Study of Residual Stress Effect on Hydrogen Diffusion of X-groove Flat Butt Welded Joints

Qianqian Jia, Kaixiang Sun, Hui Liu, Xiaofeng Meng

Abstract— Ships are usually large-welded structures, and residual stress would inevitably occur in the welding process. At present, high-strength steel has been more and more widely used in ship structures, and it has high sensitivity to residual stress. At the same time, in the high temperature during the welding process, the hydrogen-containing compound in the arc welding is decomposed into monoatomic hydrogen, which is dissolved in the molten pool in a large amount. Uneven weld residual stresses in such structures can promote the diffusion and accumulation of hydrogen in the steel, resulting in excess hydrogen at the weld joint. This behavior can lead to hydrogen embrittlement, threatening the safety and reliability of the ship's structure. In this study, a three-dimensional finite element analysis thermodynamic model for the flat butt welding joints of high-strength steel was established, the welding process was simulated, and the distribution law for the welding residual stress field was obtained based on the thermal elastic-plastic theory. Then the sequential coupling calculation of hydrogen diffusion was performed by defining the welding residual stress field of flat butt welding joint of high strength steel as the pre-defined field, and the hydrogen diffusion behavior under the welding residual stress field was obtained based on the theory of residual stress-induced hydrogen diffusion. The results show that the welding residual stress level decreases rapidly with the increase of the weld distance. The welding residual stress affects the hydrogen diffusion behavior, hydrogen is enriched in the zone where the residual stress is high, and the heat affected zone is the region with high residual stress. These results could provide theoretical support for ensuring the safety and reliability of large ship structures.

Index Terms— Hydrogen Diffusion, Residual Stress, High-Strength Steel, Numerical Simulation

I. INTRODUCTION

Flat butt welding is the most common welding form on ships, usually large welding structures. During the welding process, the hydrogen-containing compound in arc welding decomposes into monoatomic hydrogen at a high temperature in the arc and is dissolved in the molten pool in a large amount. When the molten pool solidifies, a part of the hydrogen escapes, and another part of the hydrogen exists in the weld, forming a gap solid solution with the weld metal. Since the hydrogen radius is small, a part of hydrogen is freely diffused in the crystal lattice of the weld metal to become diffused hydrogen. Another part of the diffusion is concentrated in the voids of the lattice defects, microcracks

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and non-metallic inclusions, and is combined into molecules, which cannot be freely diffused, and is called residual hydrogen. The chemical potential gradient is the fundamental cause of hydrogen diffusion in steel, and both the hydrogen concentration gradient and the stress gradient can lead to the generation of chemical potential gradient [1]. The main sources of hydrogen in welding are shown as follow: the moisture contained in the coating, the core or the flux in the welding material; the damage to the product packaging, the humid environment or the long storage time can lead to a significant increase in the diffusion hydrogen content; The surface paint, rust, coating, anti-splash compound and grease, surface lubricant of the wire can affect the diffusion hydrogen content; the temperature and humidity of the welding environment have a great influence on the diffusion hydrogen content, and the moisture in the air can enter the arc, thus increase the diffusible hydrogen content[2].

The essence of hydrogen-induced failure is that hydrogen enters the interior of the material and causes crack nucleation and expansion [1]. Hydrogen has different diffusion properties in different metals or in different structures of the same metal. The diffusion rate slows down with decreasing temperature, but also diffuses at room temperature. In different parts of the joint, due to the existence of different plastic deformation, there are different dislocation densities, which will capture different amounts of hydrogen. The diffusion and accumulation of hydrogen in the material are not only related to the heterogeneity of the structure [3], but also related to the stress concentration in the material [4-6]. The results show that hydrogen accumulation in the notched sites such as roots and weld toes will directly affect the generation of cold cracks [2].

Zhang Xianhui et al. [7] determined the diffusion coefficient and solubility of hydrogen in various areas of welded joints by gas phase infiltration method, and based on the extension of Fick's second law, the diffusion of hydrogen in 20MnNiMo steel welded joints was carried out by ABAQUS finite element analysis software. The simulation results show that the hydrogen concentration in the weld metal gradually decreases with time, and the concentration of hydrogen outside the fusion zone undergoes a peak change process. Jiang Wenchun et al. [8-10] based on the basic theory of hydrogen diffusion induced by welding residual stress, a coupled finite element calculation program for hydrogen diffusion under welding residual stress was developed by the finite element software ABAQUS. The distribution of hydrogen-diffusion induced by welding residual stress in 16MnR steel liquefied petroleum balloon tank welded joints under wet hydrogen sulfide environment was numerically simulated and compared with hydrogen diffusion under unstressed state. The results show that the welding residual stress is one of the main reasons leading to the accumulation of hydrogen in the welded joint. Lv Liangxinbu et al. [11]

used COMSOL Multiphysics to numerically simulate the stress and internal hydrogen redistribution in titanium alloy welds in the deep sea environment based on differential equations. The results show that the welding process will generate residual stress at the weld, and under the action of residual stress, hydrogen will be enriched in the high stress region and finally stabilized.

