Research Article

Effects of Temperature, Time, Magnesium, and Copper on the Wettability of Al/TiC System

Halil Ibrahim Kurt and Murat Oduncuoglu

Technical Sciences, University of Gaziantep, 27310 Gaziantep, Turkey

Correspondence should be addressed to Halil Ibrahim Kurt; hiakurt@gmail.com

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The effects of temperature, time, and the additions of magnesium and copper on the wetting behavior of Al/TiC are studied theoretically. Mathematical formula is presented in explicit form. The effect of each variable is investigated by using the obtained equation. It is observed that the time and temperature have a stronger effect on the wetting of TiC in comparison to other input parameters. The proposed model shows good agreement with test results and can be used to find the wetting behavior of Al/TiC. The findings led to a new insight of the wetting process of TiC.

1. Introduction

One of the most important phenomena is the wetting of ceramic particles by molten metals, when metal matrix nanocomposites (MMNCs) are produced. During the processing stages of MMNCs, the wetting behavior plays an important role in the evolution of the microstructure and mechanical properties [1]. Titanium carbide (TiC) is an attractive reinforcing phase because of high chemical and thermal stability, extremely high hardness, low density, high melting point, and low coefficient of thermal expansion [2].

Wettability studies usually include the measurement of contact angles, which indicates the degree of wetting when a solid and a liquid interact. While large contact angles ($>90^\circ$) correspond to low wettability, small contact angles ($<90^\circ$) correspond to high wettability [3]. The wetting of ceramic particles by molten metals usually includes interfacial reactions [4]. The transfer and distribution of the load from the matrix to the reinforcement come true with a strong interfacial bonding. The interface reaction is dependent not only on temperature but also on time, the composition of the liquid, the volume of the liquid drop, and the size of the reaction zone. A change in any of these parameters will result in a change in the wetting process [5]. For example, if the temperature, time, and composition of the molten metal are

changed, how does the wettability vary? Experimentally, this phenomenon is costly and time consuming. In many studies, the mathematical formulation is derived by researchers to reduce cost and save time [6–10].

The aim of this study is to investigate the effects of temperature, time, and chemical composition on the wettability of Al/TiC and to obtain an explicit formulation. For this purpose, the contact angles were formulated by using MATLAB program.

2. Experimental Procedures

An extensive literature survey is performed for available experimental results [11–14]. The experimental results are divided in two sets, train and test data sets. The data sets for train and test are randomly selected from among experimental results where 94 sets are train set and 40 sets are test set, as shown in Tables 1 and 2, respectively. The input variables are temperature (T), time, aluminum (Al), magnesium (Mg), and copper (Cu) and the output variable is the contact angle (θ). Each input variable is scaled to the range of 0 to 1 by the following formula:

$$x_N = \frac{x - x_{\min}}{x_{\max} - x_{\min}}, \quad (1)$$

TABLE 1: Train data set.

Number	T (°C)	Time (min.)	Al (wt.%)	Mg (wt.%)	Cu (wt.%)	θ
1	750	90	79,25	20,75	—	64
2	750	60	79,25	20,75	—	60
3	900	60	79,25	20,75	—	36
4	900	—	—	100	—	119
5	900	120	91,64	8,36	—	57
6	800	20	100	—	—	86
7	750	—	79,25	20,75	—	122
8	900	30	—	100	—	20
9	800	80	79,25	20,75	—	55
10	900	80	79,25	20,75	—	35
11	750	60	91,64	8,36	—	110
12	800	15	96	—	4	115
13	1000	15	96	—	4	78
14	800	15	92	—	8	113
15	750	40	98,91	1,09	—	123
16	800	15	99	—	1	93
17	900	60	100	—	—	58
18	800	150	79,25	20,75	—	50
19	900	10	—	100	—	41
20	800	40	91,64	8,36	—	90
21	900	40	95,86	4,14	—	61
22	750	80	98,91	1,09	—	122
23	900	15	67	—	33	85
24	800	15	80	—	20	103
25	1000	30	67	—	33	63
26	900	80	91,64	8,36	—	62
27	800	80	95,86	4,14	—	83
28	1000	30	80	—	20	69
29	1000	15	92	—	8	71
30	800	150	95,86	4,14	—	64
31	800	10	—	100	—	118
32	900	150	95,86	4,14	—	58
33	900	15	80	—	20	90
34	750	120	79,25	20,75	—	59
35	900	60	95,86	4,14	—	60
36	750	60	98,91	1,09	—	123
37	850	40	—	100	—	89
38	900	—	79,25	20,75	—	113
39	800	20	91,64	8,36	—	101
40	900	40	91,64	8,36	—	89
41	900	120	100	—	—	47
42	800	15	67	—	33	100
43	800	—	91,64	8,36	—	120
44	900	20	95,86	4,14	—	73
45	750	150	95,86	4,14	—	110
46	900	30	67	—	33	75
47	800	150	91,64	8,36	—	65

