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Effect of alloying elements on the concentration of atomic pairs in the ferrite

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Abstract

Ecobalance of heat resistant ferritic steels can be improved by the minimum alloying through saving energy and mineral resource. In the present study, the optimum ferrite compositions was sought through maximizing M-C atomic pair concentrations which control the long term creep strength of ferritic steels. The proposed alloy composition is the Fe-0.0017at%C-1.0at%Mn-1.6at%Ni-0.01at%Mo. The creep rupture life of the alloy is estimated to be 260000h at 88MPa/773K from the previously reported regression equation.

1. INTRODUCTION

For metallic materials, reduction of alloying elements is desirable from view points of saving energy and mineral resource. One of present authors[1] has suggested the possibility of the minimum alloying from the analysis of NRIM Creep Data Sheets for ferritic steels where the long term creep strength depends mainly on the minutes contents of Mo and C. Furthermore, the present authors[2] have found a good correlation between the long term creep strength of carbon steels and the concentrations of Mn-C and Mo-C atomic pairs. These atomic pairs seem to reduce the climb velocity of dislocations due to their large interaction energies with dislocations, suggesting that the long term creep strength of ferritic steels is controlled by these atomic pairs.

Thus, the target of the present study is to seek the optimum ferrite compositions by examining effects of alloying elements on the concentrations of these atomic pairs.

2.CALCULATION OF THE CONCENTRATIONS OF ALLOYING ELEMENTS

The equilibrium concentration of solute elements and atomic pairs in the ferrite matrix for Fe-C-M (M=Mn, Mo, and Cr) systems were estimated by thermodynamic calculations with the sublattice model (Thermo-Calc[3]) and the central atoms model[4] (CAM), respectively. Effect of quaternary additions (Mo, Ni, Si, and Cr) on the concentrations of various atomic pairs was also examined for the alloy which has the maximum concentration of the atomic pairs among the three ternary alloys. Wagner interaction parameter between i and j atoms, ε_{ij}, used in the calculation of the concentration of M-C atomic pairs is given by

$$\varepsilon_{ij} = \left. \frac{\partial \ln \gamma_i}{\partial x_j} \right|_{x_{Fe} \to 1} \qquad (1)$$

where γ_i is an activity coefficient of i atom, x_i is the mole fraction of j atom in the ferrite matrix. The Wagner interaction parameters were calculated by the Thermo-Calc in which related thermodynamic parameters are optimized with experimental data[5,6,7,8].

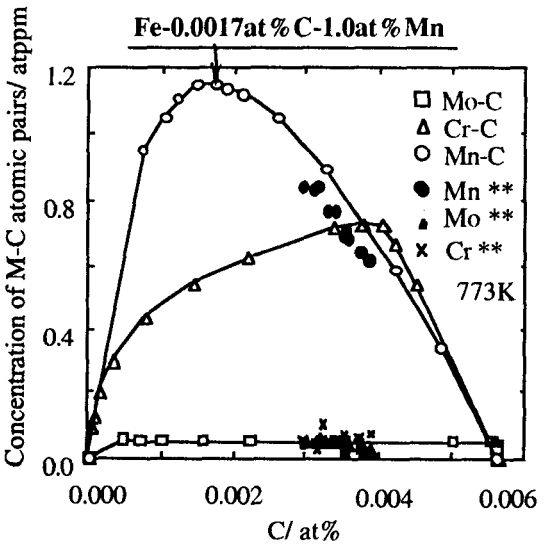

Fig.1 Concentrations of the M-C atomic pairs (M=Mn, Mo and Cr) at the ferrite/carbide phase boundary.
**Alloys in NRIM creep data sheet

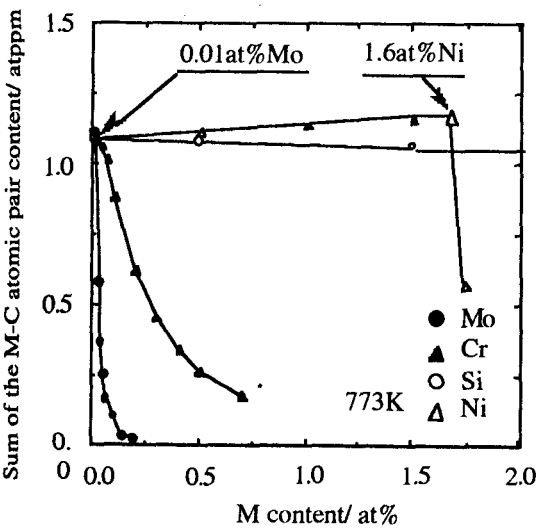

Fig.2 Effect of quaternary addition to the Fe-0.0017at%C-1.0at%Mn alloy on sum of the concentration of M-C. atomic pairs.