It can be seen from the above literatures that most of the researches are on the hydrogen diffusion of the welded joints of pressure vessels or pipeline steels in the field of chemical engineering, while there are few researches on the hydrogen diffusion of the welded structures in the field of ships. Therefore, the results obtained in this paper on the influence of residual stress on hydrogen diffusion in the most common butt welding joints of ship structure laid a foundation for the study on the influence of residual stress on hydrogen crack.

II. BASIC THEORY AND ANALYTICAL METHODS

A. Basic theory

The diffusion phase should satisfy the law of mass conservation in diffusion [12]:

$$\int_V \frac{dc}{dt} dV + \int_S n \cdot J dS = 0 \quad (1)$$

Where: V represents the volume; S represents the surface of the volume V; n represents the vector of the vertical surface S; J is the concentration flow of the diffusion phase; $n \cdot J$ represents the concentration flow leaving the S surface.

In a heterogeneous medium, the constitutive equation for hydrogen diffusion caused by a chemical potential gradient is:

$$J = -sD \cdot \left[\frac{\partial \varphi}{\partial x} + k_s \frac{\partial}{\partial x} (ln(\theta - \theta_z)) + k_p \frac{\partial p}{\partial x} \right] \quad (2)$$

$$\varphi = \frac{c}{s} \quad (3)$$

where D represents the diffusion coefficient of hydrogen, φ represents the hydrogen activity, c represents the concentration of hydrogen, s represents the solubility of hydrogen, k_s represents the "Soret effect" coefficient driven by the temperature gradient, θ represents the temperature, θ_z represents the absolute temperature zero on the temperature scale used, k_p represents the stress coefficient driven by the stress gradient, and $P = -\text{trace}(\sigma)/3$ is the equivalent stress.

$$P = -\frac{\sigma_{11} + \sigma_{22} + \sigma_{33}}{3} \quad (4)$$

Assuming that the ambient temperature is constant and the influence of the temperature gradient on hydrogen diffusion is not taken into account, (2) becomes (5), and the stress influence factor k_p can be calculated using (6).

$$J = -sD \cdot \left(\frac{\partial \varphi}{\partial x} + k_p \frac{\partial p}{\partial x} \right) \quad (5)$$

$$k_p = \varphi \cdot \frac{V_H}{R(\theta - \theta_z)} \quad (6)$$

where R is the general gas constant and V_H is the partial molar volume of hydrogen in steel.

B. Analysis steps

The sequential coupling calculation steps and the hydrogen diffusion process under the welding residual stress field are shown in Fig. 1. Firstly, the welding temperature field is calculated, and then the temperature field result is used as the pre-input to calculate the welding stress field. Finally, the result of the welding stress field is used as the sequential coupling calculation of hydrogen diffusion for the predefined field of hydrogen diffusion [13]. In this paper, ABAQUS finite element software was used for numerical simulation of

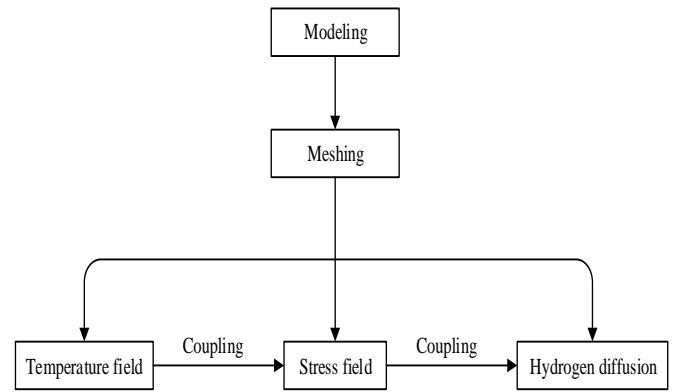hydrogen diffusion induced by welding residual stress.

