

Description of hydrogen transport through a metal wall, and prediction of embrittlement risk

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Abstract

Minute amounts of hydrogen cause the embrittlement of some high strength alloys. Because of the safety, technological and economic issues involved, research efforts have intensified in recent years to improve our understanding of such phenomena.

A physical model describing the diffusion of interstitial atoms was developed and has been used to study the redistribution of hydrogen in alloys during manufacturing. In particular, the model contemplates diffusion in its most comprehensive description, i.e., atom diffusion is driven by the gradient in chemical activation, instead of simply occurring down the composition gradients. The model incorporates the influence of thermal history, microstructure, matrix solubility, multiple trap typologies and distributions, and interaction with the atmosphere. It has been successfully applied to describe casting processes, heat treatments like baking, and to design a novel method for hydrogen extraction, as well as to predict the risk and location of hydrogen damage.

This work presents another application of interest to various industries, including nuclear energy. The case studied is that of hydrogen transport through a metal wall separating one volume with high hydrogen pressure and temperature from another volume with low hydrogen pressure and temperature. By using such comprehensive physical model, it is possible to study the effects of hydrogen pressure and temperature gradient, wall thickness, metal microstructure and trap distribution on the flux across the wall and on the accumulation of hydrogen within the metal. Furthermore, it makes possible to estimate the embrittlement risk and when necessary the time to fracture.

Keywords: Hydrogen transport, embrittlement, fracture, prediction

Introduction

It is well known hydrogen causes severe damage to high performance alloys [1-4]. Because of the economical, technological and safety repercussions, this phenomenon has driven research efforts for over a century [5-7].

The way hydrogen redistributes and the sites where it becomes trapped influence metal embrittlement. Therefore, understanding the redistribution of hydrogen correctly would permit the prediction and, subsequently, prevention this type of material degradation.

This is an overview on the development of a physical model of interstitial diffusion and its application to the study of hydrogen redistribution in several metallurgical processes. These include from casting and various heat treatments, to the permeation of hydrogen through a metal wall. The later is of interest in several industries, including in some designs of nuclear power generation. With better understanding of the behaviour of hydrogen within the metal, it is possible to predict when, where and what type of damage will take place. Lastly, during this research project has also produced a new method to remove hydrogen from alloys [8-10].

Description of the model

A physical model describing the diffusion of interstitial atoms has been developed and used to study the redistribution of hydrogen in steels[8,11]. Phase transformations during any treatment are modelled using thermodynamic and kinetics criteria as described in elsewhere [12-13].

Hydrogen diffusion

Strictly, diffusion, is driven by the gradient of **chemical potential** (and not just to the composition gradient, as often seen in simpler model)[14]. Then, as long as we assume dilute solution of the interstitial elements, the gradient in chemical potential of an interstitial atom is related to the gradient in partial saturation in the matrix phase [5-6,15]. Consequently, the actual flux of atoms becomes a function of the relative saturation, that is, interstitial atoms will tend to flow from regions with high levels of saturation to regions with lower levels of saturation (*i.e.* down-hill the partial saturation gradient). For instance, in the case of uniform temperature this would lead to atoms flowing from regions with high concentration to regions with low concentration. However, in a system with large temperature (and therefore solubility) gradients, or with phases with distinct solubilities, a correct diffusion model still describes other possibilities, like diffusion happening up-hill the composition gradient [8,11,14].

Hydrogen distribution is determined from thermal agitation and atom mobility by relating it to a random walk process. The distance covered by each atom, the mean random walk distance, Δx , in a time interval Δt , is related to the thermal agitation, via the diffusion coefficient D , using the random walk expression [16]:

$$\Delta x = \sqrt{\Delta t D} \quad (1)$$

The effect of thermal activation is captured by an Arrhenius-type description of diffusion[7, 17-19].

If each atom jump were totally random, the probability, P_j , of an atom ending its random walk in the adjoining cell in each direction j would be similar. However, when temperature gradients, phase, trap distributions and partial saturation are taken into account, these probabilities change, and the model takes that into account. The differences in partial saturation in adjoining regions are used to determine the probability of atoms diffusing. Last, by considering partial saturation the issue of site saturation is also dealt with.[8].

Supersaturation of the microstructure

The alloy's microstructure is only able to store a small amount of hydrogen between the lattice and various types of lattice defects. In some cases, these defects consist in subtle distortions of the lattice itself, like the distortion around dislocations, or on the surfaces of a coherent precipitates. Othertimes, defects represent a severe rupture of the lattice structure, like for instance voids, microcracks or the surfaces of specific incoherent precipitates.

