Diffusive Hydrogen Distribution Simulation on Microstructure Scale in High Strength Weld Metal Containing Retained Austenite

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Abstract. In this study, hydrogen diffusion in high strength steels with martensite and retained austenite phase was evaluated by numerical simulation. A numerical simulation method for hydrogen diffusion that takes into consideration the difference in diffusion properties between martensite phase and austenite phase was proposed. In the simulation, the effect of microscopic stress distribution caused from martensite and austenite phases was also incorporated. In order to import temperature profile and residual stress distribution in welds, multi-scale analysis procedure was adopted. It was confirmed by the proposed hydrogen diffusion simulation that hydrogen concentration in martensite phase is constant for a certain period after welding and starts to decrease in high strength steel welds with martensite and retained austenite.

Introduction

In order to apply more widely 980 MPa class high strength steels, needed is an improvement of weldability. Especially, prevention of cold cracking is essential as the susceptibility to cold cracking becomes high for high strength steels. Heat treatment such as preheating and post weld heat treatment is a common measure to suppress cold cracking, however, it leads to the increase of fabrication cost. Therefore, a new method for suppressing cold cracking was proposed: development of Ni- and Cr-based welding wire [1]. As the wire has lower martensitic transformation temperature compared to conventional one, reduction of tensile residual stress in weld metal and induction to compressive stress are expected. In addition, due to the low martensitic transformation temperature, retained austenite also exists. The retained austenite is expected to have the effect of improvement of fracture toughness and trapping of diffusive hydrogen, one of the factors of cold cracking. However, because of the difficulty in the measurement of diffusive hydrogen in microscopic scale, the distribution of hydrogen in the weld metal of high strength weld metal containing retained austenite has not been clarified. In this study, the microscopic hydrogen distribution was discussed by numerical simulation.

Simulation Model

Diffusive hydrogen distribution was calculated considering the residual stress distribution and microstructure of high strength steel welds. In this chapter, the simulation method for hydrogen diffusion and weld residual stress distribution are described.

Diffusive Hydrogen Simulation. In this study, hydrogen diffusion after martensitic transformation occurred during cooling of welds was simulated. Shown in Fig. 1 is the simulation model for diffusive hydrogen distribution. The simulation model considered being austenite phase at initial state as shown in Fig. 1(a). The initial temperature of the simulation model is set to just above martensitic transformation temperature, M_s. In this paper, M_s was set to 400°C. The temperature of the model was lowered from the initial temperature to room temperature. Temperature profile during cooling was taken from the simulation result of the residual stress simulation. Martensitic phase transformation occurs at M_s during cooling, the initial austenite phase changes to martensite phase as shown in Fig. 1(b). In this case, part of austenite phase still remains at room temperature and the fraction of the retained austenite is 9.6%. The hydrogen concentration in the simulation model is preserved before and after phase transformation and was set to 1 ppm through out the model. In addition, a case where no retained austenite exists was also calculated for comparison. As a boundary condition for hydrogen diffusion simulation, hydrogen concentration at top and bottom surface were set to 0 ppm.

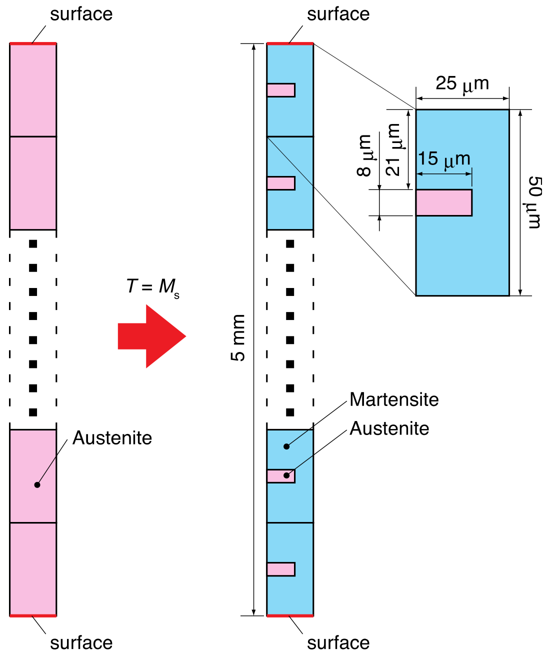


Fig. 1. Hydrogen diffusion simulation model.