Fig. 1. Steps for numerical simulation of hydrogen diffusion

III. NUMERICAL SIMULATION OF THE RESIDUAL STRESS FIELD

A. Finite Element Model

A welded plate of high-strength steel was formed by butt welding two plates with a size of 250 mm × 125 mm × 20 mm, and X-type groove was used in the welded plate. The sketch of the welded joint was presented in Fig. 2. In this paper, a double-sided continuous weld was used according to the thickness of the plate, and the weld is simplified to five layers along the thickness direction, and the geometric model of the welded plate was shown in Fig. 3.
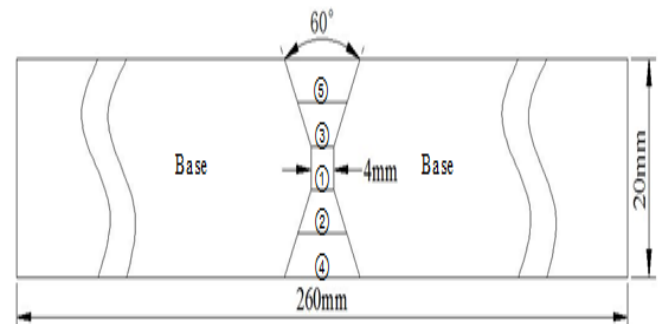

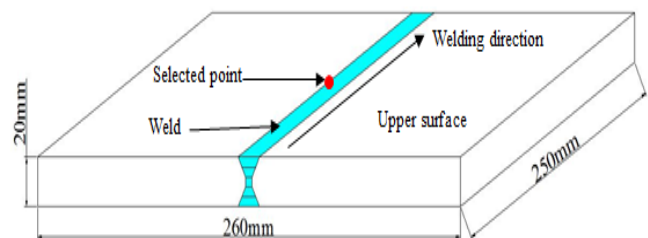**Fig. 2.** Sketch of the welded joint.

Fig. 3. Geometric model of the welded plate.

B. Thermal Physical Properties and Mechanical Properties

The flat butt welded joint (Fig. 3) was made of high-strength steel, and the thermal physical properties of this material are shown in Table Ⅰ. The stress–strain characteristics at different temperatures are shown in Fig. 4

Table Ⅰ. Physical properties of the joint material.

Temper ature	Elastic modulus	Poisson's ratio	Thermal expansion coefficient	Heat transfer coefficient	Specific heat
°C	MPa		1/°C	W/(m·°C)	J/(kg·°C)
20	2.1×10^5	0.3	1.1×10^{-5}	46	——
200	2.06×10^5	0.3	1.22×10^{-5}	45	550
400	1.71×10^5	0.3	1.35×10^{-5}	41	610
600	0.87×10^5	0.3	——	35	710
800	0.39×10^5	0.3	1.48×10^{-5}	24	865
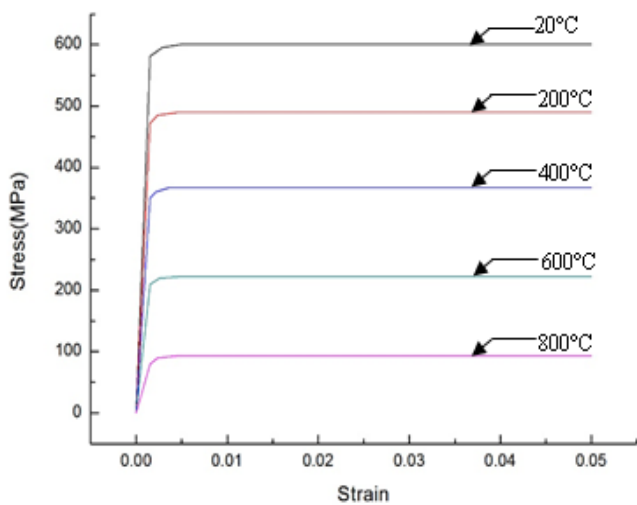
Fig. 4. Stress–strain characteristics of high-strength steel material

C. Meshing and Boundary Conditions

The finite element meshing is shown in Fig. 5, with a total of 25,245 nodes and 22,000 elements
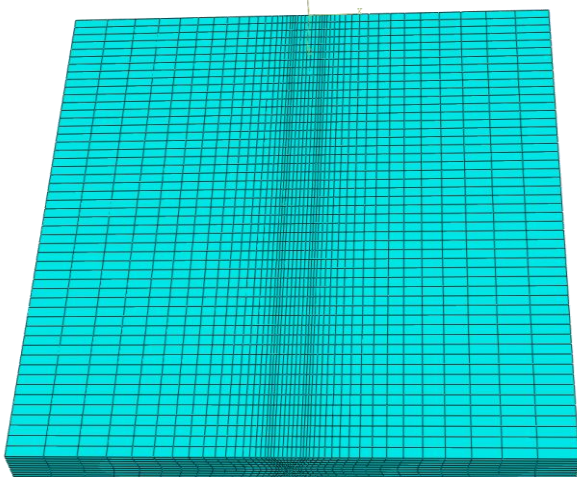
Fig. 5. Finite element meshing.