The resulting effect of hydrogen on the mechanical properties of the alloy depends directly on the type of trapping site and the amount of hydrogen that contains. As several types of trapping sites coexist, different and competing embrittlement mechanisms might be at work simultaneously [5].

Hydrogen trapped in microcracks, for instance, when in large concentrations, may transform into molecular form (gas), and produce an increase in pressure inside the defect, potentially leading to irreversible damage in the form of cracking and plastic deformation (fisheyes, flaking, etc.) [5, 20].

An illustrative parameter to gauge the risk of hydrogen embrittlement is the equivalent gas pressure in a microcavity due to supersaturation. Moreover, even though the physical meaning of the equivalent gas pressure becomes less clear for trapping sites other than microcavities, it is still a useful measure of the embrittlement risk from superaturation. Therefore, this *equivalent gas pressure* is calculated for each the lattice and each of the traps considered, not necessarily as a physical prediction of actual pressure, but as a convenient estimate of the potential embrittlement risk, as described elsewhere [21].

Nevertheless, one could develop this parameter to obtain a physically meaningful estimation of the risk of embrittlement, accounting for the effect of evolving mechanical properties, microstructure and defect distribution, as described later.

Trapping

The model describes the redistribution of hydrogen into various types of trap assuming that any hydrogen contained in the metal either stays in solution up to the lattice phase's solubility limit or it is expelled from the lattice and becomes *trapped* into various types of lattice defects available. Also, a diffusing hydrogen atom may become trapped as it comes across with lattice defects while partitioning [18-19, 22].

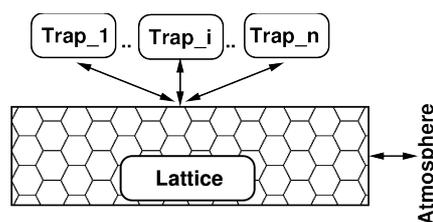


Figure 1: Hydrogen redistribution fluxes between the atmosphere, the lattice and n trap site types.

The nature of trapping sites vary, but they can all be described as a potential well, in the same way as lattice diffusion sites. Each trap type is then characterised by the specific activation energy, necessary for the release of an hydrogen atom contained in them [5, 22]

Hydrogen desorption

To include the effect of free surfaces on the behaviour of interstitial atoms, specially those as mobile as hydrogen, hydrogen desorption is estimated assuming local equilibrium at the surface. Then, the relationship between hydrogen dissolved in the metal at the surface and the partial pressure of hydrogen gas in the atmosphere follows Sievert's law [5-6, 17]. Additionally, the flux of hydrogen atoms across the surface is still restricted by the atom mobility conditions and by site saturation (*i.e.* partial saturation), as described earlier [8, 21].

Prediction of permanent hydrogen damage

Hydrogen embrittlement is a complex phenomenon with multiple and often competing mechanisms, including HIE (Hydride-induced embrittlement), AIDE (Adsorption-induced dislocation-emission), HELP (Hydrogen enhanced localised plasticity), HEDE (Hydrogen enhanced decohesion mechanism) and others [23-24].

However, having a set of criteria able to predict the threshold of permanent damage in real structural components and during industrial practices would perform an invaluable service during component manufacturing and process supervision.

In summary, permanent damage in ductile materials occurs when the capacity of elastic (*i.e.* reversible) deformation is exceeded and plastic (*i.e.* irreversible) deformation develops. Brittle fracture, on the other hand, takes place when the energy required to create fresh fracture surfaces is lower than the energy to activate any of the available deformation mechanisms which would reduce the stress distribution by yielding under the stress [23-24]. In the first case, and for a general ferrous alloy, the onset of plastic deformation occurs around the point where shear stress τ reach G , where G is the Shear Modulus of the metal for that alloy composition, phase and temperature [25]. In engineering terms it is usually expressed as 0.1% of shear deformation ($\gamma = \tau / G = 0.001$) [24].

As described previously, hydrogen supersaturation could be represented as a stress distribution equivalent to an hydrostatic pressure on the lattice structure, akin to the real pressure within existing micro-defects like micro-cracks, voids and incoherent interfaces [21]. By determining the equivalent pressure in the lattice and then applying the criterion described above, it is possible to estimate the risk of irreversible deformation and therefore, the onset of permanent damage in the metal component [26].

Results and discussion

Using this model the influence of manufacturing parameters and material conditions on the redistribution of hydrogen in steel have been studied for several real industrial applications. Of these, a few are summarised below. This project started with the need to describe accurately hydrogen redistribution during accelerated cooling, in particular, during casting. Another treatment studied has been *baking*, a commonly used method against of hydrogen embrittlement. The prediction of

permanent damage in the alloy has also been analysed, paying special attention to the effect of mechanical properties, microstructure and defect distribution. Most importantly, the improved understanding of hydrogen redistribution has allowed to design a novel method for the elimination of hydrogen in metallic alloys, with the aim to reduce the risk of hydrogen embrittlement at a lower cost. Finally, the same model has been applied to the case of hydrogen diffusion across a metal wall separating two volumes presenting different hydrogen partial pressure and temperatures.