3.RESULTS AND DISCUSSION

Figure 1 shows concentrations of M-C atomic pair (M=Mn, Mo, and Cr) calculated at ferrite/carbide phase boundary for the Fe-C-M ternary systems at 773K. The maximum atomic pair concentration (1.10atppm) is obtained in the Fe-0.0017at%C-1.0at%Mn alloy. In this figure, the concentration of the atomic pair is also calculated for 0.2, and 0.3 carbon steels in NRIM creep data sheets[9,10] and plotted in fig.1. As shown in this figure, the concentration of the atomic pairs of these alloys is smaller than the maximum value in the ternary systems, suggesting that the long term creep strength of these alloys can be improved by the optimization of alloying elements.

Furthermore, in order to improve the long term creep strength, effect of the quaternary additions on the atomic pair concentration in the Fe-0.0017at%C-1.0at%Mn alloy was examined by the thermodynamic calculations (fig.2). Additions of Mo up to 0.01at%, and Ni up to 1.6at% showed slight increases in the amount of atomic pairs while an addition of Cr showed decreases in them. Addition of Si makes no changes in the concentration of atomic pairs. Then, for the Fe-C-Mn system added with 1.6at%Ni and 0.01at%Mo, the concentration of the atomic pairs was calculated for the ferrite compositions at the ferrite/carbide phase boundaries at 773K. The result is compared with the concentrations of the atomic pairs in the

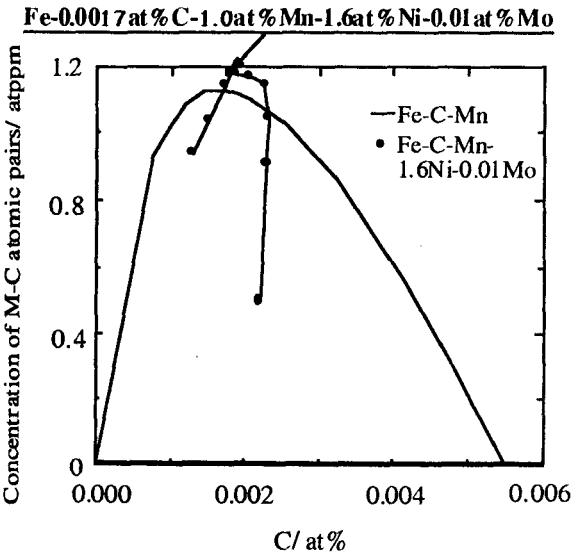

Fig.3 Effect of Ni and Mo addition on the sum of the M-C atomic pairs at the ferrite/carbide phase boundary.

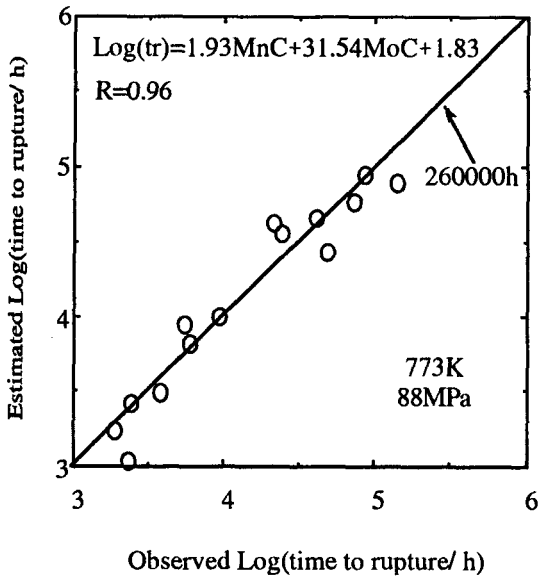

Fig.4 Correlation between estimated values by the regression equation and observed values. The closed circle shows the time to rupture for the alloy designed in the present study.

Fe-C-Mn ternary system in Fig.3. The maximum value of the total concentration of the atomic pairs was obtained in the Fe-0.0017at%C-1.0at%Mn-1.6at%Ni-0.01at%Mo alloy.

The creep rupture life of this alloy was estimated to be 260000h at 88MPa/773K from the regression equation as shown in fig.4.

4. CONCLUSION

The effect of the alloying elements on the atomic pair concentration at the ferrite/carbide phase boundary was studied by the thermodynamic calculations with the Thermo-Calc and CAM. The main results obtained can be summarized as follows.

1) Among three ternary systems, Fe-C-Mn, Fe-C-Mo, and Fe-C-Cr, the maximum concentration of the M-C atomic pair of 1.10atppm was obtained in the Fe-0.0017at%C-1.0at%Mn alloy.

2) The quaternary additions of Mo up to 0.01at% and Ni up to 1.6at% showed slight increases in the concentration of the M-C atomic pairs in the Fe-0.0017at%C-1.0at%Mn.

3) The maximum value of total concentrations of the M-C atomic pairs, 1.20atppm, was obtained in the Fe-0.0017at%C-1.0at%Mn-1.6at%Ni-0.01at%Mo alloy.

4) The creep rupture life of the alloy was estimated to be 260000h at 88MPa/773K from the previously reported regression equation.

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