TABLE 1: Continued.

Number	T (°C)	Time (min.)	Al (wt.%)	Mg (wt.%)	Cu (wt.%)	θ
48	1000	15	80	—	20	88
49	900	20	79,25	20,75	—	42
50	800	—	—	100	—	121
51	800	40	95,86	4,14	—	114
52	800	150	98,91	1,09	—	41
53	800	60	95,86	4,14	—	97
54	900	—	91,64	8,36	—	117
55	750	150	79,25	20,75	—	56
56	800	30	96	—	4	110
57	750	60	95,86	4,14	—	115
58	800	20	98,91	1,09	—	83
59	900	150	79,25	20,75	—	31
60	900	30	96	—	4	90
61	800	30	92	—	8	103
62	850	30	—	100	—	91
63	800	30	—	100	—	107
64	800	60	79,25	20,75	—	58
65	900	15	96	—	4	100
66	900	15	99	—	1	80
67	800	30	99	—	1	81
68	900	80	95,86	4,14	—	60
69	850	10	—	100	—	101
70	900	30	99	—	1	72
71	1000	15	99	—	1	67
72	900	—	100	—	—	125
73	800	20	95,86	4,14	—	123
74	900	150	91,64	8,36	—	52
75	1000	30	96	—	4	61
76	750	120	91,64	8,36	—	87
77	800	20	79,25	20,75	—	77
78	750	20	79,25	20,75	—	98
79	750	—	98,91	1,09	—	127
80	750	30	91,64	8,36	—	120
81	900	15	92	—	8	102
82	800	120	79,25	20,75	—	52
83	900	30	80	—	20	78
84	800	120	95,86	4,14	—	76
85	900	150	100	—	—	45
86	800	40	—	100	—	100
87	750	80	95,86	4,14	—	114
88	800	150	100	—	—	55
89	900	30	92	—	8	86
90	800	60	100	—	—	78
91	900	—	95,86	4,14	—	118
92	800	—	95,86	4,14	—	130
93	800	120	100	—	—	57
94	750	150	91,64	8,36	—	82

TABLE 2: Test data set.

Number	T (°C)	Time (min.)	Al (wt.%)	Mg (wt.%)	Cu (wt.%)	θ
1	750	30	95,86	4,14	—	118
2	800	—	100	—	—	125
3	800	80	100	—	—	63
4	900	120	95,86	4,14	—	60
5	900	60	91,64	8,36	—	77
6	1000	30	99	—	1	57
7	750	—	95,86	4,14	—	120
8	900	20	98,91	1,09	—	70
9	800	—	98,91	1,09	—	120
10	900	20	91,64	8,36	—	98
11	800	—	79,25	20,75	—	136
12	750	120	98,91	1,09	—	121
13	800	120	98,91	1,09	—	44
14	900	80	98,91	1,09	—	50
15	750	120	95,86	4,14	—	114
16	900	60	98,91	1,09	—	55
17	900	80	100	—	—	52
18	900	—	98,91	1,09	—	120
19	800	40	98,91	1,09	—	67
20	800	40	79,25	20,75	—	64
21	800	80	91,64	8,36	—	77
22	900	40	79,25	20,75	—	38
23	800	60	91,64	8,36	—	80
24	800	30	67	—	33	88
25	750	150	98,91	1,09	—	120
26	900	120	79,25	20,75	—	32
27	800	30	80	—	20	93
28	900	40	98,91	1,09	—	58
29	1000	30	92	—	8	58
30	900	150	98,91	1,09	—	46
31	750	20	98,91	1,09	—	125
32	750	—	91,64	8,36	—	127
33	750	90	91,64	8,36	—	90
34	850	—	—	100	—	120
35	800	80	98,91	1,09	—	57
36	900	120	98,91	1,09	—	47
37	800	120	91,64	8,36	—	70
38	1000	15	67	—	33	82
39	900	20	100	—	—	72
40	800	60	98,91	1,09	—	60

