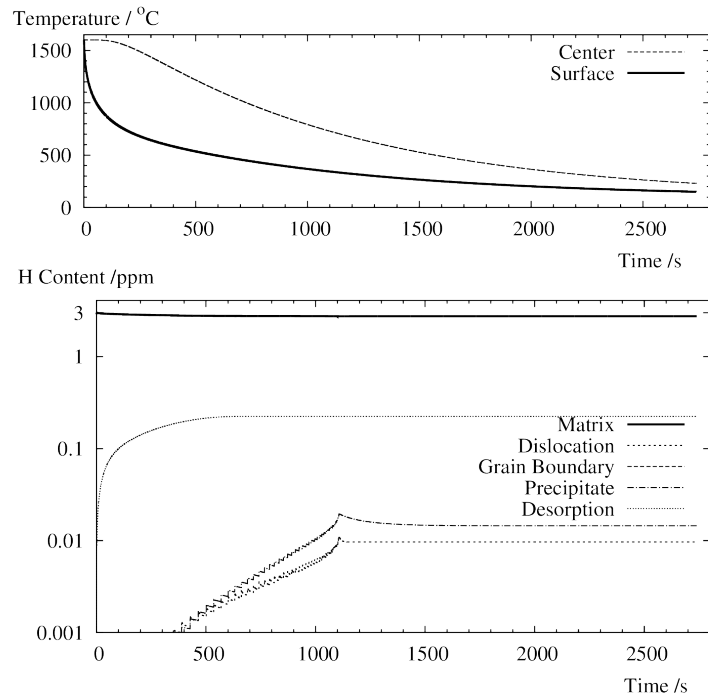


Figure 1: Temperature evolution and hydrogen redistribution into different trap sites for a standard cooling process.

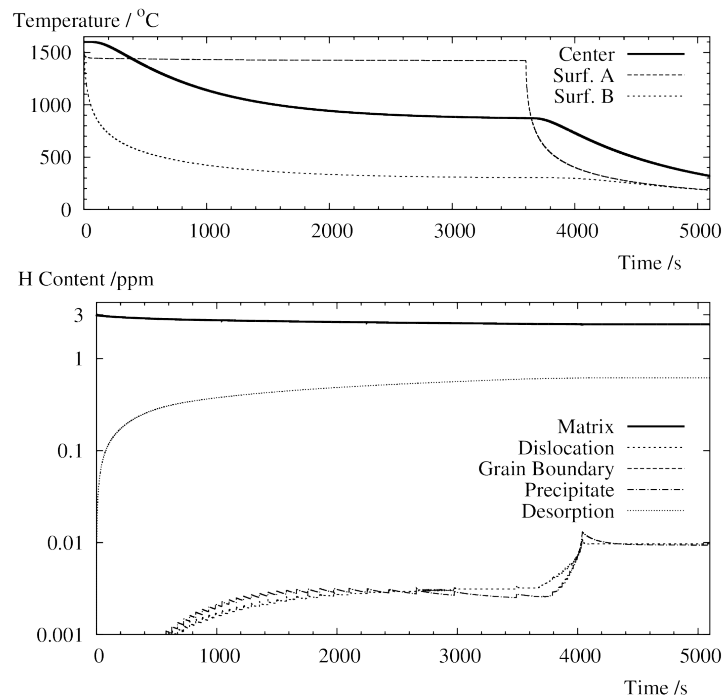


Figure 2: Temperature evolution and hydrogen redistribution into different trap sites using H extraction process[6].