Diffusive hydrogen distribution was calculated by the formulation proposed by Sofronis et al. introduced in the commercial finite element analysis software Abaqus [2, 3]. The driving force of hydrogen diffusion is the gradient of chemical potential as described in Eqs. 1 and 2.

$$\mathbf{J} = -s\mathbf{D}\cdot\left\{\frac{\partial \phi}{\partial \mathbf{x}} + \kappa_s \frac{\partial}{\partial \mathbf{x}}\left(\ln\left(\theta - \theta^{Z}\right)\right) + \kappa_p \frac{\partial p}{\partial \mathbf{x}}\right\} \quad (1)$$

$$\int_V \frac{dc}{dt} dV + \int_S \mathbf{n}\cdot\mathbf{J}\, dS = 0 \quad (2)$$

where,

s (θ, f): solubility (ppm)
$\mathbf{D}$(c, θ, f) : diffusivity (mm^2/s)
κ_s(c, θ, f) : Soret effect factor
κ_p(c, θ, f) : pressure stress factor
$\overline{V}_H$: partial molar volume of hydrogen in the solid solution (= 2×10^{-6} m^3/mol)
R : gas constant (= 8.3143 J/K·mol)
θ : temperature (K)
θ^{Z} : absolute zero temperature (K)
ϕ : normalized concentration (= c/s)
c : concentration (ppm)
p : equivalent pressure stress (= – trace(σ)/3, MPa)
f : number of microstructure ()
V : arbitrary volume (mm^3)

S : surface of V (mm^2)
n : normal vector of S
J : flux of concentration (ppm·mm/s)

Based on the above formulation, temperature and microstructure dependent material properties related to hydrogen diffusion were determined in order to simulate the effect of retained austenite on hydrogen concentration distribution. Material properties used in this study are shown in Fig. 2. The temperature distribution in the hydrogen diffusion model was considered to be uniform in this study; therefore, the second term in Eq. 1 is negligible. Temperature distribution in the model was uniform, however, temperature profile in the weld metal was taken from the weld residual stress simulation results. The gradient of hydrostatic pressure was imported from the residual stress calculation described in the next section.