Description of cooling and casting processes

A generic cooling process has been modelled in order to obtain a better understanding of the effect of material and process parameters to the redistribution of hydrogen [8]. This simulation could be applied to casting, for instance, or any other cooling process. In this section, trapping is not considered.

An aspect of interstitial redistribution that often is misunderstood is the effect of different cooling rates. Fig.2 presents the different hydrogen distribution obtained with either a fast or a slow cooling processes applied to a steel plate 25cm thick and containing 2ppm of hydrogen. These calculations show how during a long and slow cooling, and while the surface is still at high temperature, a portion of hydrogen diffuses away from the subsurface region and out into the surrounding atmosphere, and as the temperature gradients within decrease the hydrogen concentration homogenises to an average content of 1.53ppm.

Conversely, during an accelerated cooling of the same component, the large temperature gradient between the surface and the core of the component encourage the hydrogen flux towards the core region. Simultaneously, as the surface temperature decreases rapidly, desorption to the atmosphere is reduced. Additionally, as the metal cools and undergoes phase transformation from FCC to BCC, the flux towards the core region is favoured as the later phase is less able to dissolve hydrogen.

During a long and slow cooling, hydrogen content remains homogeneously distributed, and although hydrogen content reaches supersaturation and increases to several times the solubility of the BCC matrix, the supersaturation is still substantially less severe than in the core region of a fast cooled component. For the example presented here, the fast cooled component starting with a hydrogen content of 2.0ppm would reach in its core region supersaturation over 40 times the solubility limit of the BCC matrix. Of course, in the real material some of that hydrogen would end up in various trapping sites, but much of it would still be insoluble, with the foreseeable embrittlement risk.

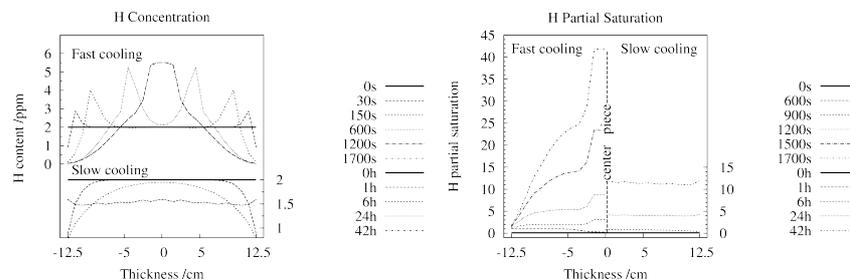


Figure 2: Hydrogen redistribution during fast and slow cooling of a 25cm thick plate with 2ppm start H content. Concentration and partial saturation (or supersaturation if above 1.0).

Component size intensifies this effect, as a larger volume implies larger absolute hydrogen content for the same average content. The FCC to BCC transformation temperature, also influence the intensity of this redistribution. Both effects are presented in Fig. 3 [8].

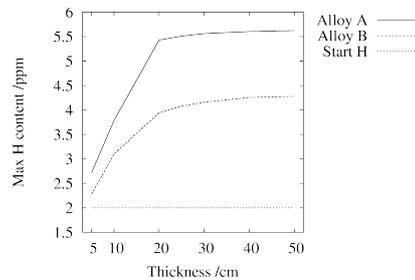


Figure 3: Effect of component size and FCC/BCC phase transformation temperature on hydrogen concentration after fast cooling. Steel A transforms at 700C and Steel B at 450C.

Design of hydrogen extraction method

The deeper understanding of the fluxes of hydrogen in metals obtained using the model described above has allowed to design a novel method to eliminate hydrogen from metallic alloys [8, 10].

As already discussed earlier, during the process of cooling a metal component the flux of hydrogen occurs towards the core of the metal component, because it stays at higher temperature as heat is extracted from all the surface of the component. However, if we consider a case where a small region of the surface of that component were to be kept at high temperature during the cooling process, hydrogen would still flow towards the hot regions of the component, with the difference that in this case, it would not accumulate in the core region but under the heated surface from where it would eventually diffuse to the atmosphere, as illustrated in Fig.5 [8, 10].

The evolution of hydrogen distribution during such an operation is summarised in Fig.6. A 25cm thick plate, as in the calculation shown earlier is cooled from 1600°C to just above room temperature. However, in this case while one face of the plate is severely cooled the one opposite is kept at 1500°C for 7200s. (2 hour). During this process the overall hydrogen content decreases to less than half the starting content (*i.e.* from 2ppm to 0.99ppm).