In the analysis of temperature field, the initial temperature and the ambient temperature were both set to 20°C, and the convection heat release coefficient was set to 25 W/m²·°C. In the analysis of stress field, in order to simulate actual conditions, the four sides of the welded plate were rigidly fixed.

D. Welding Process Parameters

The welding parameter for simulation is shown in Table Ⅱ, and the welding thermal efficiency constant was 0.75. A double ellipsoid heat source was used, as shown in Fig. 6. The parameters of double ellipsoid heat source are shown as follow: $a = 0.008$ m, $b = 0.006$ m, $c_f = 0.0032$ m, $c_r = 0.0064$ m, $f_1 = 0.8$, and $f_2 = 1.2$.

Table Ⅱ. Welding procedure.

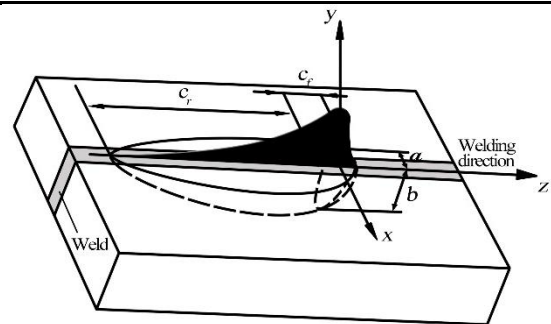| Welding layer	Voltage	Current	Speed
	V	A	mm /s
1	18	106	2.5
2	18	106	3
3	22	166	3
4	22	166	3
5	30	210	3

Fig. 6. Double-ellipsoid heat source model.

E. Calculation of the Welding Residual Stress Field

The life-and-death element technique was used for the numerical simulation of residual stress field in butt welded joint of flat plate. The temperature field after welding is shown in Fig. 7.
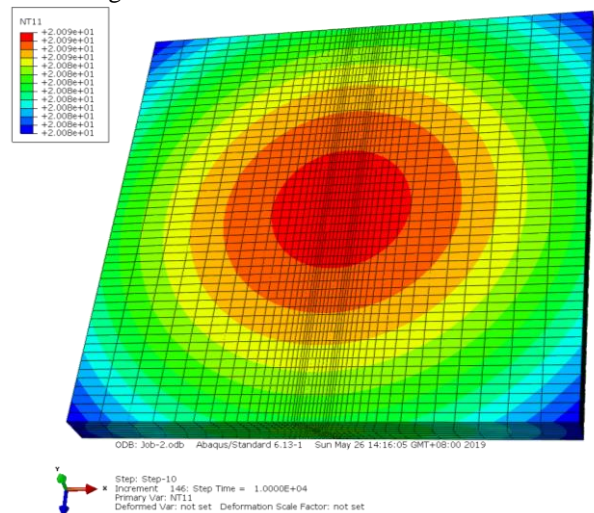

Fig. 7. Temperature field.

The temperature change curve at a selected point (Fig. 3) on the upper surface near the last weld is shown in Fig. 8. It can be seen from Fig. 8 that at a certain point in the welding process of the last weld, the maximum value of the welding temperature was reached, and the maximum value was about 1500 °C, and then cooled rapidly to room temperature. Before reaching the maximum temperature, the point has a maximal

value, because the heat source is close to the last weld when welding the weld adjacent to the last weld, so that its temperature is higher. Then, when welding the penultimate weld, the temperature of the point decreases. On the temperature curve, it shows a bimodal curve, which first reaches the maximal value, then falls back and then rises to the maximum value. This is consistent with the actual welding process.
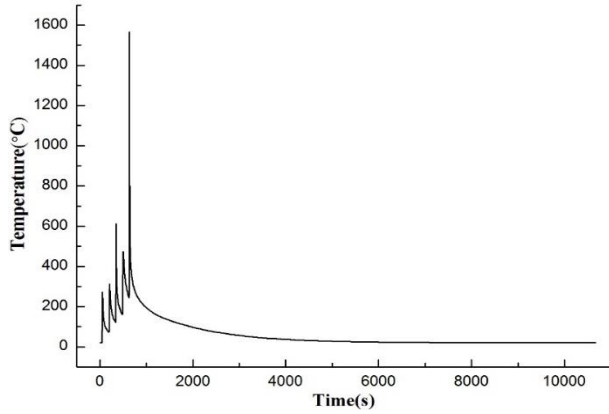

Fig. 8. Temperature curve of a point on the upper surface.

