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Artificial neural network modeling of phase volume fraction of Ti alloy under isothermal and non-isothermal hot forging conditions

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Abstract

An artificial neural network (ANN) model was applied to simulate the phase volume fraction of titanium alloy under isothermal and non-isothermal hot forging condition. For isothermal hot forging process, equilibrium phase volume fraction at specific temperature was predicted. For this purpose, chemical composition of six alloy elements (i.e. Al, V, Fe, O, N, and C) and specimen temperature were chosen as input parameter. After that, phase volume fraction under non-isothermal condition was simulated again. Input parameters consist of initial phase volume fraction, equilibrium phase volume fraction at specific temperature, cooling rate, and temperature. The ANN model was coupled with the FE simulation in order to predict the variation of phase volume fraction during non-isothermal forging. Ti-6Al-4V alloy was forged under isothermal and non-isothermal condition and then, the resulting microstructures were compared with simulated data.

Keywords: Artificial neural network; Ti alloy; Phase volume fraction; Forging

1. Introduction

Ti-alloys are widely used in many industries due to their attractive combination of properties like low density, excellent strength to weight ratio and superior corrosion resistance. The main phases of titanium alloys are well known as alpha (HCP) and beta (BCC) phases [1]. The properties of Ti-alloys significantly depend on the type of phase present and its volume fraction, and consequently determine the application of the alloys [2]. For example, the phase volume fraction between alpha and beta phases has great influence on the high temperature deformation behaviour of Ti-alloys because the flow stress and ductility of alpha and beta phases are very different to each other. Thus, hot workability can be improved via controlling alpha/beta phase volume fraction.

Hence, it is very important to know the thermodynamics and kinetics of the phase transformation as well as the prediction of phase volume fraction. The thermodynamics of the phase transformation in binary and ternary titanium alloys is generally well studied and known [3]. However, at present there is no comprehensive knowledge on the kinetics of the phase transformation for various titanium alloys at different temperatures. It is because there are so many controlling factors such as chemical composition (Al, V, Fe, O, C, N, and etc) and temperature and so on. Especially, phase transformation phenomena during hot forging of Ti-alloys and its prediction have never been reported. Unfortunately, it is very difficult to develop models to predict or estimate the amount of phase volume fraction. The reason is that the relationships among the controlling factors and ther-

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modynamics of the phase transformation are very complex and nonlinear. An alternative approach is based on an artificial-neural-network (ANN) methodology. It comprises a mathematical model/algorithm that emulates certain aspects of information processing and the knowledge gathering methods of the human nervous system [4, 5]. The objective of the present work is to demonstrate the applicability of the ANN method for the prediction of the alpha, beta phase volume fraction during isothermal and non-isothermal condition. For this purpose, the ANN model was implemented into FE simulation to predict the distribution of phase volume fraction of hot forged product.

2. Artificial neural network

The collection of suitable database describing the pertinent phase equilibria and kinetics of the phase transformation was made and then ANN codes were implemented. The ANN codes were consisted of two parts; first one is for the phase volume fraction change under isothermal condition and second one is for non-equilibrium state. Established ANN models were applied into FE code (DEFORM-3D) to predict the phase volume fraction.

Table 1. Input data (alloy composition in weight percent and heat treatment temperature) and output (beta-phase volume percent) used for equilibrium phase volume fraction.