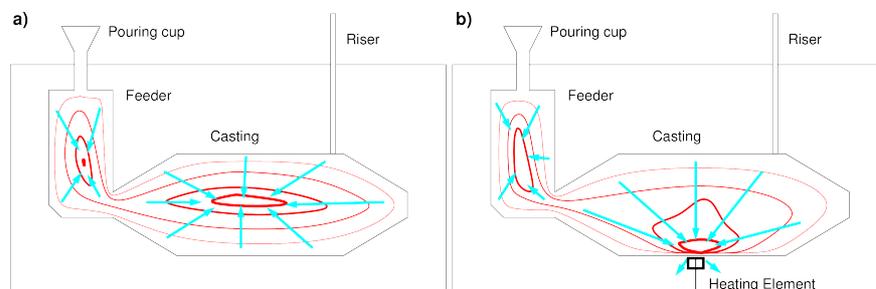


Figure 5: a) Schematic of hydrogen redistribution during a standard casting process. b) Modified hydrogen redistribution when diffusion fluxes are redirected to a heated region at the surface.

During the treatment a severe concentration peak still occurs. However, on this case it occurs only while the material is at high temperature and it is able to dissolve the large interstitial content. Fig 6 illustrates how the partial saturation remains below saturation during all the treatment, only increasing slightly during cooling to room temperature after the treatment. Even then, the final supersaturation is similar to what would result of an extremely slow cooling.

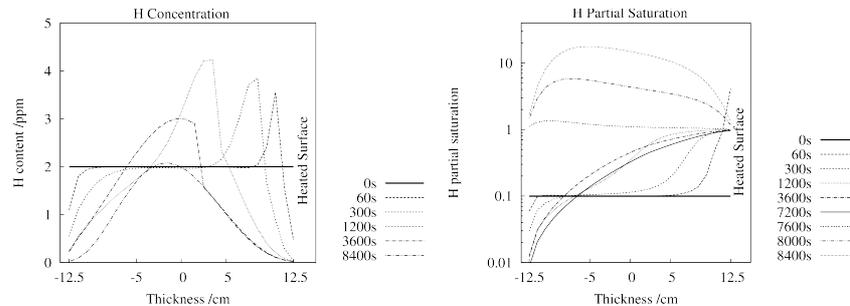


Figure 6: Hydrogen redistribution during directional cooling of a 25cm thick steel plate, where one of its surfaces is kept at 1500°C for 7200s. Concentration and partial saturation (or supersaturation if above 1.0).

While the treatment proceeds hydrogen is released to the atmosphere through the surface at the heated region, and the overall content and the magnitude of the concentration peak both decrease. At the end of the treatment the overall hydrogen content has been halved, to reach 0.99ppm. This is sensibly lower than the 1.53ppm obtained during extremely slow cooling, and taking only 8400s (2 hours and 20 minutes) instead of 42 hours by slow cooling or over 12h by an equivalent baking treatment.

Furthermore, by taking into account the geometry of the component and the hydrogen content requirements and with tools like the model presented here, it is possible to design tailored heat treatments optimising the final hydrogen content and distribution, and even limiting the maximum concentration peaks by adjusting parameters like the temperature of treatment and severity of cooling.

Description of baking

Baking is a common heat treatment used to try and minimise the detrimental effect of hydrogen on the mechanical properties of metallic components. Typically, the treatment consists in treating the component at *low* temperature (*i.e.* 150 to 230°C) for a long period of time (typically 12 to 48 hours) [27].

The aim of the treatment is that a fraction of the hydrogen in the lattice diffuses to the atmosphere. However, and as clearly described by the simulations, the picture is more complex. On one hand, because a fraction of the hydrogen becomes stored in microstructure defects, or *traps*. Hydrogen atoms in such *trap* sites need to overcome the detrapping energy barrier characteristic to the type of site, while at the low temperature of the treatment, this is not always possible [9, 28-30]. On the other hand, saturation of the lattice impedes the diffusion of hydrogen atoms.

The capacity of hydrogen to diffuse is, *a grosso modo*, inversely dependent on the degree of saturation of the lattice. Therefore, any baking treatment will only be effective when applied to an alloy presenting a microstructure largely unsaturated. For instance an alloy able to absorb large amount of

hydrogen before becoming saturated will fare better than an alloy that is already saturated at the start of the treatment.

The role played by different types of traps is on one hand, function of their partial saturation related to the lattice and on the other, of their characteristic energy barrier to the release of hydrogen. While the lattice presents lower partial saturation and the temperature allows the release of hydrogen from the trap distribution, the flux of hydrogen will occur towards the lattice (and eventually to the atmosphere). However, for traps with a large energy barrier (*deep traps*) it is possible that they keep absorbing hydrogen while the rest of the microstructure releases hydrogen to the atmosphere [9].