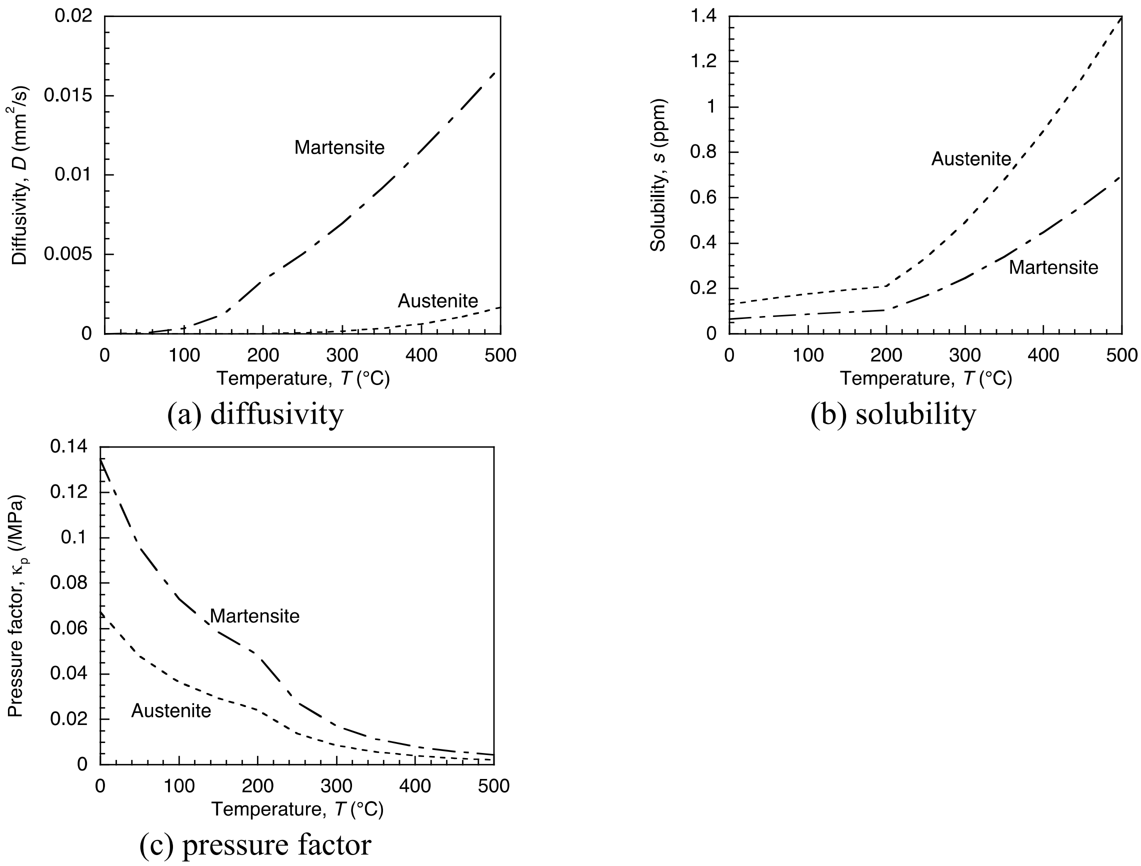


Fig. 2. Material properties used in hydrogen diffusion analysis.

Residual Stress Calculation. In order to obtain the hydrostatic pressure component appears in Eq. 1, a residual stress calculation was performed. The simulation model of residual stress distribution is shown in Fig. 3. The finite element model used was a half model with symmetry axis at the center of the weld metal. The edge of base plate is rigidly fixed. The model is usually used to evaluate the residual stress occurs in weld metal under a certain constraint condition to discuss cold cracking. The constraint condition varies with different constraint length, L. In this paper, the case for L = 200 mm is presented.

The hydrogen diffusion model described in the previous section is supposed to be located in the center of the weld metal as shown in Fig. 4. In order to obtain the stress distribution at the region corresponding to the hydrogen diffusion model, a multi-scale analysis procedure was adopted in the residual stress simulation as shown in Fig. 5 [4, 5]. The displacement at nodes of the boundary of models were transferred from macroscopic model to microscopic model; from (a) to (b), from (b) to (c), etc. The temperature at nodes was also transferred from macroscopic models to microscopic models except the transfer to the hydrogen diffusion simulation model. In this transfer step, temperature at nodes corresponds to the hydrogen diffusion simulation model were averaged and uniform temperature was used. In this study, as the simulation was performed for the temperature lower than M_s = 400°C, the temperature distribution becomes almost uniform, so that the procedure have little effect on the simulated results.

The temperature and microstructure dependent material properties used in the residual stress simulation are shown in Fig. 6. Two phases, martensite and austenite were defined in order to take into consideration the effect of phase transformation.

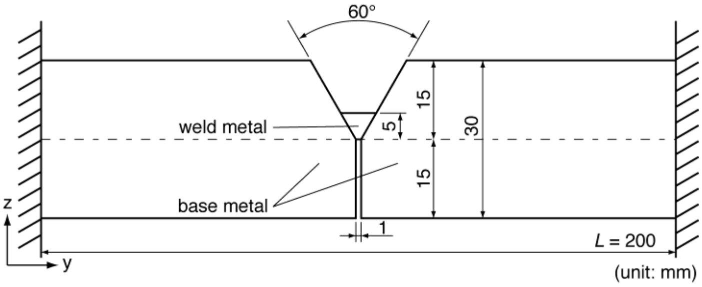


Fig. 3. Residual stress simulation model.

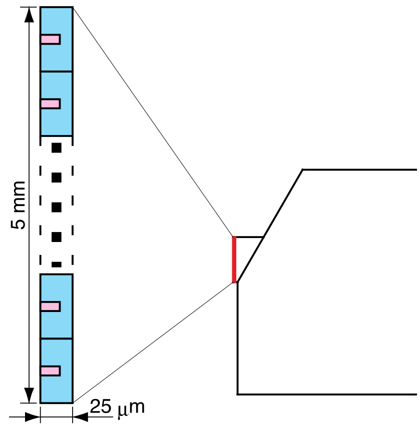


Fig. 4. Location of hydrogen diffusion model.