The results of temperature field were used as pre-input to calculate the stress field, and the residual stress distribution of butt welded joint of flat plate is obtained, as shown in Fig. 9. Among them, σ_x is the transverse residual stress, which is σ_{11} in (4); σ_y is the residual stress in the thickness direction, which is σ_{22} in (4); σ_z is the longitudinal residual stress, which is σ_{33} in (4); and P_s is the residual stress component that affects hydrogen diffusion, which is P in (4). Thus, in accordance with (4):

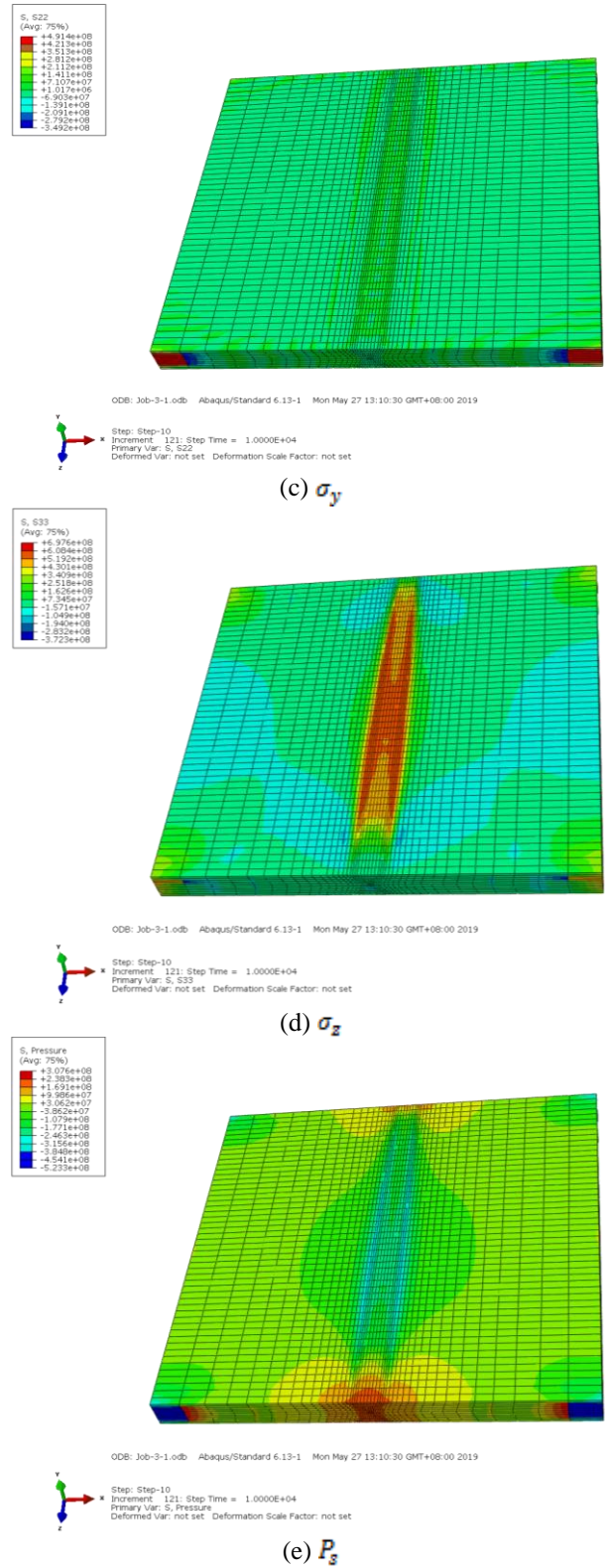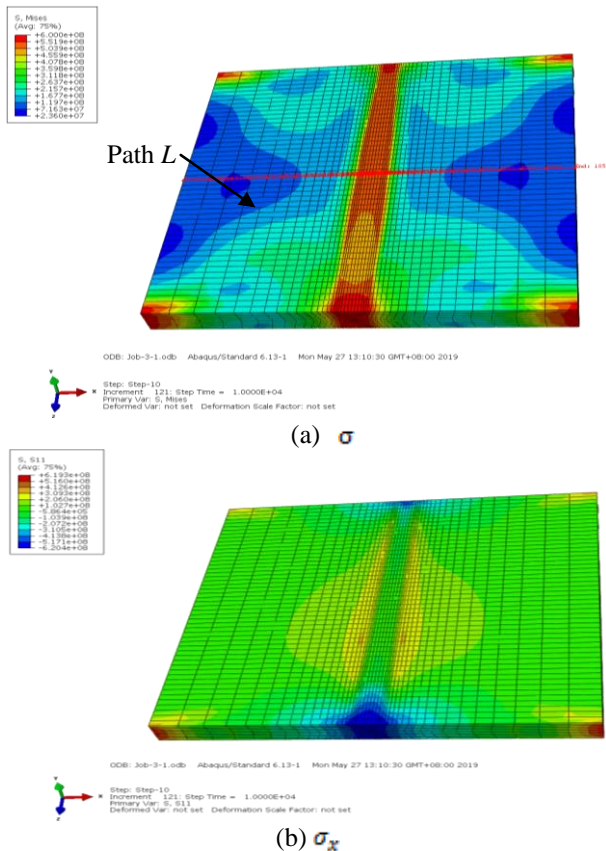$$P_s = -\frac{\sigma_x + \sigma_y + \sigma_z}{3} \quad (7)$$

