Research on the Effect of Alloy Elements on the A_1 Critical Transition Temperature of P91 Heat-resistant Steel Based on JMat Pro Software

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Abstract. The A_1 critical transition temperatures (Hereinafter referred to as A_1) of P91 heat resistant steels (Hereinafter referred to as P91) with different alloy elements were simulated by the continuous cooling simulation method of JMat Pro (JMP) software, and the statistical analysis tool of the JMP was used to analyze the simulation results, and the effects of the content of alloy elements Cr, C, Mo, Mn, Ni, V on the A_1 of P91 were studied. Obtained results indicated that the A_1 of P91 decreases firstly and then increases with the increasing of the content of Cr and Mo, the content of Cr has a great effect on the A_1 of P91, the effect of the content of Mo is almost negligible; when the content of Cr is 8.8wt%, the A_1 of P91 has the minimum 814 ℃; the A_1 of P91 decreases almost linearly as the content of Mn increases, when the content of Mn increases from the minimum to the maximum, the A_1 of P91 is reduced by about 7℃; the A_1 of P91 increases firstly and then decreases as the content of Ni increases, and when the content of Ni is 0.2 wt%, the A_1 of P91 has the maximum 815℃; the A_1 of P91 decreases firstly and then increases with the increasing of the content of V, it has the minimum 814℃ when the content of V is 0.2wt%.

Introduction

The P91 is a new kind of 9Cr-1Mo Markov heat-resistant steel developed by Oak Ridge National Laboratory of America. It has much lower thermal expansion coefficient, lower stress corrosion cracking sensitivity and higher thermal conductivity than austenitic heat-resistant steel, which is the ideal material for manufacturing the main stream pipe of ultra-supercritical boiler, super-heater and header [1,2]. It should be high-temperature tempered after welding. A higher heat treatment temperature of high temperature tempering must be chosen due to its high tempering resistance as well as reducing the heat treatment time in engineering. But, if the heat treatment temperature is higher than the A1 of P9, tempered structure is not all the tempered marten site structure. Therefore, it is necessary to investigate the effect of alloy elements on the A_1 of P91 [3,4].

JMat Pro(JMP) software is the simulation software with a powerful function for simulating the properties of metal materials, developed by the Sente Software Company in the UK. It has the functions including steady state and the metastable state phase equilibrium calculation, solidification process simulation, calculation on the physical properties of materials, it can provide the property parameters of materials for computer aided Engineering (CAE) software in molding materials. It can also be used to aid the researchers to resign the alloys and material processing technology including casting, forging and extrusion. Therefore, it can supply important reference direction and design basis for experiment design; much experimental time and cost can be saved [5,6]. In this work, the JMP was used to investigate the effect of the main alloy elements of Cr, Mo, Mn, Ni, V on the A1 of the P91.

Computing Model for Thermodynamics

To get the $A_1$of P91, one must know the critical temperature of ferrite by simulating the equilibrium

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phase transition of ferrite and austenite. Firstly, the Gibbs free energy relationship of each equilibrium phase in the goal system must be build up; the mole Gibbs free energy of any phase at the constant pressure is the function of element and temperature, as the Eq.1:

$$G_m = \sum_{i=1}^{c} x_i G_i^0 + RT \sum_{i=1}^{c} x_i \ln x_i + G_m^E \quad (1)$$

Where, the first item of the Eq.1 is the mole Gibbs free energy of each constituent element of the phase, x_i is the mole fraction, G_i^0 is the standard Gibbs free energy of constituent element i; the second item is contribution of ideal mixing entropy to free energy, which is the contribution of the entropy; the third item G_m^E is excess Gibbs free energy, and indicates the degree that the solution deviates from the ideal solution and can be calculated using different solution models[7].

The Thermo-Calc software can obtain interaction coefficients between the elements in the real system through fitting contrastively the data simulated by different mathematical models and the experimental data. As long as knowing the temperature of the system (T), pressure (P) and composition (X), you can calculate the free energy of combination system by every possible generated phase through the model mentioned above (Eq.1). At the constant temperature and constant pressure system, it is the basic criterion of phase equilibrium system that the total Gibbs free energy is minimum. That is:

$$G_{system} = \sum_{\emptyset=\alpha}^{\varphi} n^{\emptyset} G^{\emptyset} = \text{Min} \quad (2)$$

Where G_{system} is the total free energy of the system; $\emptyset$ is the phase, $\emptyset = \alpha, \beta, \gamma \ldots$; $G^{\emptyset}$, $n^{\emptyset}$ represents the mole Gibbs free energy and mole content of the $\emptyset$ phase, respectively. Then, the expression of describing the relationship between the Gibbs free energy of ferrite (α) and austenite (γ) phases of the system at different temperatures Gibbs free energy and the composition change is obtained. Secondly, the equilibrium phase composition at the different temperature based on the Eq.2 by the method of the computer simulation is calculated by computer simulation. At last, the critical temperature of A_1 of P91 comes out.