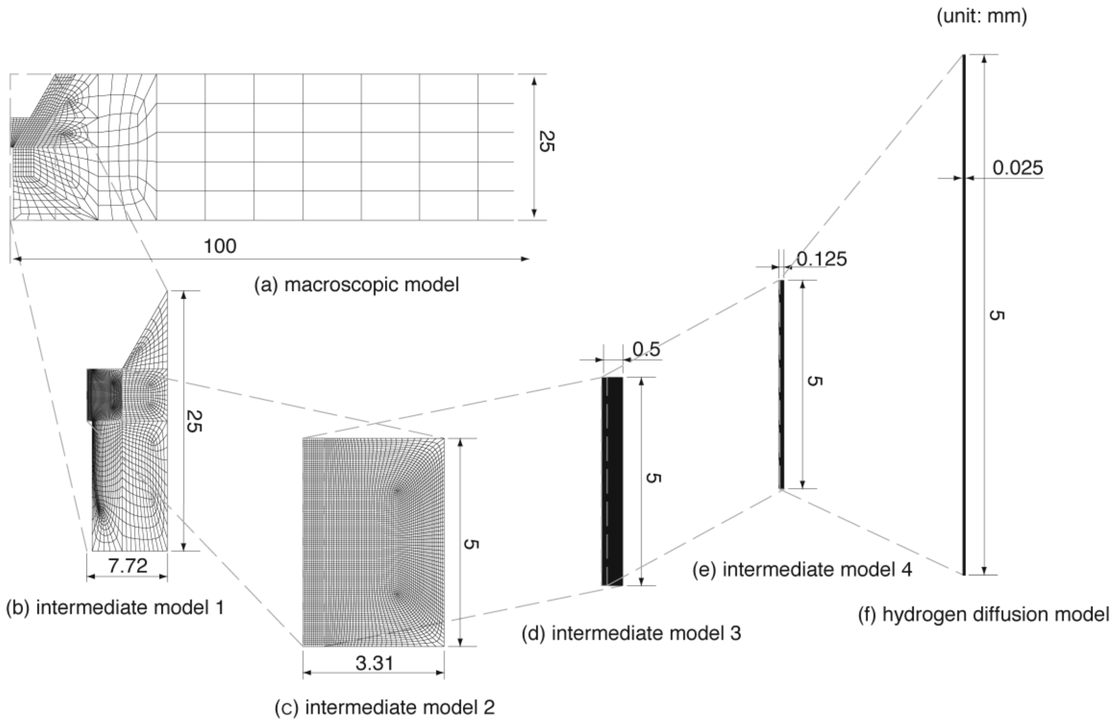


Fig. 5. Multi-scale analysis procedure.

