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

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Abstract:

Determining the distribution of hydrogen among different microstructure features and trapping site types, and the degree of saturation developed at each of them is of paramount importance to understand the risks and mechanisms of hydrogen embrittlement in steel.

A physically sound model describing traps as potential energy pits and considering the characteristic energy barrier to release an hydrogen atom from them has been used to describe the redistribution of hydrogen in ferrous alloys. In the model, hydrogen diffusion is driven by a reduction of the Gibbs energy of the system, and not only occurring to reduce the concentration gradient, as is usually considered in simplified systems at constant matrix composition and temperature.

Such a model permits the study of the effect of different microstructure characteristics on the trapping, de-trapping 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 finally obtain the degree of saturation at the matrix and each trapping site type during and after a simple heat treatment.

Finally, the results obtained are compared with those resulting after the application of a novel hydrogen removal treatment developed during this work, which is based on the deliberate application of temperature gradients to the cast metal.

Description of the Model:

A simple but physically robust model is used to describe the redistribution of hydrogen in steel. As this model incorporates a description of thermal and microstructure evolution it can be used to study 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 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 up to the matrix phase's solubility limit or is expelled from the matrix and becomes *trapped* into various types of lattice defects available.

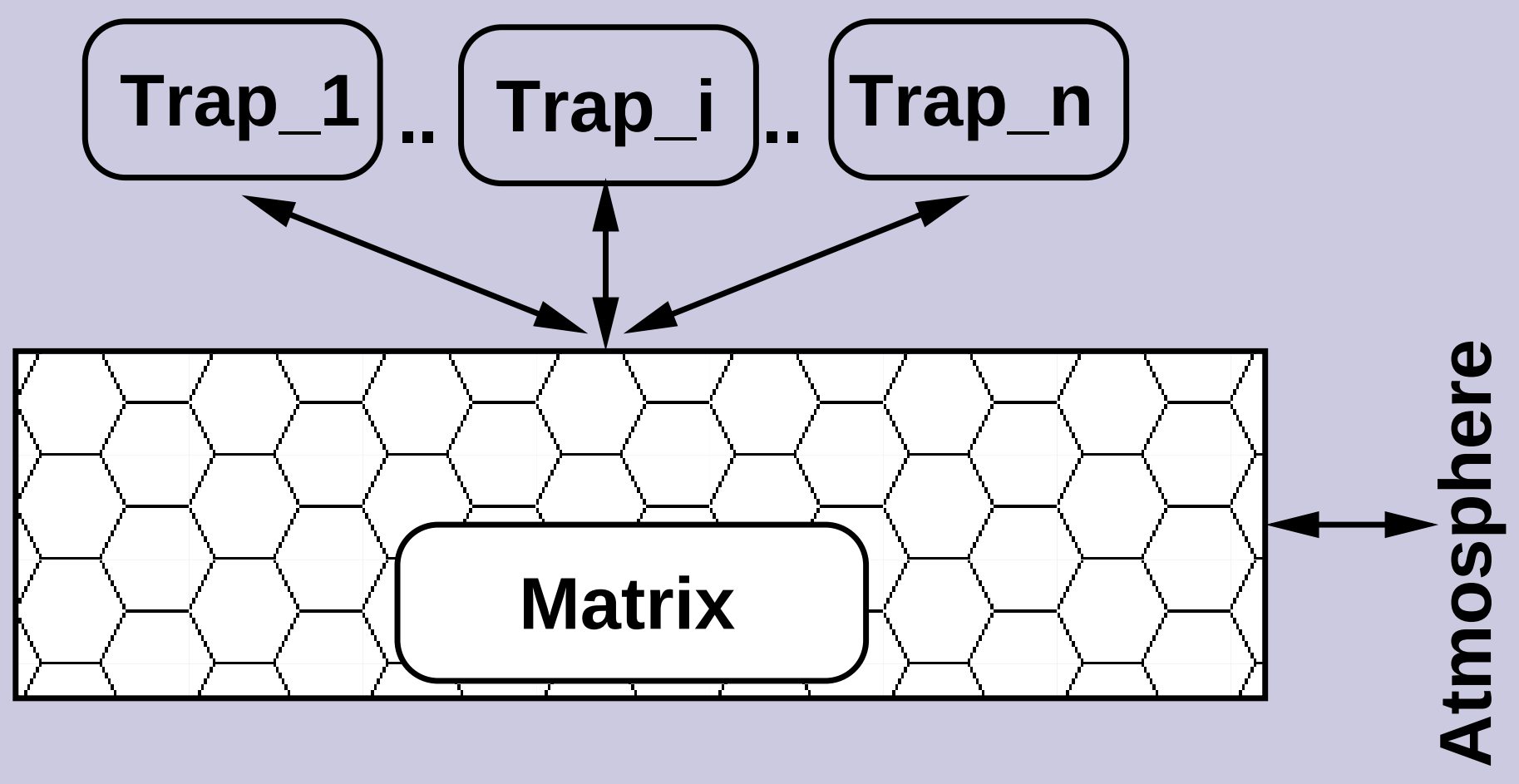


Figure: Hydrogen redistribution fluxes between the atmosphere, the matrix and ***n*** trap site types.

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 difusion jump and the release from a trap site.

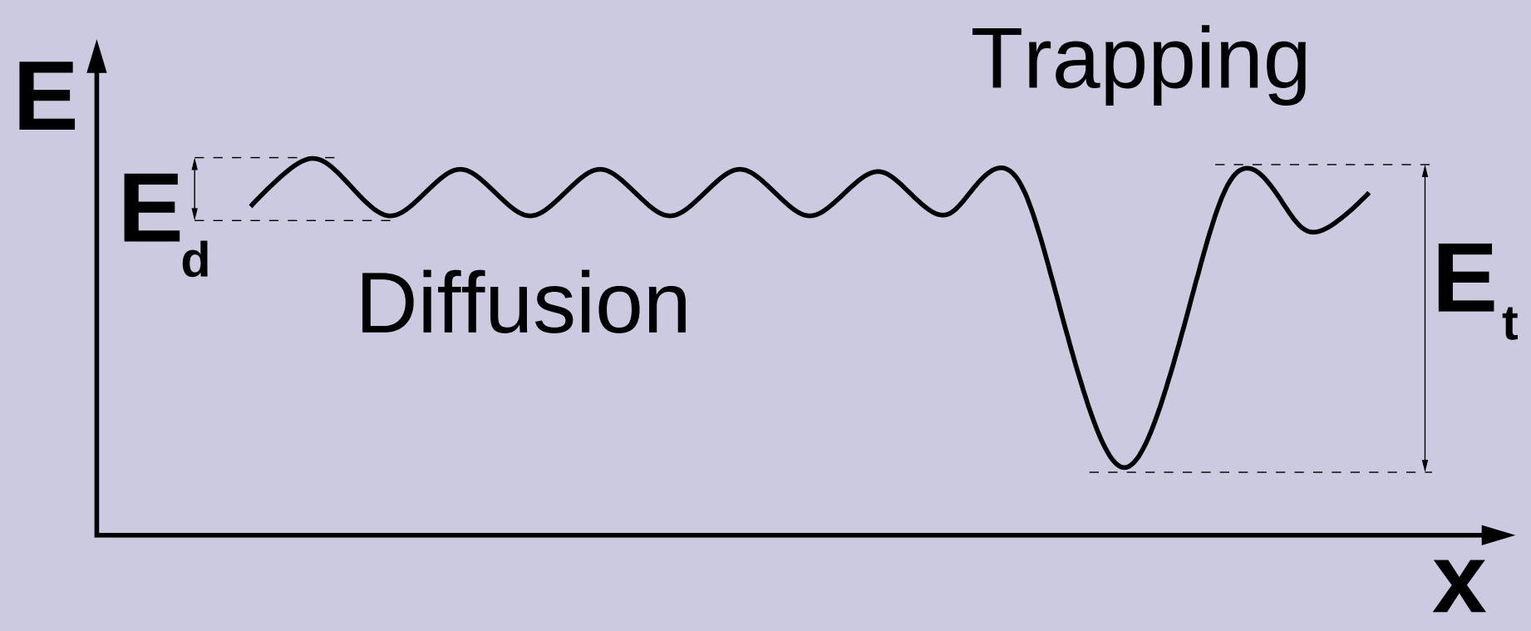


Figure: Diagram comparing the lattice position energy well (diffusion) and a generic trap site energy well.