where x_N is the normalized value of variable x and $x_{\max}$ and $x_{\min}$ are the maximum and minimum values of the variables, respectively.

Output values resulted from the model also in the range $[0, 1]$ and transformed to its equivalent values based

FIGURE 1: The model architecture.

on reverse method of normalization technique [15]. The unnormalized method is as

$$x = x_N (x_{\max} - x_{\min}) + x_{\min}. \quad (2)$$

MATLAB neural network (NN) toolbox is employed for the network training. Backpropagation (BP) learning algorithm with sigmoid function (Levenberg-Marquardt-Trainlm), the most popular and effective supervised learning method, is used for training stage [16, 17].

3. Results and Discussion

One of the most important duties in NN works is the determination of layer numbers and neurons in the hidden layers. There is no well-defined procedure to find the optimal parameter settings and network architecture. The trial and error approach is used to determine the number of neurons in the hidden layer. The various neuron numbers (5–15) and hidden layers (1 and 2) are used in this study. It is observed that the optimal NN architecture is found to be 5–7–1 NN architecture, as shown in Figure 1.

Figure 2 shows the correlation of NN and test data for train and test sets. R^2 values of train and test sets are 0.8311 and 0.8146, respectively. R^2 value compares the accuracy of the model and a high R^2 value ($R^2 = 1$) tells that all points lie exactly on the curve with no scatter and the result has a perfect correlation [18]. It is clear that all R^2 values are higher than 0.81 and the proposed model has high accuracy. In all stage of NN work, the effects of the temperature, time, and percent weights of Mg and Cu elements on the wetting behavior of Al/TiC are quantified. It is clear from Figure 2 that there are deviations between the experimental and theoretical results. It is normal that the deviations are observed in NN works. These can be attributed to the formation and

FIGURE 2: Correlation of NN and experimental results for (a) training set and (b) test set.

TABLE 3: Statistical parameters.

	R	MAE
Train	0.911	9.090
Test	0.903	10.205

FIGURE 3: Sensitivity of input vectors.

volume fraction of the oxides and variation in experimental conditions. It is well known that the wettability of ceramic surfaces by metals and alloys is affected by some parameters such as time, temperature, composition, volatilization of Mg, oxides (MgO , MgAl_2O_4 , Al_4C_3 , and Al_2O_3), and volume fraction of the oxides [11, 19]. It is difficult to estimate the effect of each parameter on the wettability and it needs extensive studies. Nevertheless, " R^2 ," shown in Figure 2, and " R ," shown in Table 3, values of training and test sets, indicate that the learning ability of NN is well enough.

Figure 3 demonstrates the sensitivity of input vectors on the wettability of Al/TiC system. The different methods are used in order to estimate the sensitivity analysis [20]. A sensitivity analysis is done using the system to identify the effects of input parameters and their degree of importance on the output parameter. The training data set are used to estimate the sensitivity. It is well known that increasing data used in training process of NN enhances the ability of NN. The basic idea of the analysis is that the input variables are shifted slightly and the corresponding change in the output

is reported as a percentage. So, the relationship between the inputs and outputs of the network is revealed. As mentioned before, wetting behavior is affected by some parameters such as time, temperature, composition, volatilization of Mg, oxides (MgO , MgAl_2O_4 , Al_4C_3 , and Al_2O_3), and volume fraction of the oxides. According to the done sensitivity analysis, it is observed that the time and temperature have a dominant effect on the wettability. In other words, any change in time and temperature in comparison to Mg and Cu levels will have significantly affected the wettability.