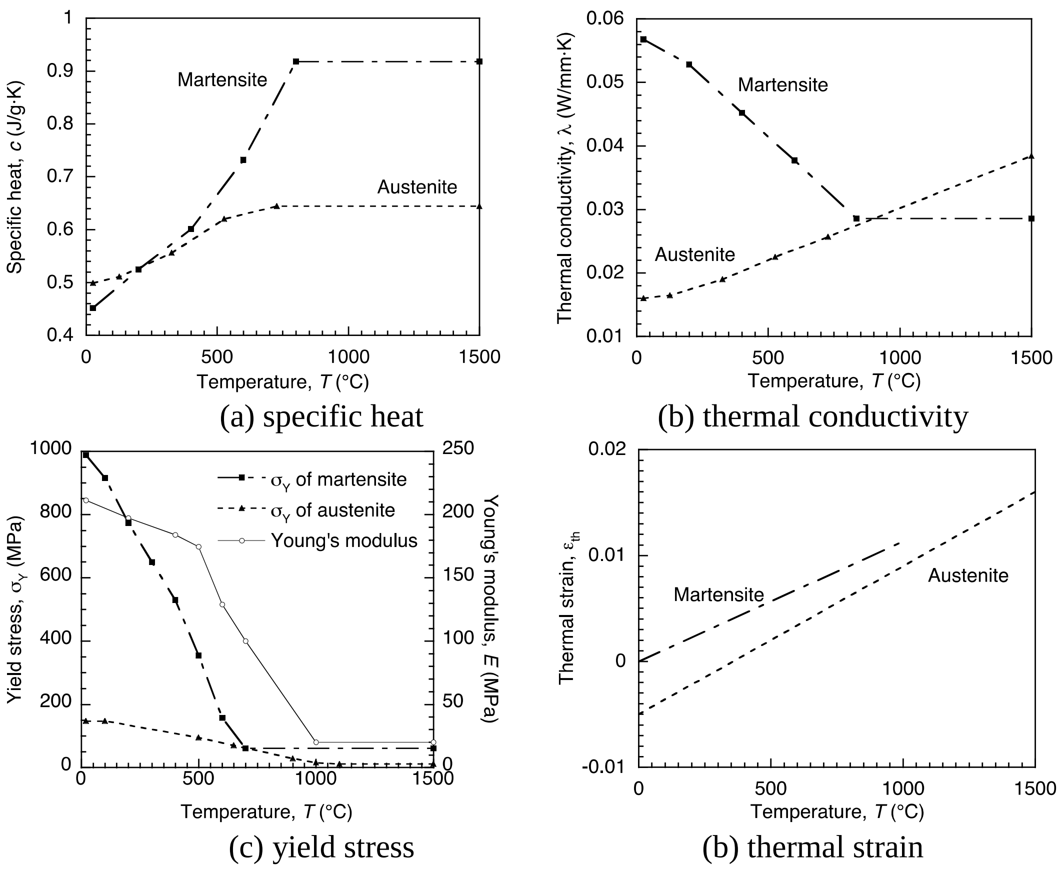
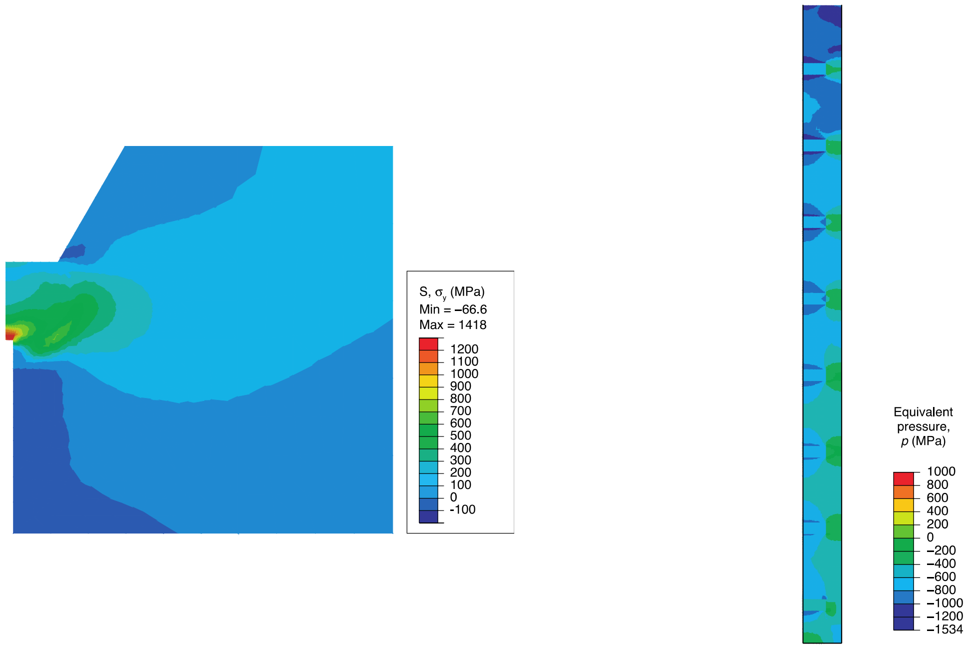


Fig. 6. Material properties used in the residual stress simulation.

Results and Discussion

Residual Stress Distribution. The residual stress distribution in welds is shown in Fig. 7. Shown in Fig. 7(a) is the residual stress distribution in macroscopic scale, and in Fig. 7(b) is that in microscopic scale considering austenite and martensite phase. The result was taken into the hydrogen diffusion simulation.



(a) macroscopic scale

(b) microscopic scale
(bottom of hydrogen diffusion model)

Fig. 7. Residual stress distribution in welds.

Hydrogen Release Curve. Released hydrogen from the simulation model is shown in Fig. 8. Hydrogen involved in the model is gradually released, and finally, all hydrogen introduced into the model is completely released through the surface. As shown in Fig. 8, the release curve shows retardation when the retained austenite exists. This is because the diffusion coefficient of the austenite phase is lower than that of martensite phase.

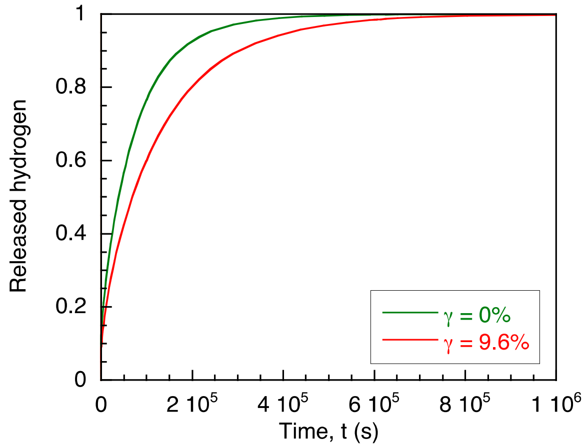


Fig. 8. Evolution of released hydrogen.

