

# 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. 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.

A physically accurate description models traps as potential energy pits with a characteristic energy barrier to release an hydrogen atom from it. This 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 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.

## Model:

A physical model for the redistribution of hydrogen in steel has already been presented, which incorporates a description of thermal and microstructure evolution during a simple heat treatment.

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.

The new model of hydrogen diffusion 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 vary, but they can all be modelled as a potential well. 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.

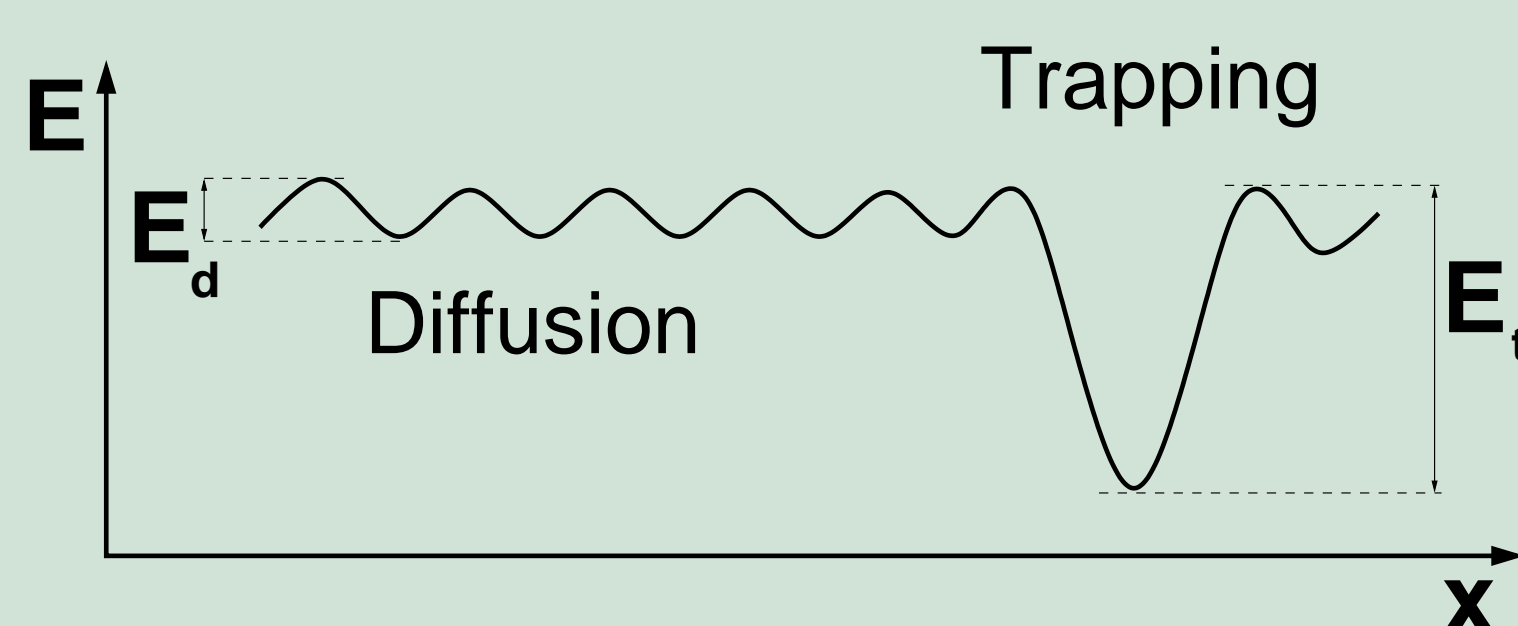


Figure: Diagram comparing the lattice position energy well (diffusion) and a generic trap site energy well.

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.

Trap type	$E_t$ [kJ · mol <sup>-1</sup> ]
Dislocation distortion	20.6
Grain boundary	58.6
Precipitate surface	84.0
Diffusion in ferrite	13.4

Table: Characteristic release energy,  $E_t$ , for each trap site type considered in this work, as well as lattice diffusion activation energy for comparison.

## Process & steel studied:

### Process:

- Continuous cooling of an alloy piece of 25 cm in thickness, from 1600°C to approximately 200°C.
  - Heat extraction by radiation and intense convection.
  - Convection severity as  $h = 2000 \text{ Wm}^{-2}\text{K}^{-1}$ .
- With these conditions, the alloy cools from 1600°C to roughly 200°C in  $\approx 45$  minutes (2740 s).