Prediction of permanent hydrogen damage

Most industrial alloys are polycrystalline and often multiphase. The availability of deformation mechanisms able to reduce an applied stress vary with metallographic orientation in the grain, and this varies from grain to grain. Therefore, any internal stress distribution will also depend to a certain extent on the grain orientation distribution. For this reason, any criteria on the onset of permanent damage in the metal necessarily can only be approximate. Nevertheless, the development of criteria predicting the inception of permanent damage in structural components is invaluable in component production and process design and supervision.

Simulations used

This section presents calculations of hydrogen redistribution on a large component (1.5m in thickness) during solidification and constant forced cooling to room temperature. Two different alloys have been simulated: *Steel A* with FCC to BCC transformation at 725°C producing ferrite characterised by larger grain size (100 μm) and an intermediate dislocation density, and *Steel B* with FCC to BCC transformation at 450°C producing ferrite characterised by smaller grain size (10 μm) and high dislocation density. The starting hydrogen content levels considered are 1.0 and 3.5 ppm.

Lattice hydrogen supersaturation and microplasticity damage

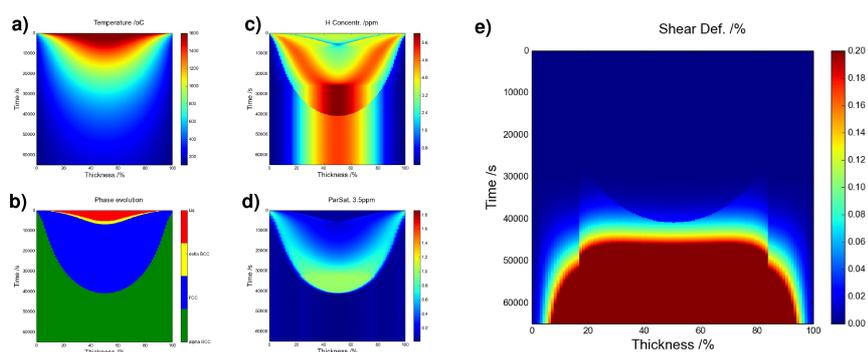


Figure 7: Plots presenting the evolution of a) temperature, b) phase, c) hydrogen concentration, d) hydrogen partial saturation in the metal lattice and e) shear deformation (as criteria for microdamage risk) during solidification and cooling of a 1.5 m thick steel component with a homogeneous starting hydrogen concentration of 3.5 ppm. FCC to BCC phase transformation occurring at 450°C.

Fig. 7 illustrates the application of the criterion described earlier. A component made with alloy *Steel B* and containing 3.5 ppm of hydrogen solidifies and is forcefully cooled to room temperature. The evolution of temperature as well as the phase evolution during cooling and at any position across the thickness of the component are shown respectively in Fig. 7 a) and b). During this cooling process hydrogen redistributes, and different regions in the ferritic lattice attain a range of hydrogen partial saturation levels or in some regions even supersaturation. By determining the equivalent hydrogen gas pressure related to those regions where supersaturation occurs, and then applying the criterion of $0.1\%G$, (with G the Shear Modulus of the metal) it is possible to estimate the risk of permanent damage to the component due to microplasticity. $\tau=10^{-3} G$ is equivalent to shear deformation $\gamma=0.1\%$ [24, 26].

In this example it is observed the apparition, just before 30 ks, of two regions around 20% and 80% of the thickness of the component where the shear strain starts to build up towards the yield shear strain limit defined above. As the process progresses, at around 45 ks, these two regions converge into a larger region comprising the whole core of the component. Within this region strain levels reach values considered to be unsustainable. Either cracking or some other type of permanent damage would be then expected.

Hydrogen saturation in dislocation distribution

Another criterion proposed here to estimate the risk of embrittlement of an alloy under the influence of hydrogen consists in observing the degree of partial saturation of the dislocation distribution [26]. A dislocation distribution presenting a large partial saturations in hydrogen is expected to behave differently than when free of hydrogen presence [24, 31].

Fig. 8 illustrates the calculations for a component of the same alloy and geometry as in the example above but containing only 1.0 ppm of hydrogen. The evolution of temperature as well as the phase evolution during cooling are identical as shown in Fig. 7 a) and b).