Alloy Code	Al (I_1)	V (I_2)	Fe (I_3)	O (I_4)	N (I_5)	C (I_6)	Heat-Treatment Temperatures (°C, I_7)	Respective Beta Volume Percent	Reference
1	5.72	4.04	0.15	0.08	0.005	0.03	725, 763, 802, 834, 850, 889, 913, 932, 949, 969, 973	18, 22, 27, 34, 38, 51, 61, 70, 79, 91, 94	6
2	6.20	4.1	0.18	0.17	0.02	0.02	603, 699, 800, 851, 901, 951, 983	12, 12, 15, 23, 38, 66, 98	7
3	6.10	4.1	0.03	0.24	0.01	0.02	622, 736, 850, 901, 949, 983, 992	10, 11, 21, 32, 48, 78, 98	7
4	6.10	4.1	0.08	0.3	0.01	0.03	631, 724, 850, 901, 950, 994, 1001	8, 9, 18, 28, 44, 76, 97	7
5	6.56	4.44	0.1	0.046	0.01	0.046	875, 900, 925	27, 38, 50	8
6	6.20	5	0.1	0.135	0.01	0.03	750, 800, 850, 900, 950	15, 21, 31, 56,78	9
7	6.18	4.37	0.115	0.085	0.003	0.03	775, 825, 875, 895, 925, 940	16, 20, 33, 47, 70, 71	10
8	5.92	4.2	0.534	0.087	0.003	0.03	825, 875, 895, 925, 940, 975	25, 40, 58, 81, 81, 100	10
9	6.16	4.22	0.965	0.08	0.006	0.03	775, 825, 875, 895, 925, 940	42, 48, 59, 71, 86, 93	11
10	6.29	4.35	2.07	0.081	0.003	0.03	775, 825, 875, 895, 925, 940, 975	52, 55, 67, 86, 100, 100, 100	11
11	5.88	4.35	3.04	0.084	0.004	0.03	775, 825, 875, 895, 925, 940, 975	64, 65, 72, 91, 100, 100, 100	11
12	6.40	4.2	0.14	0.19	0.005	0.016	739, 810, 851, 899, 924, 953, 983, 1000	21, 25, 33, 46, 56, 69, 84, 94	12
13	6.34	4	0.19	0.17	0.01	0.03	700, 750, 800, 850, 875, 905, 930, 955, 980, 990, 996	12, 13, 17, 24, 31, 49, 58, 72, 89, 97, 100	10
14	8.10	0	0	0.06	0	0.06	1025, 1030, 1035, 1040, 1045, 1050	88, 90, 94, 95, 97, 100	13
15	7.60	0	0	0.03	0	0.12	1050, 1100, 1150, 1200	82, 87, 92, 100	13
A	7	1.5	0.01	0.15	0.01	0.03	600, 650, 700, 750, 800, 850, 900, 950	0, 0, 0, 0, 0, 0, 0, 0	Present work
B	6.85	1.6	0.13	0.17	0.01	0.03	650, 700, 750, 815, 900	3, 4, 5, 6, 9	
C	6.19	4.05	0.19	0.12	0.01	0.03	650, 700, 750, 815, 900	25, 26, 29, 37, 55	
D	6.3	4.1	0.21	0.168	0.005	0.03	700, 815, 900, 950	23, 34, 54, 80	
E	6.32	4.0	0.20	0.17	0.01	0.03	954, 982, 996	82, 95, 100	

2.1. Database collection

Present NN model requires for two kinds of dataset and they were collected from the published literature [6-13] as well as from own experimental results. Table 1 shows the dataset for the isothermal condition. Input parameters are chemical compositions (Al, V, Fe, C, O, and N) and quenching temperature of titanium alloys, and output parameter is the corresponding volume fraction of alpha and beta phases. The majority of the data sets used were for α+β Ti alloys and the remaining were near α and single phase α Ti alloys. Both the input and output variables were normalized within the range of 0.1 to 0.9. Fifteen data sets randomly chosen used for validation and 9 data sets of alloy C (Ti-6.19Al-4.05V-0.19Fe-0.12O-0.01N) and alloy D (Ti-6.3Al-4.1V-0.21Fe-0.168O-0.005N) were kept for testing. After the collection of database for equilibrium phase volume fraction at specific temperature, the effect of initial volume fraction before forging, hot forging temperature, and hot forging time on the variation of phase volume fraction were investigated. For this purpose, alloy E (Ti-6.32Al-4.0V-0.2Fe-0.03C-0.17O-0.01N) was heated to various temperatures (750°C~993°C) for 30 minutes and then, rapidly exposed to lower temperature for a certain time period (0~60 seconds) followed by water quenching. Table 2 shows measured phase volume fraction after experiments.