(a) σ

(b) σ_x

(c) σ_y

(d) σ_z

(e) P_s

**Fig. 9.** Residual stress distributions.

Fig. 10 (a) shows the residual stress σ_L along path L of the butt welded joint of the plate, and path L is the center line of the plate width on the upper surface where the last weld is located, as shown in Fig. 9(a). Fig. 10 (b) shows the transverse residual stress σ_{Lx} along path L on the butt welded joint of the plate. Fig. 10 (c) shows the longitudinal residual stress σ_{Lz} along path L, Fig. 10 (d) shows the residual stress in the thickness direction σ_{Ly} along path L, and Fig. 10 (e) shows

the residual stress component that affects hydrogen diffusion P_{Ls} ($P_{Ls} = -\dfrac{\sigma_{Lx} + \sigma_{Ly} + \sigma_{Lz}}{3}$) along path L.

As shown in Fig. 9 and Fig. 10, on path L of the butt welded joint:

(1) The maximum value of residual stress σ_L is 529MPa, which was located in the weld toe and close to the yield stress of the material. As the distance from the weld increases, the level of weld residual stress decreases rapidly;

(2) The transverse residual stress σ_{Lx} exhibits a symmetric bimodal distribution, and the maximum value appears in the heat affected zone, which is about 288 MPa and is tensile stress;

(3) The maximum value of longitudinal residual stress σ_{Lz} appears in the heat affected zone, which is about 597 MPa and is tensile stress;

(4) The maximum value of residual stress in the thickness direction σ_{Ly} appears in the heat-affected zone, which is about 19.3 MPa and is compressive stress;

(5) The maximum value of residual stress component that affects hydrogen diffusion P_{Ls} appears in the heat-affected zone, which is about 275 MPa and is tensile stress.
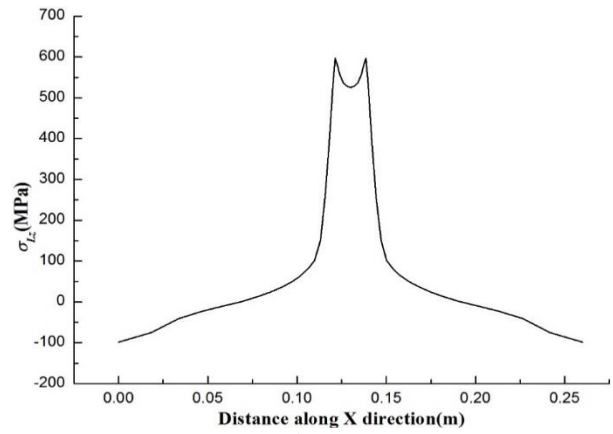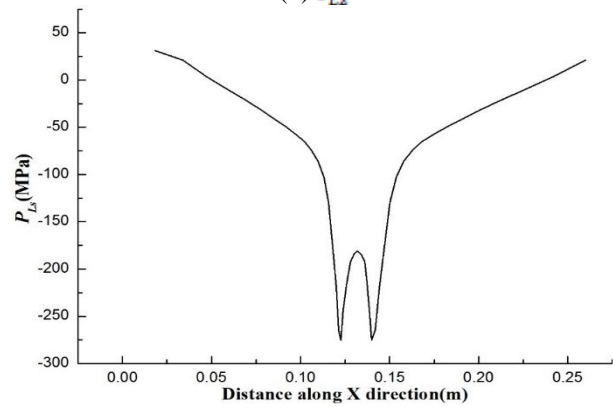