The Experimental Methods

The experimental material in this work is P91. The chemical compositions of P91 specified in ASTM A355 are shown in the Table 1.

Table 1 The chemical composition of P91 steel specified in ASTM A355 (wt%)

Element	C	Mn	Si	Cr	Mo	V	Nb	N	Ni	P	S
Min	0.06	0.30	0.20	8.00	0.85	0.15	0.06	0.03	-	-	-
Max	0.12	0.60	0.5	9.50	1.05	0.25	0.10	0.07	0.4	0.02	0.01

The P91 with different alloy elements including Cr, Mo, Mn, Ni, V was designed by the experimental design method based on thermodynamic simulation (Design of, Experiment, DOE,). The content of the alloy elements is in the specified range of the ASTM A355. The A_1 of P91 with different alloy elements was calculated by the thermodynamics software JMP. The relationship between the content of the alloy element and the A_1 of P91 was analyzed by the statistical analysis tool of JMP. The expression of describing the relationship between the content of alloy element and the A_1 of P91 was obtained by the least-squares method.

Results and Discussion

The Effect of the Cr on the A_1 Of P91. The effect of the Cr on the A1 of P91 was shown in Fig.1.

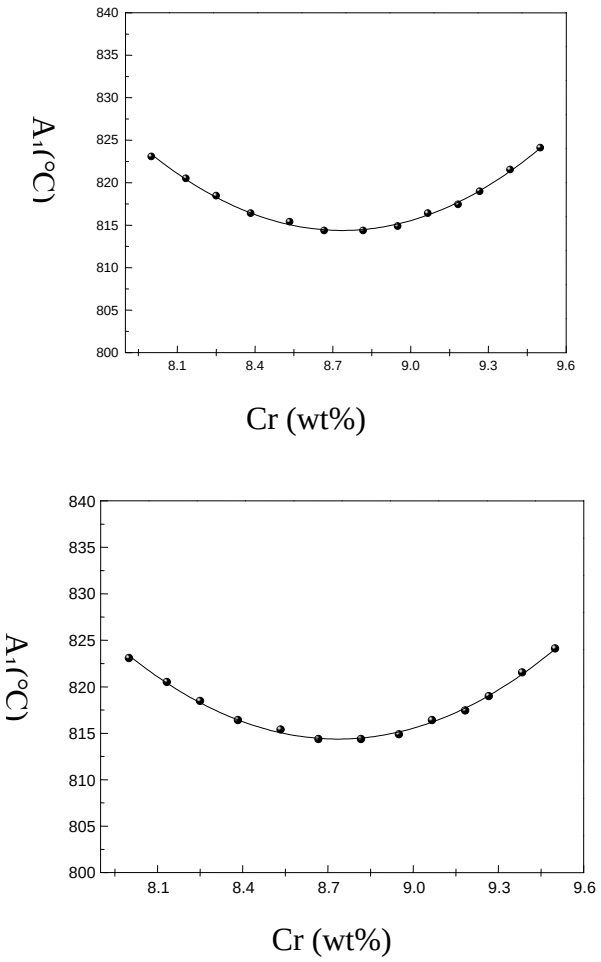

Fig.1 The effect of alloy element Cr on A_1 of P91 steel

It can be seen from Fig.1 that the A_1 of P91 decreases firstly and increases with increasing of the content of the Cr with the filling fraction in the range of 8.0~9.5wt%. when the content of the Cr is 8.8 wt%, the A_1 has the minimum 814℃; when it is 9.5wt%, the A_1 has the maximum 824℃. To describe the relationship between the content of the Cr and the A_1 of P91, the A_1 and the content of the Cr were fitted by the method of the least-squares method. The fitting result is as following:

$$A_1=2080-289.8Cr+16.6Cr^2 \quad (3)$$

The Effect of the Mo on the A_1 of P91. Fig.2 showed the effect of the Mo on the A_1 of P91.

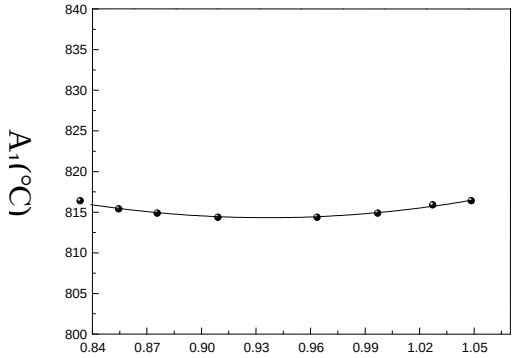

Fig.2 The effect of Mo on A_1 of P91

From Fig.2, one can see that A_1 of P91 decreases slowly and then increases as the content of the Mo increases with the content in the range from 0.85 to 1.05wt%. but the difference of the

maximum and the minimum of A_1 is 2℃. That is to say, the effect of the Mo on the A_1 of P91 is negligible.

The Effect of the Mn on the A_1 of P91. The effect of the Mn on the A_1 of P91 was shown in Fig.3.