2.2. Model overview

Since feed-forward neural network (FFNN) with a back-propagation (BP) learning algorithm is most commonly used among the several training algorithms, the FFNN was employed in this work. The FFNN model consists of an input layer, an output layer, and one or two hidden layers. A detailed description of the back-propagation algorithm is summarized in detail elsewhere [4, 5]. The model training was started with two hidden layers with 2-15 hidden neurons in each layer. The minimum mean sum squared error (MSE) was set as 0.0001 and the number of iterations to be executed was set as 120000. Initially the learning rate and the momentum rate were taken as 0.25 and 0.9, respectively, for training. The numbers of hidden neurons are fixed for each model based on MSE and for all patterns, p, the global error function; MSE is given by:

$$MSE = \sum_p E_p = \frac{1}{p}\sum_p \sum_i (T_{ip} - O_{ip})^2 \quad (1)$$

where T_{ip} is the target output and O_{ip} is the predicted output for the i^{th} input neuron for the p^{th} pattern.

Based on MSE of the training the learning rate was selected for each model. The number of hidden neurons in the layer and the learning rate for each model was fixed. It was tried with varying momentum from 0.1 to 0.9 with the 0.05 steps. Based on MSE the momentum rate was selected. Finally, the optimum architecture achieved through the above procedure was chosen for predictions and analysis of phase transformation behaviour in Ti alloys.

3. Result analysis

3.1. ANN model for phase volume fraction change under isothermal forging

From the training and testing of ANN model, weight factors for the prediction of steady-state phase volume fraction were calculated. The formulations of the outputs are given by Eqs. (2)~(4), where W^1_{ij}, W^2_{ij}, W^3_{ij} mean weight factors between input layer and 1st hidden layer, 1st hidden layer and 2nd hidden layer, and 2nd hidden layer and output layer, respectively. Also, I_i and O_i indicate i^{th} input and output parameter, respectively.

$$N^1_i = \frac{1}{1+\exp^{-(W^1_{ij} \cdot I_j)}} \quad (2)$$

$$N^2_{ij} = \frac{1}{1+\exp^{-(W^2_{ij} \cdot N^1_j)}} \quad (3)$$

$$O^1_i = \frac{1}{1+\exp^{-(W^3_{ij} \cdot N^2_j)}} \quad (4)$$

Since the output parameters O^1_1 and O^1_2 are normalized values of beta and alpha phase volume fraction, they should be converted into original values by the following equations.

$$\text{Phase vol. fraction of alpha phase} = \frac{(O^1_2 - 0.1) \times (\text{Output}_{max} - \text{Output}_{min})}{0.8} + \text{Output}_{min} \quad (5)$$

$$\text{Phase vol. fraction of beta phase} = \frac{(O^1_1 - 0.1) \times (\text{Output}_{max} - \text{Output}_{min})}{0.8} + \text{Output}_{min} \quad (6)$$

where $Output_{max}$ and $Output_{min}$ denote maximum and minimum output values in Table 1. In order to verify the ANN model, the wing-shaped Ti alloy product (Ti-6.33Al-4.0V-0.2Fe-0.03C-0.017O-0.01N) sketched in Fig. 1 was isothermally hot forged using an 800 ton hydraulic press. To reduce die friction and prevent the sticking between the die and workpiece, boron nitride lubricant was spread out to Alloy 718 dies. The preforms were glazed before heating to minimize the formation of α-place during heating. In isothermal forging, die forging temperature was 850 °C and the forging speed was 2 mm/s.