(a) σ_L

(b) σ_{Lx}

(c) σ_{Ly}
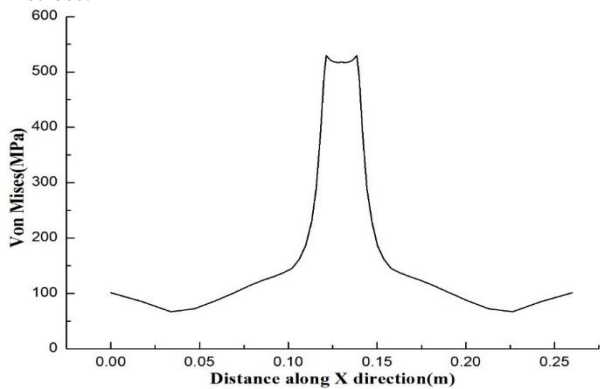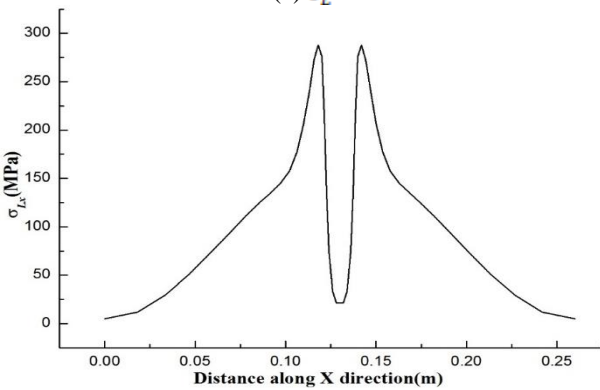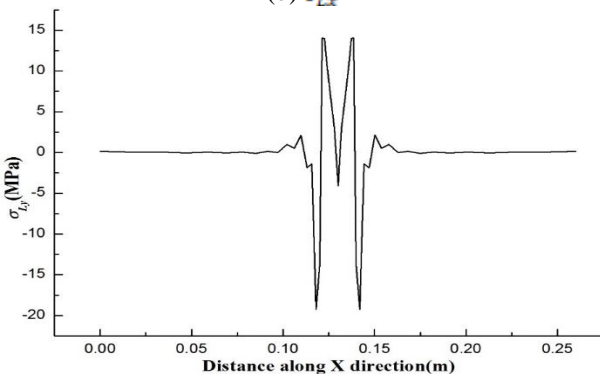
(d) σ_{Lz}

(e) P_{Ls}

Fig. 10. Stress distribution curves along path L.

IV. ANALYSIS OF HYDROGEN DIFFUSION

In the hydrogen diffusion analysis, the hydrogen activity φ is the parameter characterizing the boundary condition. The main source of hydrogen in the butt welded joint of flat plate (Fig. 3) is the electrode. According to the test results, the hydrogen concentration c at the weld is 0.1233 ppm and the solubility s is 0.078. Thus, according to (3), the hydrogen activity φ at the weld is 1.581. The distribution of hydrogen in the butt welded plate before diffusion, during diffusion and after diffusion were obtained, as shown in Fig. 11, Fig. 12 and Fig. 13. Fig. 14 shows the distribution curves for the hydrogen concentration before and after diffusion along path L (Fig. 9(a)).
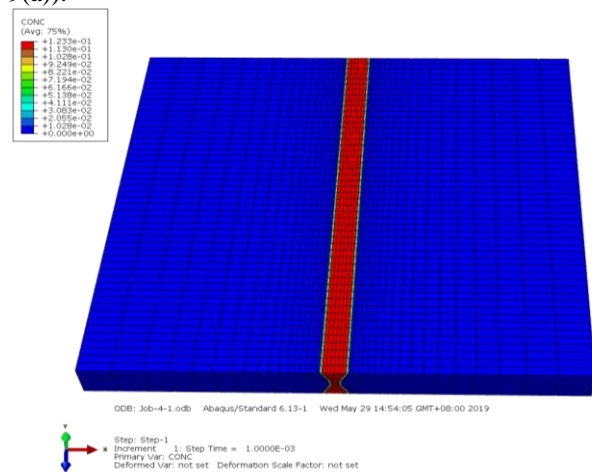

