§2. Diffusion Model of the Er₂O₃ Coating Process for Liquid Blanket Application

Muroga, T., Tanaka, T., Zhang, D. (Grad. Univ. Advanced Studies)

Previous studies by the authors showed that hydrogen permeation reduction factor (PRF) of Er_2O_3 coating on ferritic steels by Metal Organic Decomposition (MOD) depends on the Cr level of the substrate steels and the annealing conditions. The reason of the dependence was attributed to the composition of the oxide layer formed beneath the coating. The PRF was shown to be larger when Cr_2O_3 layer was formed than when Fe_2O_3 layer was formed. This paper reports further investigation of the effect of temperature and oxygen partial pressure of the annealing on the composition of the oxide layer. A diffusion modeling of Cr and O was performed to account for the experimental data.

The experimental procedure was explained elsewhere [1]. In this study, the temperature and the oxygen partial pressure during the annealing were systematically changed by controlling Ar/air ratio of the flowing gas. After fabrication of the coating, composition of the oxide layer beneath the coating was analyzed by XPS depth profiles including peak-shift analysis.

Fig. 1 summarizes the results. Both for JLF-1 and SUS430 substrates, Cr_2O_3 layer was formed at higher temperature and with lower partial pressure of O_2 . In the case of SUS430 substrate, Cr_2O_3 layer was formed at much lower temperature and higher partial pressure of O_2 than that of JLF-1. Expected boundaries of Fe₂O₃ and Cr_2O_3 layer formation for JLF-1 and SUS430 substrates are drawn by broken lines in the figure. This map would be valuable as a guide to avoid formation of Fe₂O₃ layer.

Fig. 2 illustrates the model employed in this study for Cr diffusion in substrate during the annealing when a Cr_2O_3 layer is formed. The growth of Cr_2O_3 layer takes place when balanced influx of oxygen anion from the oxide layer, J_{Ox} , and Cr cation from the substrate, J_{Cr} , took place at the interface between the Cr_2O_3 layer and the substrate by inner diffusion.

The formation of Cr_2O_3 layer needs both the chromium cation diffusion from the substrate and supply of oxygen anions at the Er_2O_3 coating/substrate interface. Figure 3 shows summary of the J_{Cr} and the oxide compositions. Broken lines show $J_{Cr}t^{1/2}$ calculated using a set of diffusion equations. The symbols on the broken lines show compositions of oxide layers formed by annealing in (a) air and (b) Ar, respectively, after Fig. 1.

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In summary, a diffusion model analysis showed that the data can be explained assuming that Cr_2O_3 layer is formed when supply of Cr exceeds that of O at the substrate surface.

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Fig. 1 The dependence of oxide composition on temperature and atmospheric partial pressure of oxygen during the annealing for JLF-1 and SUS430 substrates. Expected conditional boundaries for Cr₂O₃ and Fe₂O₃ layer formation for JLF-1 and SUS430 substrates are shown in broken lines.







Fig. 3 Temperature dependence of J_{Cr} normalized by multiplying $t^{1/2}$, shown by broken lines for (a) annealed in air and (b) annealed in Ar. The oxide composition data obtained by the experiments are indicated. The solid lines shows conditional boundaries for Fe₂O₃ and Cr₂O₃ layer formation common to JLF-1 and SUS 430 substrates.