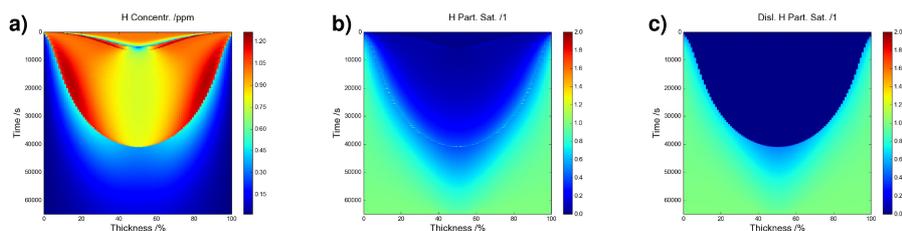


Figure 8: Plots presenting a) the evolution of hydrogen concentration in metal lattice, b) hydrogen partial saturation in lattice and c) hydrogen partial saturation in dislocation distribution, during solidification and cooling of a 1.5 m thick steel component with a homogeneous starting hydrogen concentration of 1.0 ppm. Temperature and phase evolution identical to those shown in Fig 7 a) and b). FCC to BCC phase transformation occurring at 450°C.

In this example, lattice partial saturation stays close to saturation but never reaching severe supersaturation, and therefore (by applying the microplasticity criterion above) without expected risk of embrittlement due to that mechanism. On the other hand, the dislocation distribution in the ferrite phase also becomes close to saturation. It is at this moment that needs to be pondered what could be the effect of a hydrogen saturated dislocation distribution. If dislocations become blocked due to

hydrogen then the metal would be expected to develop hardening and decreased ductility, eventually producing embrittlement of the material. At the same time, the severity of this effect is ultimately related to the ability of the alloy to create new dislocations and therefore accommodate new deformation [26].

Hydrogen saturation at grain boundaries

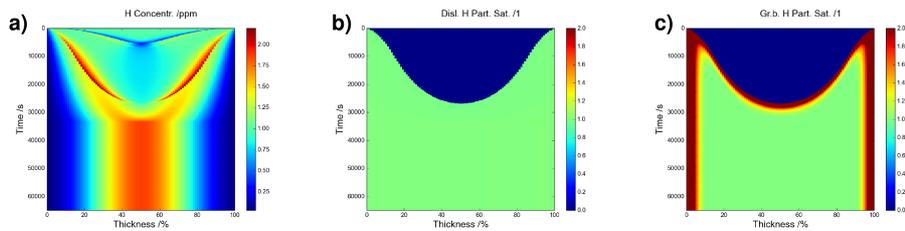


Figure 9: Plots presenting the a) evolution of hydrogen concentration in metal lattice, b) hydrogen partial saturation in dislocation distribution, and c) hydrogen partial saturation at grain boundaries during solidification and cooling of a 1.5 m thick steel component with a homogeneous starting hydrogen concentration of 1.0 ppm. Temperature evolution identical to that shown in Fig 7 a). FCC to BCC transformation occurring instead at 725°C.7

The last criterion proposed in this work for the estimation of the embrittlement risk of an alloy under the influence of hydrogen is based on determining the hydrogen partial saturation at grain boundaries (and similarly for precipitate interfaces) [26]. A grain boundary with hydrogen supersaturation could become embrittled due to various mechanisms, ranging from the obstruction of the deformation mechanisms characteristic of grain boundaries, to the apparition of microplasticity damage similar to what is described earlier for the metal lattice[2].

Fig. 9 illustrates the calculations for a component of the same geometry as in the examples above, but in a different alloy, *Steel A*. In *Steel A* austenite transforms to ferrite at higher temperature than in *Steel B* and with different characteristics (larger grain, lower dislocation density). For this calculation, the steel contains only 1.0 ppm of hydrogen. The evolution of temperature is identical as for other examples in this work, and already shown in Fig. 7 a).

Steel A's microstructure is less able to dissolve hydrogen in its trap site distribution than *Steel B* of earlier examples. In this case, the hydrogen dissolved in the lattice tends to concentrate at the core of the component, while the dislocation distribution become immediately saturated after transformation from austenite to ferrite. The interesting aspect though is the distribution of hydrogen at the grain boundary trapping sites. Actually, grain boundaries become severely supersaturated on transformation to ferrite. As the process proceeds, hydrogen in grain boundaries at a distance from the surface redistributes elsewhere reducing grain boundary supersaturation to levels close to full saturation. Grain boundaries close to the surface however, where the temperature does not allow sufficient redistribution of hydrogen, remain supersaturated till the end of the process (Fig. 9 c)). In both cases, the degree of supersaturation would strongly suggest serious risk of embrittlement. In particular, for the surface grain boundaries, this could explain various mechanisms of intergranular brittle fracture and crack formation in the surface and immediate subsurface regions (*i.e.* leading to *flaking*).