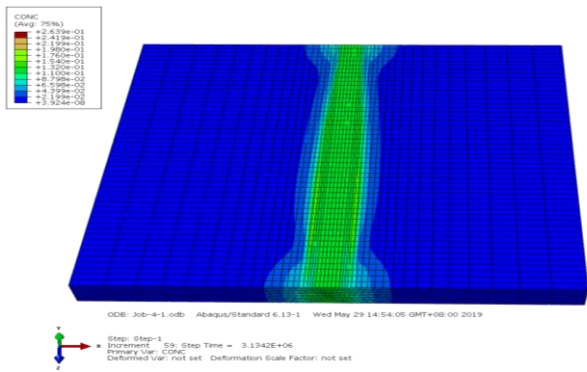**Fig. 11.** Hydrogen concentration before diffusion.

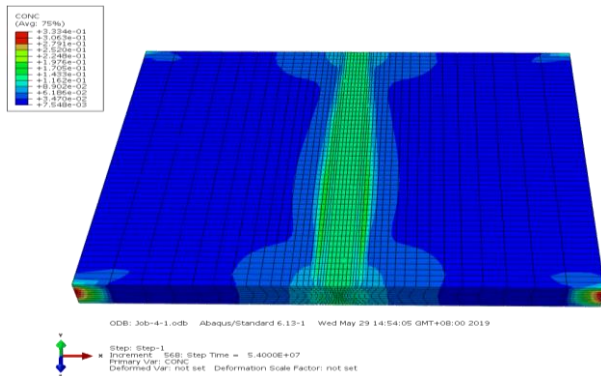**Fig. 12.** Hydrogen concentration during diffusion.

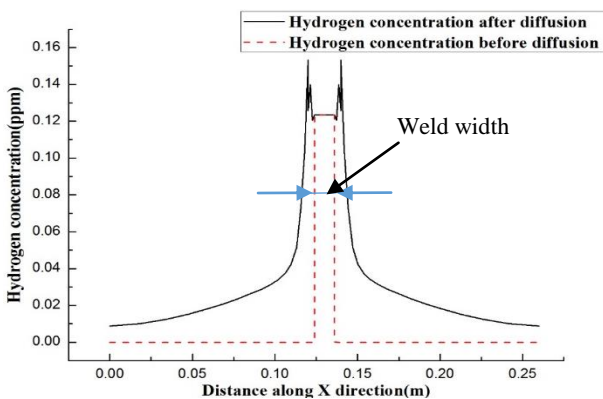**Fig. 13.** Hydrogen concentration after diffusion.

Fig. 14. Hydrogen concentration before and after diffusion along path *L*.

As shown in Figs. 11 to 14, the hydrogen before diffusion is mainly concentrated at the weld and the concentration is 0.1233 ppm. The concentration of hydrogen after diffusion reached the highest in the heat affected zone, with a maximum of 0.1532 ppm.

The results in Fig. 10 (e), Fig. 13, and Fig. 14 show that under the action of residual stress, hydrogen is concentrated in the high stress region, and after a period of time, it is stabilized. The distribution law of hydrogen concentration is basically consistent with the residual stress distribution law. And the hydrogen concentration is higher in the region with higher tensile stress. Far away from the weld and heat affected zone, the diffusive hydrogen concentration is gradually reduced. In the heat-affected zone, the tensile stress is the largest and the concentration of diffusive hydrogen is the highest.

It can be seen from the above analysis that due to the existence of welding residual stress, hydrogen will be diffused and aggregated into the weld and the heat affected zone, so that the hydrogen concentration in the weld and the heat affected zone is too high. Therefore, in the subsequent research, the area will be focused on, because this area is easy to produce hydrogen-induced cracking and threatens the safety and reliability of ship use.

V. CONCLUSIONS

In this paper, hydrogen diffusion under the residual stress of X-groove flat butt welded joints of in high-strength steel was analyzed, and the following main conclusions are listed.

(1) The welding residual stresses in the weld and the heat-affected zone are larger, with the maximum value approaching the yield strength of the material, and the level of the residual stress decreases rapidly as the distance from the weld increases.

(2) Hydrogen diffuses and accumulates in the high stress zone under the effect of welding residual stress. The final maximum hydrogen concentration appears in the heat-affected zone which coincides with the maximum level of residual stress. Therefore, hydrogen-induced cracking can easily occur in this area, adversely affecting the safety and reliability of the welded structure.

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