The microstructure of isothermally forged component was observed and no surface defect was found. Also, the average α grain size in isothermal forged body was very similar to that in Ti-6Al-4V billet. This microstructure change during the forging processes were related closely to the plastic strain and temperature varying at different positions. In order to predict the volume fraction change of α and β phases, FE simulation was used to obtain temperature distribution of wing-panel product. The ANN model was implemented into a user-defined subroutine of a commercial FE code (DEFORM-3D). Friction coefficient and interface heat transfer coefficient were given as 0.3 and 5 kW/m^2°C. Using the chemical composition information and temperature distribution calculated in the FE simulation, contours of alpha phase volume fraction was calculated. Fig. 2 shows comparison of experimental data and ANN simulation results, and good agreement was found between them.

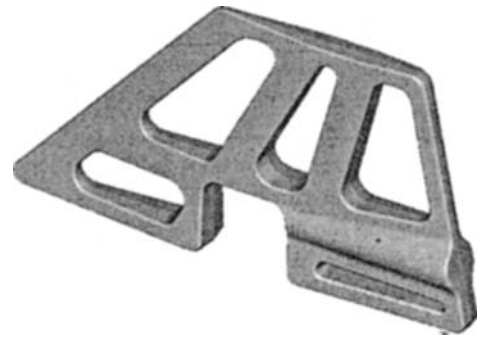

Fig. 1. Contours of volume fraction of alpha phase for isothermal forged Ti-alloy wing-panel: 'ANN' and 'Experiment' symbol indicate artificial neural network model and measured data, respectively. Number in circle indicates the location of modelling and measurement in wing-panel product.

Table 2. Samples for Input data (initial phase volume fraction, equil. phase volume fraction at exposed temperature, exposed temperature, soaking time) and output (beta-phase volume percent) used for non-equilibrium phase volume fraction. The entire tests were conducted using same Ti-6Al-4V alloy.

Test Code	Initial phase volume fraction	Equilibrium phase volume fraction at exposed temperature	Exposed temperature Temperatures (°C)	Soaking time(sec)	Respective Beta Volume Percent
1	86	67	650	0	14
2	86	67	650	25	15
3	72	62	850	0	28
4	72	62	850	25	38
5	80	62	850	5	28
6	80	62	850	0	20
7	77	62	850	3	28
8	77	62	850	0	23
9	69	24	959	2.4	61
10	69	24	959	0	31
11	87	44	886	5.3	31
12	87	44	886	0	13
13	10	37	936	3.7	87
14	10	83	805	3.7	86
15	10	37	936	0	90
16	10	83	805	0	90
17	0	2	993	0.4	99
18	9	72	866	1.6	93
19	0	85	750	55.8	15
20	0	69	850	55.3	31

3.2. *ANN model for phase volume fraction change under non-isothermal forging*

When applying the above ANN model to non-isothermal forging condition, calculated results exhibits significant deviation between prediction and measured data. Obviously, it is because the prediction of meta-stable phase volume fraction requires the consideration of the time dependent characteristics such as cooling speed and forging time. Thus, ANN model for non-isothermal forging was newly developed. Same approach mentioned in Section 4.1 was adopted again.

After training of weight factors, formulations for the phase volume fraction change under non-isothermal forging can be obtained in the similar form of Eqs. (2)~(4). Also, output parameter calculation follows similar method presented in Eqs. (2)~(6).

$$\text{Phase vol. fraction of alpha phase} = \frac{(O^2{}_2\text{-}0.1)\times(\text{Output}_{max}\text{-}\text{Output}_{min})}{0.8} + \text{Output}_{min} \quad (7)$$

$$\text{Phase vol. fraction of beta phase} = 100\text{–}(\text{Phase vol. fraction of alpha phase}) \quad (8)$$

In order to verify the model, non-isothermal hot-die forging was carried out with a forging speed of 2 mm/sec. The workpiece and die were heated to 970 °C and 650 °C, respectively. In simulation results for isothermal forging processes, strain and temperature contours at the die contact area are lower than those at other areas. It may due to die chilling effect. On the other hand, strain and temperature contours for isothermal forging process indicated a uniform distribution at all locations. In ANN model implemented into a FE simulation, two input parameters (initial phase volume fraction just before forging and equilibrium phase volume fraction at the temperature of finish forging) were calculated via ANN model subroutine for equilibrium phase volume fraction. And the other two parameters (temperature distribution and wasted time during hot forging) were obtained from FE simulation. Fig. 3 shows the comparison of ANN model results and measured data. Maximum deviation between them was about 5 % and such amount of disagreement seems to be reasonable.