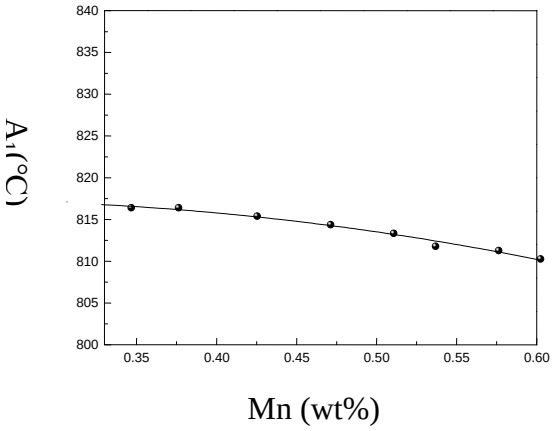

Fig.3 The effect of Mn on A_1 of P91 steel

The Fig.3 shows that the A_1 of P91 increases linearly with the increasing of the content of the Mn, when the content of the Mn ranges from 0.3 to 0.6wt%. The difference of the maximum and the minimum of the A1 of P91 is 7℃. to describe the relationship between the content of the Mn and the A_1 of P91, the A_1 and the content of the Mn were fitted by the method of the least-squares method. The fitting result is as following:

$$A_1=814.7+23Mn-50.8Mn^2 \quad (4)$$

The Effect of the Ni on the A_1 of P91. Fig.4 showed the effect of the Ni on the A_1 of P91.

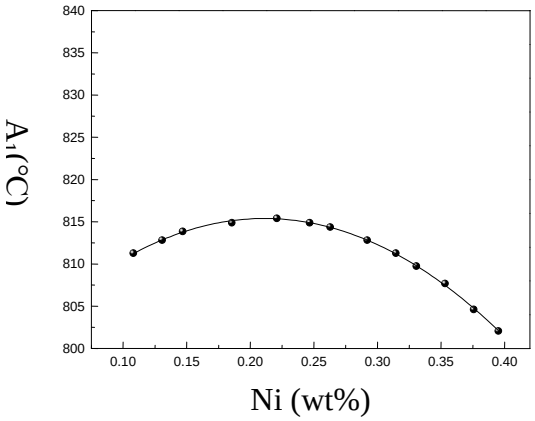

Fig.4 The effect of Ni on A_1 of P91 steel

By investigating the Fig.4, one can find out that the A_1 of P91 increases firstly and then decreases as the content of the Ni increases. The A_1 of P91 steel has the maximum 815℃ at the content of 0.2wt%,which has the minimum 802℃ as the content of the Ni is 0.4wt%. to describe the relationship between the content of the Ni and the A_1 of P91, the A_1 of P91 and the content of the Ni were fitted by the method of the least-squares method. The fitting result is shown in Eq.5:

$$A_1=798+165.6Ni-392.1Ni^2 \quad (5)$$

The Effect of the V on the A_1 of P91. The effect of content of the V on the A_1 of P91 was shown in Fig.5.

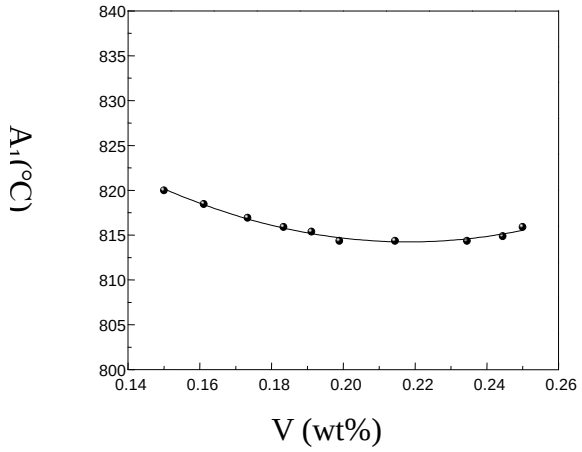

Fig.5 The effect of V on A_1 of P91

It can be seen from Fig.5 that the A_1 of P91 decreases firstly and increases with the increasing content of the V with the content in a range from 0.15 to 0.25wt%. the A_1 of P91 has the minimum 814℃ when the content of V is 0.2wt%, which has the maximum 820℃ when the content of the V is 0.15wt%. The expression of describing the relationship between the content of V and the A_1 of P91 is following:

$$A_1=875-557.3V+1277.3v^2 \quad (6)$$

Conclusions

A_1 of P91 decreases firstly and increases then with the increasing of content of Cr and Mo, the Cr has higher effect on the A_1 of P91. The A_1 of P91 has the minimum when the content of Cr is 8.8wt%; the effect of Mo on the A_1 of P91 is negligible. The A_1 of P91 decreases linearly as the content of Mn increases, the difference between the maximum and the minimum of the A_1 of P91 is 7℃. The A_1 of P91 increases firstly and decreases with the increasing of content of Ni, which has the maximum 815℃ when the content of Ni is 0.2wt%. The A_1 of P91 decreases firstly and increases as the content of V increases, which has the minimum 814℃ when the content of V is 0.2wt%.

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