### Steel & Microstructure:

	Steel A	Steel B
At temperature:	725°C	450°C
Austenite Transforms to:	Allotriomorphic Ferrite	Bainite & Martensite
Grain size:	Large 0.1 mm	Small 10 μm
Dislocation density:	Low $10^{10} \text{ m}^{-2}$	High $10^{15} \text{ m}^{-2}$
Ppt. trap site density:	$5 \cdot 10^{20} \text{ site/m}^3$	$5 \cdot 10^{24} \text{ site/m}^3$

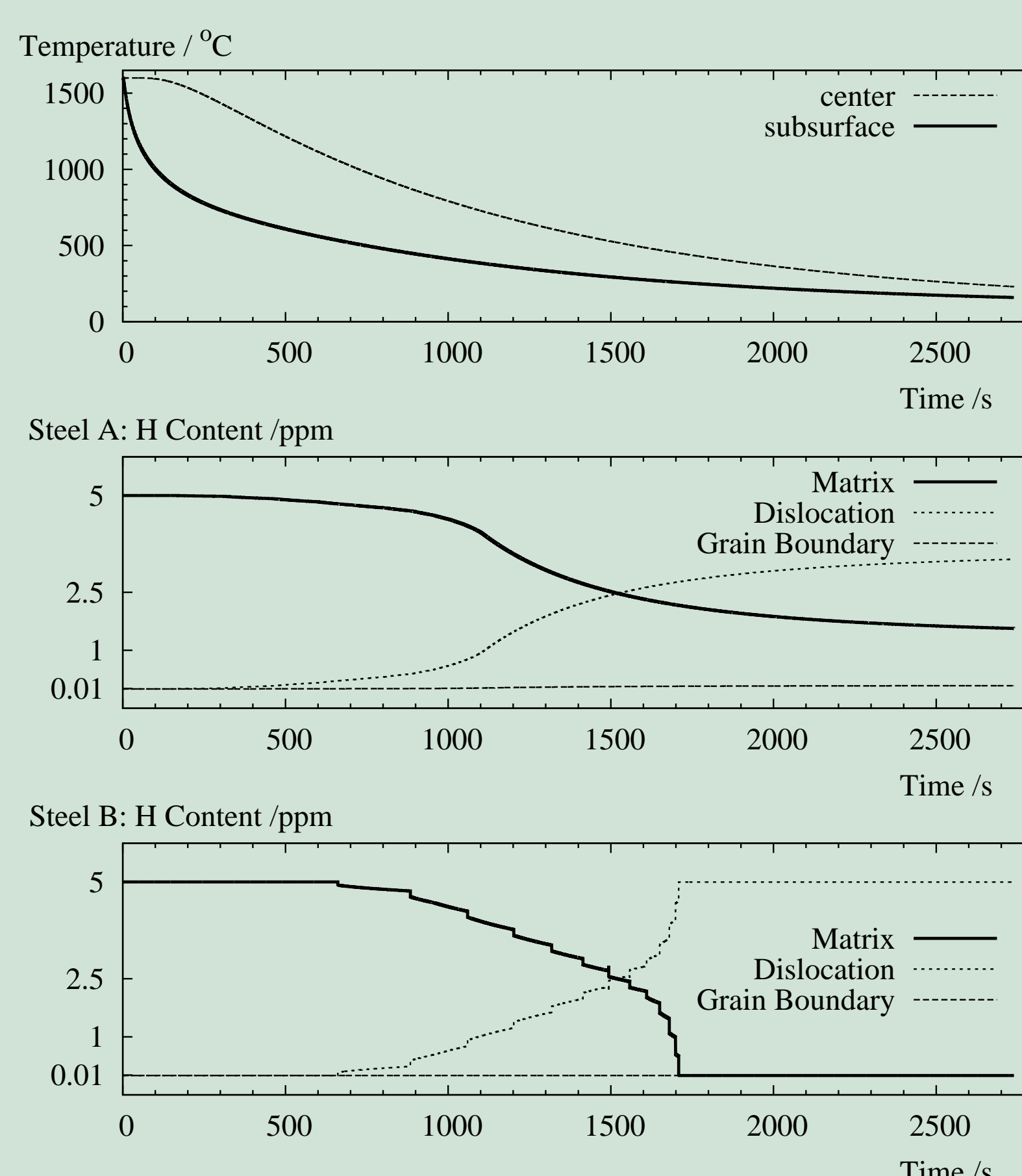
Table: Austenite transformation temperature and final microstructure obtained from the decomposition of austenite.

## Conclusions:

**Effect of Microstructure:** 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 allotriomorphic ferrite Steel A still retains some hydrogen in the matrix.

**Effect of Carbides:** 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. 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.

## Effect of Microstructure:



## Effect of carbides:

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

## To know more:

- METAL2013 Proceedings
- WebSite: <http://dgaude.sdf-eu.org>