Local Hydrogen Concentration. Distribution of diffusive hydrogen in microscopic scale is shown in Fig. 9. Diffusive hydrogen concentration is higher in austenite phase compared to that in martensite phase due to the microscopic residual stress distribution and the difference in material properties of hydrogen diffusion. The profile of hydrogen concentration in a certain austenite and martensite phase is shown in Fig. 10. Hydrogen concentration in austenite phase increases during cooling and reaches to a peak. On the contrary, hydrogen concentration in martensite phase is almost constant after welding, and finally gradually decreases. Residual stress in welds does not change after welds are cooled to room temperature; therefore, hydrogen concentration is an important factor of the occurrence of cold cracking. In the evaluation of the effect of diffusive hydrogen on cold cracking, the hydrogen content in martensite phase should be discussed. Based on the result of the simulation, hydrogen concentration in martensite starts to decrease after a certain period. If no cracking occurs in welds by the time, cold cracking unlikely to occur after that.

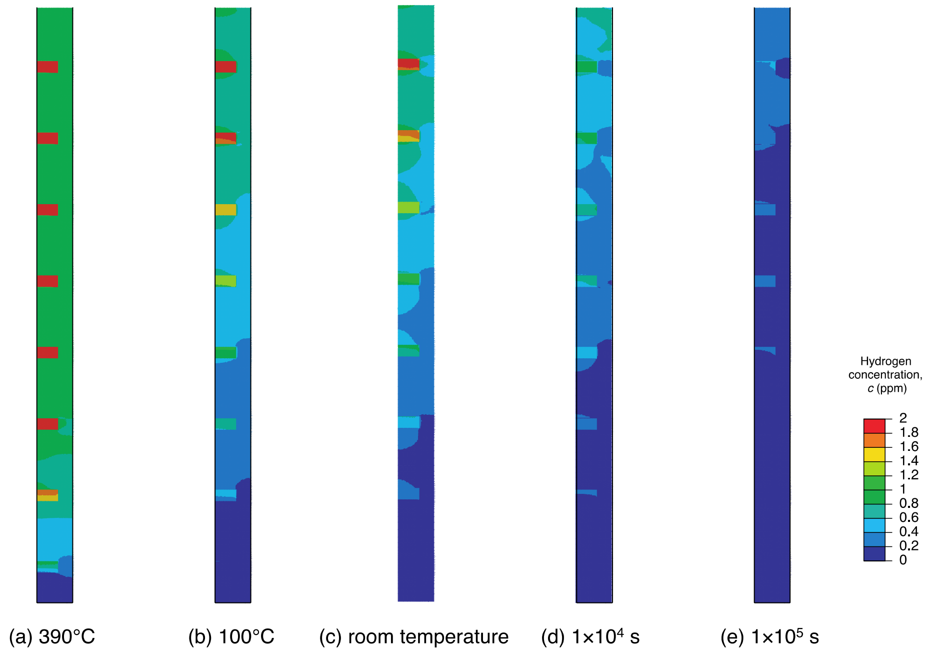


Fig. 9. Hydrogen concentration in microscopic scale.

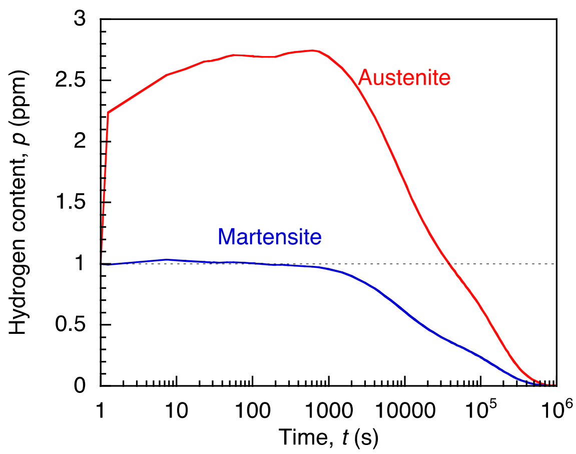


Fig. 10. Profile of hydrogen concentration in martensite and austenite phase.

Summary

In this study, a simulation method to evaluate hydrogen concentration considering residual stress distribution and microstructure was proposed. It was shown that hydrogen concentration in martensite phase, where cold cracking is supposed to occur, is almost constant after welding for a period and starts to decrease. Comparison with experimental results and validation should be needed, however, the hydrogen concentration in microscopic scale could be estimated by the proposed method.

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