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著者(和文)	LeeDosung
Author(English)	Dosung Lee
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Thesis outline

Lee Dosung

Formation behavior of C14 Laves phase under the interdiffusion of solute elements in the αFe phase

Ferritic stainless steels have been received attention for the high temperature application such as automobile exhaust manifolds and interconnect of solid oxide fuel cells. The challenging issue which I am interested in is the high temperature long-term durability regarding mechanical properties and oxidation resistance. In the ferritic stainless steels, Nb and Mo are important alloying elements mainly for the solid solution hardening. At high temperatures, these solute elements induce the precipitation of intermetallic compound (IMC) phase in the αFe matrix. Our research group has conducted a systematic research project in the Fe-Cr-Nb-Mo quaternary model alloy system to understand microstructure changes according to the IMC precipitates such as C14 Laves phase, χ, μ, and σ phases in the temperature range between 973 and 1173K under the various different heat treatment conditions as well as the oxidation conditions. All microstructure change involves atomic diffusion.

In Chapter 1, General background, motivation, problem assessment, and strategy of the present doctoral thesis research is explained. The two-fold objective of the present doctoral thesis research regarding the diffusion is stated as well. One is to quantitatively evaluate interdiffusion coefficients in the Fe-Cr-Mo and Fe-Cr-Si ternary systems as the fundamental database using the Boltzmann-Matano based Whittle-Green method. The other is to understand the formation mechanism of C14 Laves phase at the diffusion couple interface of αFe/Nb and αFe/Mo under the interdiffusion.

In Chapter 2, The both Fe-Cr-Nb and Fe-Cr-Mo ternary systems are the important subsystems from the quaternary model alloy system, however, the solubility of Nb in αFe is restricted too low to apply the Boltzmann-Matano based method. Thus, the Fe-Cr-Mo ternary system is centered to determine the interdiffusion coefficients of solute elements in the αFe. The main interdiffusion coefficients, $\widetilde{D}_{CrCr}^{Fe}$, $\widetilde{D}_{MoMo}^{Fe}$, and cross interdiffusion coefficients, $\widetilde{D}_{CrMo}^{Fe}$, $\widetilde{D}_{MoCr}^{Fe}$, in the αFe phase are determined at 1073K by diffusion couple technique and Boltzmann-Matano based analysis. It is revealed that the diffusivity of Mo is higher than Cr in the αFe in the Fe-Cr-Mo ternary system and the both cross interdiffusion coefficients have positive sings so that Cr and Mo have accelerating effect with each other on diffusion in the αFe, as calculating the average values,. Additionally, composition dependence and temperature dependence of interdiffusion coefficients were discussed.

In Chapter 3, since Si affects the precipitation of IMC phase and oxidation as reported in our research group, the Fe-Cr-Si ternary system is subjected to determine the interdiffusion coefficients as well. The main interdiffusion coefficients, $\widetilde{D}_{CrCr}^{Fe}$, $\widetilde{D}_{SiSi}^{Fe}$, and cross interdiffusion coefficients $\widetilde{D}_{CrSi}^{Fe}$, $\widetilde{D}_{SiCr}^{Fe}$, in the αFe phase are determined at 1073K. As a result, it was revealed that the diffusivity of Si is higher than Cr in the αFe. The average value of

$\widetilde{D}_{CrCr}^{Fe}$ in the Fe-Cr-Si ternary system was larger than that in the Fe-Cr-Mo system at 1073 K. The both cross interdiffusion coefficients have negative signs so that Cr and Si have suppressing effect with each other on diffusion in the αFe as calculating the average values.

In Chapter 4, the formation mechanism of C14 Laves phase Fe_2Nb was examined under the interdiffusion at the αFe/Nb interface. Diffusion couple of αFe/Nb was used to observe and to analyze microstructure, i.e. the process of phase layer formation, starting from non-equilibrium toward equilibrium state. The preformation of metastable phases is required to form the Fe_2Nb phase under the non-equilibrium condition as to help complete the diffusion path connecting between αFe and Nb since these elements have a quite low solubility with each other. The preformed metastable phases are η Fe_2Nb_3, FCC (face centered cubic) Nb, and FCT (face centered tetragonal) Nb. Additionally, the effect of Cr on the formation of C14 Laves phase was examined at the Fe-20Cr(αFe)/Nb (at.%) diffusion couple interface. It was revealed that Cr has a suppressing effect on the formation of C14 Laves phase compared to the binary αFe/Nb diffusion couple.

In Chapter 5, the formation mechanism of C14 Laves phase Fe_2Mo was examined under the interdiffusion at the αFe/Mo interface was examined. The preformation of metastable FCT Mo and stable μ phase Fe_7Mo_6 is required to form the Fe_2Mo phase. The Fe_2Mo forms at the αFe/μ interface. To understand the competitive effect of Nb and Mo, the formation of C14 Laves phase at the αFe/50Nb50Mo (at.%) diffusion couple interface was examined. The ternary C14 Laves phase Fe_2(Nb,Mo) forms at the interface between αFe and Nb-rich metastable layer. It was revealed that the diffusion of Nb is the controlling factor for the formation of C14 Laves phase.

In Chapter 6, the main results and findings obtained in the present doctoral thesis from chapter 2 through chapter 5 were summarized. The quantitative evaluation of interdiffusion coefficients can be utilized as a database which would have chance to contribute to the theoretical calculation and materials informatics. Understanding of the formation mechanism of C14 Laves phase at the diffusion couple interface not only includes important scientific findings but also enables more accurate precipitation control. Consequently, all these achievements would lead to the establishment of the new material design concept for ferritic stainless steels as the final goal.