This process is suitably described by a characteristic activation energy. Each trap type is then characterised by a speciffic activation energy, $\boldsymbol{E_t}$, necessary for the release of an hydrogen atom contained in them.

Although many different embrittlement mechanisms have been characterised, often they share a local supersaturation in hydrogen as a start. By considering the fluxes between phases and trap types and their respective saturation limits, it is possible to determine the risk of hydrogen supersaturation, and therefore, estimate an effective risk of embrittlement.

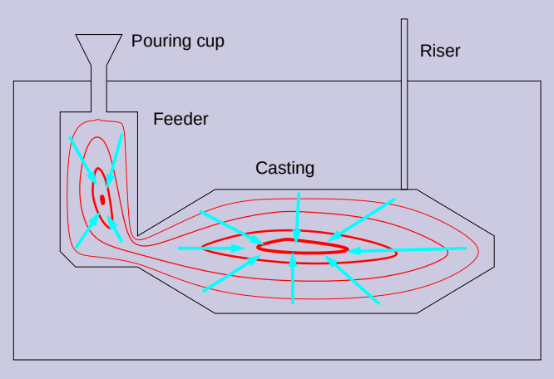
Brief Bibliography:

- HIRTH, J. P. *Effects of hydrogen on the properties of iron and steel*. Metallurgical Transactions A. 1980, 11A: 861-890
- GAUDE-FUGAROLAS, D. *Understanding hydrogen redistribution during steel casting, and its effective extraction by thermally induced up-hill diffusion*. HSLA Steels 2011 (High Strength Low Alloy Steels International Conference). (Beijing, China. 31 May-2 June 2011).
- GAUDE-FUGAROLAS, D. Journal of Iron and Steel Research International. vol.18 supl.1.1 pp.159-163 (Beijing, China. 2011).
- GAUDE-FUGAROLAS, D. *Application of a physical model on interstitial diffusion to the issue of hydrogen damage during casting and forming of ferrous alloys*. METAL2011. (Brno, Czech Republic. 18-20 May 2011).
- GAUDE-FUGAROLAS, D. *Effect of microstructure and trap typology on hydrogen redistribution in steel*. METAL2013, (Bnro, Czech Republic, 15-17 May 2013).
- Patent (US): US 8,286,692 Awarded: 16th October 2012. D. Gaude-Fugarolas. Also PCT patent WO/2010/097755, *et c*.