Consequently, it is suggested that the microstructure simulation module is very useful for hot forming process design of Ti- alloy.

4. Conclusions

In this work, the microstructure evolution of Ti-6Al-4V alloy during the isothermal or non-isothermal forging processes was predicted by coupling method between artificial neural network model and FEM simulation. The comparison of the microstructure with the actual observation of the isothermally or non-isothermally forged Ti-6Al-4V alloy wing-

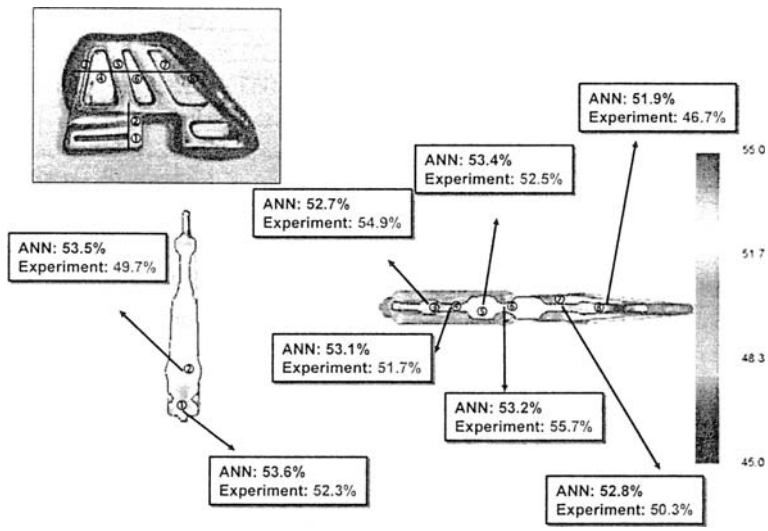

Fig. 2. Contours of volume fraction of alpha phase for non-isothermal forging: 'ANN' and 'Experiment' symbol indicate artificial neural network model and measured data, respectively. Number in circle indicates the location of modelling and measurement in wing-panel product.

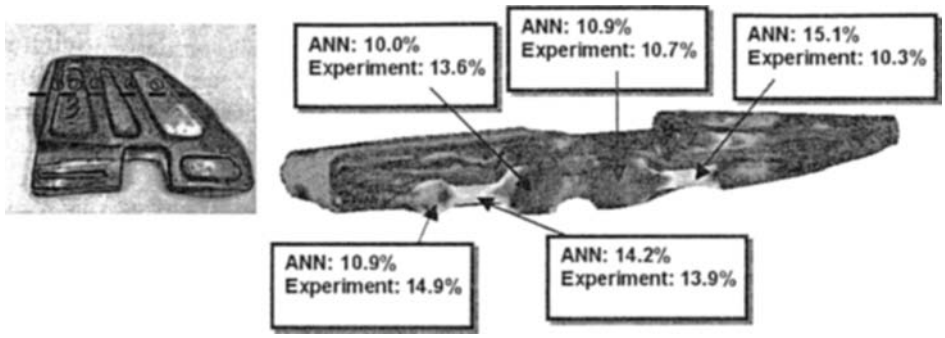

Fig. 3. Contours of volume fraction of alpha phase for non-isothermal forging: 'ANN' and 'Experiment' symbol indicate artificial neural network model and measured data, respectively. Number in circle indicates the location of modelling and measurement in wing-panel product.

panels has successfully validated the reliability of the present module for the prediction of the volume fraction.

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