Modelling hydrogen permeation across a wall

Another use of this model of great potential interest for several industries is the description of hydrogen permeation. The transport of hydrogen through a metal wall separating two volumes: one volume with high hydrogen pressure and temperature and another volume with low hydrogen pressure and temperature. By varying temperature and pressure conditions, and geometrical and microstructural parameters, this simulation would be useful, among other industries, to hydrogen storage and distribution, to petrochemical processes or in some designs of nuclear power generation.

Simulations used

The diagram in Figure 10 represents the system analysed in this section. Two volumes at different temperatures and with different hydrogen partial pressures are separated by a metal wall. The focus of the simulation is to study the transport of hydrogen through such wall, analysing the transient flux rate, the accumulation of hydrogen in the lattice and at different trapping sites and in different regions across the wall and obtaining insight on the possible saturation of the microstructure. As shown before, excess saturation at specific loci in the metal structure can potentially lead to metal embrittlement.

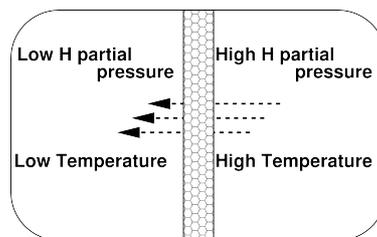


Figure 10: The diagram describes the system analysed in this section. A thin metal wall separates two volumes, one with high partial pressure of hydrogen and high temperature and another volume with lower partial pressure of hydrogen and lower temperature.

Two pairs of examples are shown below. In all cases the volume at the *hot* side of the wall stays at 290°C, while the colder side stays either at 200°C or 50°C. In one set of examples the high pressure (hydrogen partial pressure) is 0.5MPa, and in the other 1.5MPa, while, in both scenarios, the low pressure side has atmospheric conditions. The thickness of the wall is 5mm. The metal has fine microstructure and contains no hydrogen at the start of the simulation.

From the boundary conditions of the studied system, hydrogen experiences two opposing driving forces. On one hand, the pressure gradient pushes hydrogen across the metal wall, from high to low pressure volumes. Opposing that driving force, hydrogen experiences the increasing difficulty to diffuse towards regions at colder temperature, due to their lower capability to dissolve hydrogen and therefore presenting a more severe saturation.

Intermediate H partial pressure (0.5 MPa)

In both these examples, there is a trend towards saturating the structure of trapping sites before reaching some sort of adsorption-desorption steady state. In both these cases that occurs shortly before 200 hours. Grain boundaries close to the high pressure boundary saturate first, saturation that then extends to the thickness of the specimen. Similarly for the dislocation distribution. For the lattice, it only becomes partially saturated in the case with the larger temperature gradient.

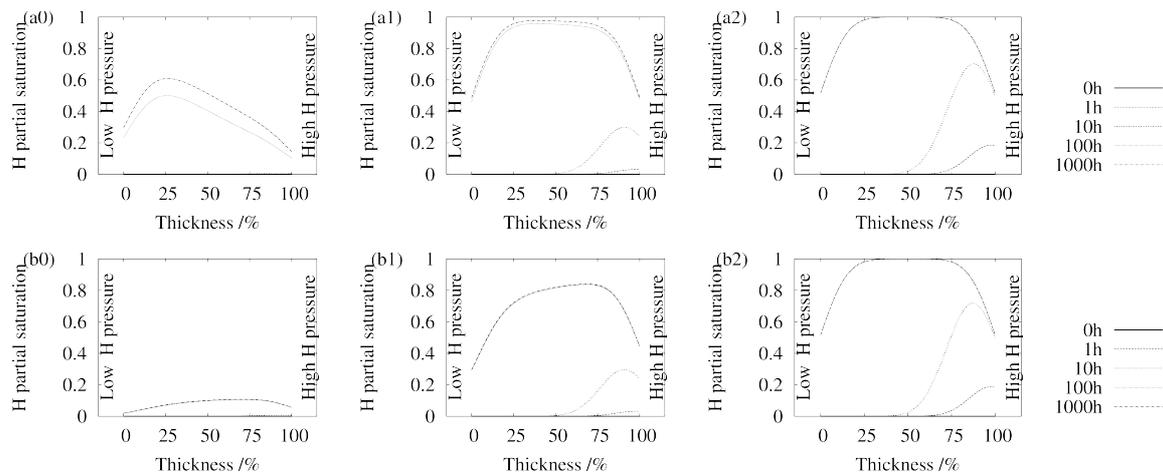


Figure 11: Hydrogen redistribution curves during permeation of a 5 mm steel wall between two volumes with different temperature and hydrogen partial pressure. High hydrogen partial pressure is 0.5 MPa. Low hydrogen partial pressure is equivalent to atmospheric conditions. Top plots (ax) present results for system with 50/290°C bounding temperatures and bottom plots (bx) for 200/290°C. Indexes **0** to **2** refer to lattice, dislocation and grain boundary trapping sites respectively.

