# Modeling of High Temperature Oxidation Behavior of FeCrAl Alloy by using Artificial Neural Network

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## 1. Introduction

After Fukushima accident in 2011, the development of new material for cladding of light water reactors has been intensively investigated to prevent steam oxidation and to increase mechanical properties of cladding in high-temperature conditions. Variety concepts have been suggested, including iron-chromium-aluminum (FeCrAl) alloys [1], silicon carbide (SiC) [2], and coating method for conventional zirconium-base alloys.

Refractory alloys are candidate materials for replacing current zirconium-base cladding of light water reactors and they retain significant creep resistance and mechanical strength at high temperatures up to 1500 ℃ due to their high melting temperature. Thermal neutron cross sections of refractory metals are higher than that of zirconium, however the loss of neutron can be overcome by reducing cladding thickness which can be facilitated with enhanced mechanical properties. However, most refractory metals show the poor oxidation resistance at a high temperature. For instance, volatilization of molybdenum trioxide $MoO_3$ at a temperature above 700 ℃ causes a material loss in synthetic air conditions (20 % of $O_2$ and 80 % of Ar) and water vapor conditions [3]. MoSiB alloys, which has a good high temperature oxidation resistance at a temperature above 1000 ℃ [4], were developed. However, their low fracture toughness caused by intermetallic phase is a big obstacle for applying MoSiB alloys as a cladding material of nuclear reactors. [5] Therefore, another alloying element needs to be investigated for the high temperature oxidation resistance of refractory alloys.

For the designing of new alloys, prediction of properties based on the statistical data can be an effective tool. In general, properties change along the composition of alloying elements might show nonlinear behavior and there might be interconnected effects between each element. As a nonlinear regression tool, artificial neural network was utilized, which is able to give a great modeling of the complex oxidation behavior of alloys. Among many kinds of neural network methods, the Bayesian neural network, modified by Mackay [6] and Neal [7], was used because it has an advantage in terms of accurate prediction with a small number of training samples.

Before selecting new alloying elements of refractory alloys, confirming applicability of the artificial neural network for the modeling of high temperature oxidation behavior of cladding material needs to be investigated. In order to confirm this, oxidation behaviors of FeCrAl alloys at high temperatures were modeled by using Bayesian neural network in advance. FeCrAl alloy is also one of the promising materials for the replacing current zirconium-base cladding. Effects of Cr and Al compositions in this alloy on the high temperature oxidation behavior were studied.

## 2. Review of FeCrAl alloys

Iron-base alloys have been continuously developed to improve their poor resistance to high temperature oxidation. Although stainless steels, which were used for the cladding material of an early type of nuclear reactor, shows comparatively good oxidation resistant at room temperature and normal operation of nuclear reactor by forming thin protective chromium oxide on the surface of alloys, it has poor oxidation resistance at a high temperature condition such as loss of coolant accident (LOCA). Therefore, investigation of new alloying elements to give high temperature oxidation resistant to the stainless still was essential.

FeCrAl alloy has strong resistance to the high temperature oxidation. At a relatively low (500 ~ 600 ℃) temperature, an oxide layer is formed which is composed of mainly chromium and aluminum. Aluminum oxide layer has a role of continuous and dense protective layer when exposed to high temperature conditions. Oxidation behavior of six different aluminum concentrations in the range of 1.2-5.0 wt% in FeCrAl alloys was investigated [8]. For the continuous aluminum oxide layer, at least 3.2 wt% of Aluminum was needed. The addition of yttrium was studied which is able to promote adhesion strength of the oxide scale on the surface of the metal [8]. Alloys with 0.1 wt% of yttrium shows much enhanced oxidation resistance behavior than alloys without yttrium. Table 1 represents the composition of several FeCrAl alloys.

Table 1. Composition of several FeCrAl alloys [8-10]

| | *1Cr13A14* | *0Cr25A15* | *0Cr23A15* | *0Cr21A14* |
|---|---|---|---|---|
| Cr [wt%] | 12.0-14.0 | 23.0-26.0 | 22.5-24.5 | 18.0-21.0 |
| Al [wt%] | 4.0-6.0 | 4.5-6.5 | 4.2-5.0 | 3.0-4.2 |
| Fe [wt%] | Rest | Rest | Rest | Rest |

## 3. Neural network modeling

Database of oxidation behavior based on the composition of each element will be sample data for modeling by using artificial neural network. A schematics diagram of the neural network is shown in Figure 1. The architecture of the neural network is composed of an input layer, a hidden layer with a undetermined number of nodes, and one output layers.

$$h_h = tanh\left(\sum_{i=1}^{I} x_i W_{ih} + b_h\right) \quad (1)$$

$$y(x) = \sum_{h=1}^{H} h_h V_h + b_0 \quad (2)$$

$W_{ih}$ and $V_h$ are weight factors from the input layer to hidden layer and from hidden layer to output layer. $b_h$ and $b_0$ are the biases of the hidden and output layer. At first, these values are set randomly. By comparing between real oxidation behavior of alloys of sample data and the output value y(x) of the neural network, each weighting factor and bias will be updated to the direction of better prediction. During neural network modeling, over-fitting should be avoided which is a phenomenon that modeling focuses on the detail noise not the tendency of training sample. To overcome this problem, Bayesian neural network which was modified by Mackay [6] and Neal [7] can be one of the best solution. In Bayesian neural network, each weighting factor and bias are not specific values but they are probability distribution of values. This flexibility can give a chance to avoid over-fitting problem in modeling and to obtain excellent prediction with a small number of training samples.

Radford Neal's [11] program will be used in prediction of oxidation behavior of alloys. To figure out which number of hidden node shows the best performance of prediction, neural networks which have from 2 to 30 number of hidden nodes will be tried to make modeling. Automatic relevance determination (ARD) which is built in function of Neal's program will be applied to figure out which components in alloy give a great influence on the oxidation resistance of alloys.

Several sets of different compositions of chromium and aluminum in FeCrAl alloys and followed oxidation behavior will be training samples of neural network.

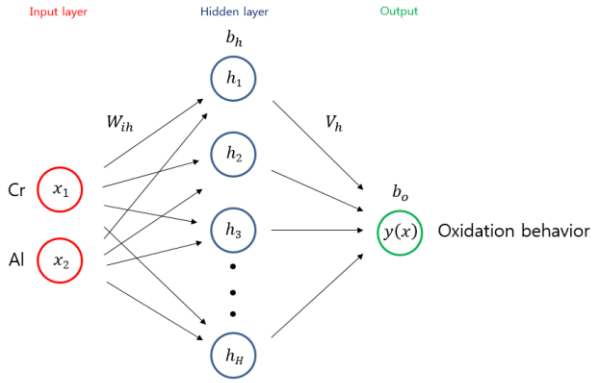


Figure 1. Schematics of neural network architecture

## 4. Conclusions

Oxidation behaviors of the various compositions of FeCrAl alloys in high temperature conditions were modeled by using Bayesian neural network. The automatic relevance determination (ARD) technique represented the influence of the composition of alloying elements on the oxidation resistance of FeCrAl alloys. This model can be utilized to understand the tendency of oxidation behavior along the composition of each element and prove the applicability of neural network modeling for the development of new cladding material of light water reactors.

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