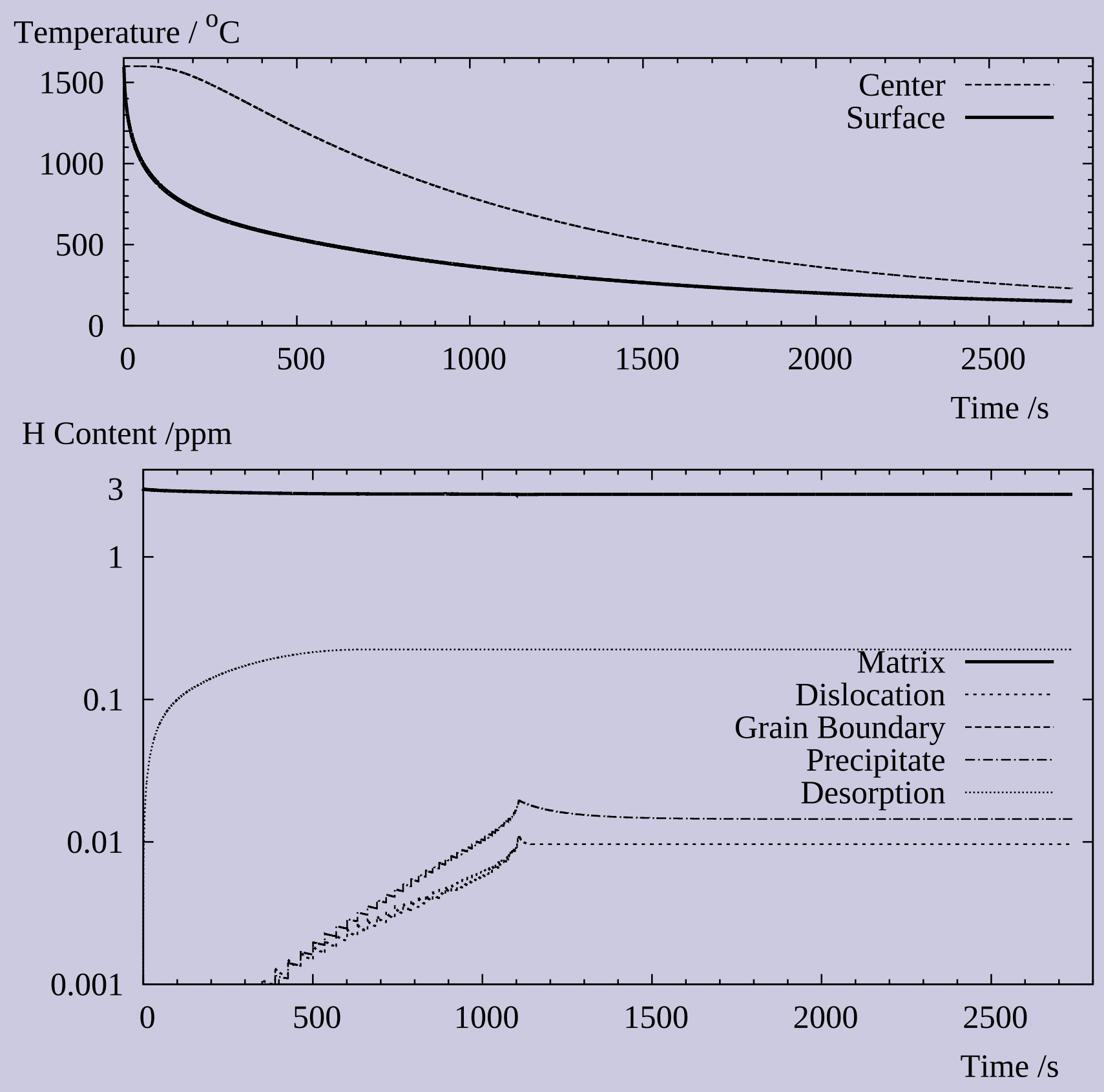
Further details:

- Accompanying Article: SteelYHydrogen2014 Proceedings
- Comprehensive project results and publications: **http://www.primeinnovation.net**

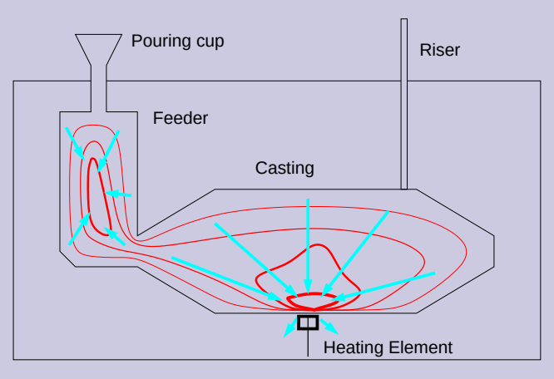
Standard cooling process:



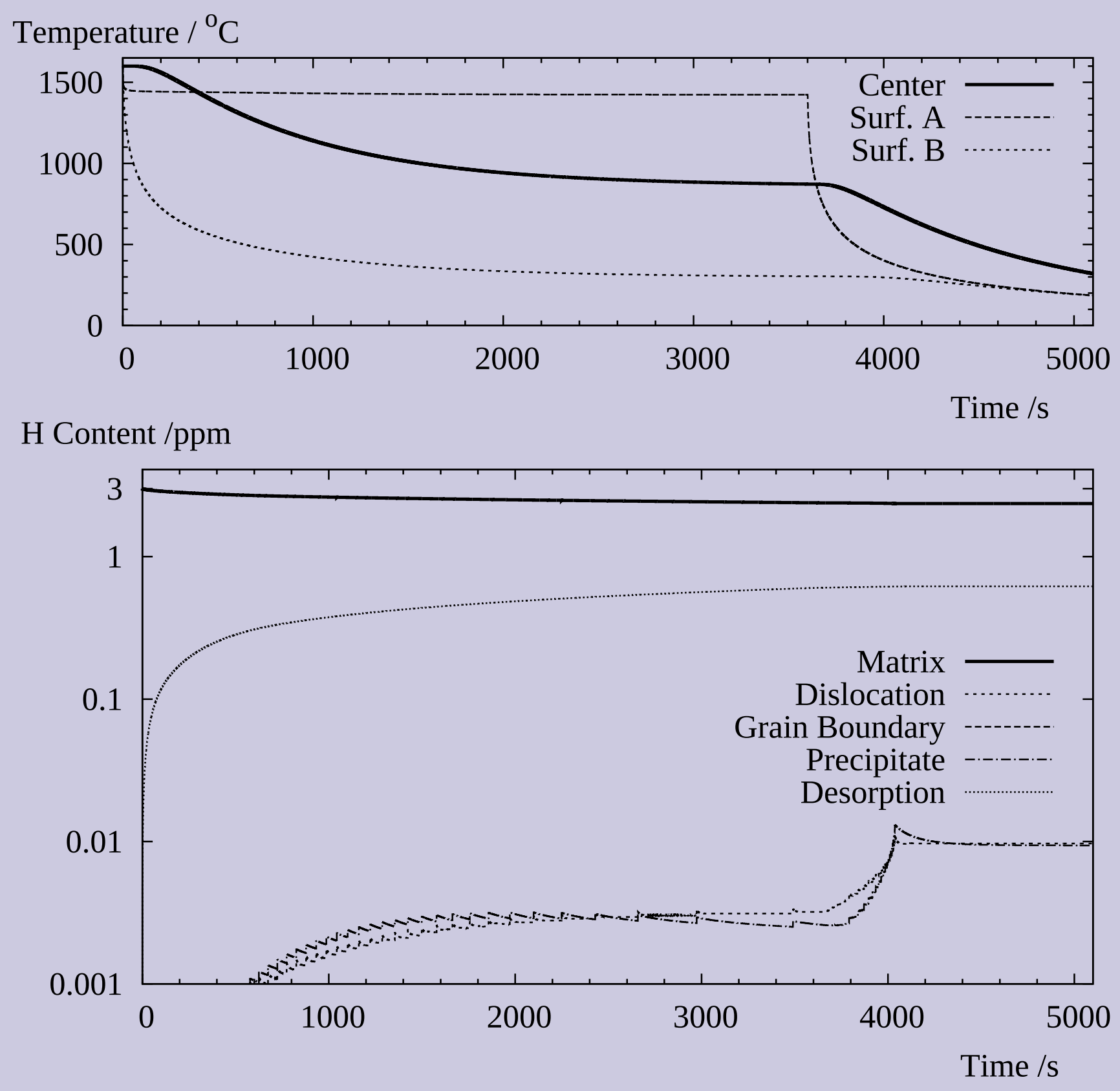
Cooling from liquid
Standard process
Start H content: 3.0 ppm
Thickness: 25 cm



Hydrogen removal treatment:



Cooling from liquid
H reduction process
Start H content: 3.0 ppm
Thickness: 25 cm



Final H content:

Final hydrogen content at each microstructure sites after cooling from solidification. The difference in hydrogen reduction between a standard process and one aplying a patented modiffied treatment, imposing a severe thermal gradient to the cooling solid, is evident and show how the final supersaturation in trapping sites can be effectively reduced.

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