High H partial pressure (1.5 MPa)

In the present example, and for the case of a smaller temperature gradient, and similarly to the previous example with lower partial hydrogen pressure, the lattice never experiences large partial saturation, while both trapping distributions reach towards saturation, starting from the boundary at higher temperature and pressure, and then growing to the whole thickness.

On the other hand, the case subjected to a larger temperature gradient experiences a rapid supersaturation at the grain boundary level, while the rest of the structure grows richer in hydrogen till reaching a sort of adsorption-desorption steady state shortly after 100 hours. As the degree of supersaturation experienced by the grain boundaries in this set of boundary conditions reaches well above saturation, these calculations suggest that this region of the metal could possibly suffer from severe embrittlement if subjected to similar conditions to the ones considered in this example. Similarly, and according to the calculations, the metal's lattice also becomes supersaturated suggesting also a risk of embrittlement. Using the level of maximum supersaturation at each site type, it would be possible to predict the risk of embrittlement, by using the criteria described previously [26].

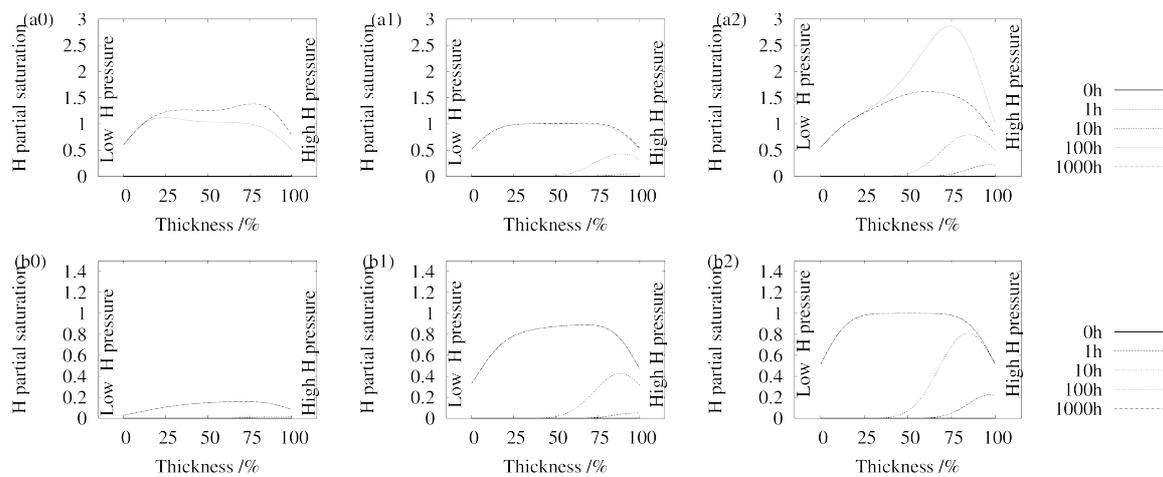


Figure 12: Hydrogen redistribution curves during permeation of a 5 mm steel wall between two volumes with different temperature and hydrogen partial pressure. High hydrogen partial pressure is 1.5 MPa. Low hydrogen partial pressure is equivalent to atmospheric conditions. Top plots (ax) present results for system with 50/290°C bounding temperatures and bottom plots (bx) for 200/290°C. Indexes 0 to 2 refer to lattice, dislocation and grain boundary trapping sites respectively.

Conclusions

A model on hydrogen diffusion had been presented able to describe accurately hydrogen redistribution during manufacturing processes. Using this model it is possible to describe and predict the behaviour of hydrogen during standard industrial practices, and it has been used to explain the individual and combined effects of parameters like component size, cooling rate, microstructure, trap distribution, and phase transformation temperature on hydrogen redistribution.

Using this model, it has been possible to develop a method to reduce hydrogen content based on the deliberate application of temperature gradients. This method has recently obtained several patents [10].

The model is also able to predict, based on physical criteria, the risk of hydrogen damage based on the fact that severe supersaturation of either lattice or any defect structures in the metal is involved in damage formation and embrittlement of the metal. For this, several criteria have been presented for the prediction different embrittlement mechanisms.

For this work, this model has been applied to simulate hydrogen permeation through a metal wall, driven by a gradient in partial pressure and against a temperature gradient. This kind of simulation can be applied to predict (and therefore also prevent) hydrogen embrittlement in nuclear power generation and other industries. By obtaining a better understanding of redistribution of hydrogen within the metal, it is possible to avoid potentially damaging working conditions.

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