The performance of the model is evaluated by the correlation coefficient (R) as in the following expression [21]:

$$R = \frac{\text{cov}(t_i, \hat{t}_i)}{\sqrt{\text{var}(t_i) \cdot \text{var}(\hat{t}_i)}}. \quad (3)$$

Mean absolute error (MAE) is used as error evaluation criteria in order to facilitate the comparisons between predicted values and desired values according to the following equation:

$$\text{MAE} = \frac{1}{N} \sum_{i=1}^N |t_i - \hat{t}_i|, \quad (4)$$

where N is the total number of the data and t_i and $\hat{t}_i$ are the experimental value and predicted output values from NN model for a given input, respectively.

The statistical parameters of train and test data sets are shown in Table 3. The correlation coefficients and MAE in train and test sets are 0.911 and 0.903 and 9.090 and 10.205, respectively. A high R value means that the model has high accuracy. The proposed model is in good agreement with the experimental data and all the errors are within acceptable ranges.

3.1. Formulation of the Model. The main aim is to obtain the explicit formula of the wettability as a function of input variables. The contact angle (θ) is determined by using the formula

$$\theta = 116 * \left(\frac{1}{1 + e^{-v}} \right) + 20, \quad (5)$$

where

$$\begin{aligned} v = & (-5.413) * \left(\frac{1}{1 + e^{-u1}} \right) + (-5.039) * \left(\frac{1}{1 + e^{-u2}} \right) \\ & + (4.471) * \left(\frac{1}{1 + e^{-u3}} \right) + (5.617) * \left(\frac{1}{1 + e^{-u4}} \right) \\ & + (-3.187) * \left(\frac{1}{1 + e^{-u5}} \right) + (-5.171) \\ & * \left(\frac{1}{1 + e^{-u6}} \right) + (1.940) * \left(\frac{1}{1 + e^{-u7}} \right) + (3.251), \end{aligned} \quad (6)$$

where

$$\begin{aligned} u1 = & (12.860 * X1) + (-0.479 * X2) + (-2.663 * X3) \\ & + (4.828 * X5) + (2.791 * X6) + (3.189), \\ u2 = & (5.879 * X1) + (0.198 * X2) + (-3.548 * X3) \\ & + (-0.218 * X4) + (-2.365 * X5) \\ & + (-4.276), \\ u3 = & (1.076 * X1) + (1.848 * X2) + (-0.015 * X3) \\ & + (3.167 * X4) + (1.939 * X5) + (2.625), \\ u4 = & (-3.182 * X1) + (-6.709 * X2) + (-1.973 * X3) \\ & + (3.004 * X4) + (-1.407 * X5) + (0.792), \\ u5 = & (-2.754 * X1) + (11.393 * X2) + (3.637 * X3) \\ & + (-4.467 * X4) + (1.088 * X5) + (-1.209), \\ u6 = & (-0.053 * X1) + (-2.200 * X2) + (-4.219 * X3) \\ & + (6.404 * X4) + (-5.141 * X5) + (1.100), \\ u7 = & (-3.957 * X1) + (-4.811 * X2) + (3.341 * X3) \\ & + (-2.824 * X4) + (-0.321 * X5) + (0.639), \end{aligned} \quad (7)$$

where $X1$, $X2$, $X3$, $X4$, and $X5$ are normalized values of temperature, time, Al, Mg, and Cu (wt.%), respectively.

It should be noted that the explicit formulation is valid for the proposed ranges. The contact angles of Al, Mg, and Cu are 119, 125, and 130, respectively [22–24]. For example, by using the designed equation, it is calculated that the contact angle value of Al-1Mg-5Cu alloy at 1000°C and 60 minute is 44.5 ± 4 . It can be said that the wettability between TiC and Al matrix with Mg and Cu can be predicted by the advanced model with 90% accuracy.

4. Conclusion

In this work, the explicit mathematical formula is derived from NN model. The model has a high reliability rate and shows good agreement with experimental results. The mean absolute error for predicted values does not exceed 10.5%. The sensitivity analysis of the developed model demonstrated that the time and temperature are the significant variables in affecting the wettability. The results also showed that the

wetting of TiC by Al alloy with Mg and Cu can be predicted with 90% accuracy. Hence, it is concluded that the model is a successful and advantageous analytical tool for determining the wettability with considerable saving in cost and time.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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