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Application of artificial neural networks to predict the hardness of Ni–TiN nanocoatings fabricated by pulse electrodeposition

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ABSTRACT

A three-layer backward propagation (BP) model was used to predict the hardness of Ni–TiN nanocoatings fabricated by pulse electrodeposition. The effect of plating parameters, namely, TiN particle concentration, current density, pulse frequency, and duty ratio on the hardness of Ni–TiN nanocoatings was investigated. The morphology, structure, and hardness of Ni–TiN nanocoatings were verified using scanning electron microscopy, white-light interfering profilometry, high-resolution transmission emission microscopy, and Rockwell hardness testing. The results indicated that the surface roughness of the Ni–TiN nanocoating is approximately 0.12 μm. The average grain sizes of Ni and TiN on the Ni–TiN nanocoating are 62 and 30 nm, respectively. The optimum conditions for fabricating Ni–TiN nanocoatings based on the greatest hardness of Ni–TiN deposits are as follows: TiN particle concentration of 8 g/L, current density of 5 A/dm^2, pulse frequency of 80 Hz, and duty ratio of 0.7. We conclude that the BP model, with a maximum error of approximately 1.03%, can effectively predict the hardness of Ni–TiN nanocoatings.

1. Introduction

Pulse electrodeposition is a versatile process for depositing various protective metal and metal–ceramic coatings on metallic substrates [1–5]. Ma et al. [6] prepared the Ni–SiC composite thin films by direct current (DC) and ultrasonic pulse-current (UPC) deposition methods. The UPC Ni–SiC composite thin films presented a more compact and exiguous surface morphology, which possessed Ni and SiC grains with average diameters of 63.6 and 38.5 nm, respectively. Borkar and Harimkar [7] deposited carbon nanotube (CNT)-reinforced nickel coatings onto a stainless steel substrate using pulse electrodeposition by a nickel Watts bath. Sen et al. [8] obtained Ni–CeO_2 nanocomposite coatings employing pulse electrodeposition by a Watts-type electrolyte. Titanium nitride (TiN), a well-known metal nitride ceramic that possesses hardness as high as 21 GPa, has been widely employed as a secondary phase to improve the strength and toughness of a metal or ceramic substrate [9–11]. Pulse electrodeposition is a simple and inexpensive method for obtaining Ni–TiN coatings.

Significant attention has been focused on the morphology and performance of the formed parts, which are evidently affected by coating features during the process of pulse electrodeposition [12,13]. Coating properties such as hardness, strength, wear resistance, and corrosion resistance are influenced by processing parameters such as current density, particle concentration, on-duty ratio, stirring rate, pH value, and bath temperature. For instance, the hardness of the nanocomposite coating increased when the stirring rate was increased up to 450 rpm, after which the hardness decreased due to the agglomeration of the ceria particles in the nickel matrix [8].

Artificial neural networks (ANN) have been widely applied in mathematics, engineering, and science [14–16]. The most widely used ANN type to date is the backward propagation (BP) neural network, which is composed of simple artificial neurons that mimic some functional properties of a biological neural network when connected. An artificial neuron consists of analog inputs multiplied by weights. The neural output activation is computed by a mathematical threshold function over the weighted sum of the inputs. A typical structure of the artificial neuron is presented in Fig. 1. Successful usage of ANNs, which provides satisfactory results when compared to the experimental measurement, will significantly reduce the cost of experimental tests.

Despite many studies that have applied ANNs to material science [14–16], reports concerning their specific application to predicting the hardness of Ni–TiN coatings are limited. In this study, Ni–TiN nanocoatings were deposited on 45 steel substrates using pulse electrodeposition. The morphology and hardness of the Ni–TiN nanocoatings were characterized using scanning electron microscopy (SEM), white-light interfering profilometry (WLIP), high-resolution transmission electron microscopy (HRTEM), and Rockwell hardness testing. Moreover, experimental data were used to condition the networks. Our study aims to investigate the effect of plating parameters on the hardness of Ni–TiN nanocoatings produced by pulse electrodeposition and predict the hardness of Ni–TiN nanocoatings using an ANN.

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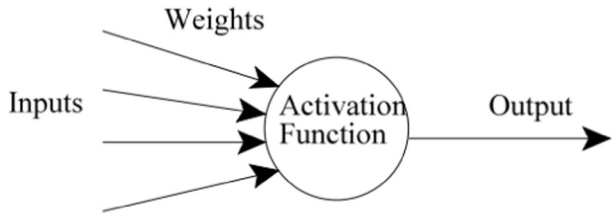

Fig. 1. An artificial neuron.

2. Experimental methods

2.1. Sample preparation

Ni–TiN coatings with thickness of approximately 70 μm were deposited on 30 mm × 20 mm × 5 mm 45 steel substrates by pulse electrodeposition. The 45 steel substrates are purchased from Anben Iron and Steel Group Corporation, which consist of 98.13% Fe, 0.42% C, 0.17% Si, 0.58% Mn, 0.25% Cr, 0.25% Ni, and 0.2% Cu. A schematic of a basic pulse electrodeposition cell is shown in Fig. 2. The 45 steel substrates were used as cathodes, and were mechanically polished with a 0.15 μm surface finish. A similar dimension of pure nickel (99.9%) plate (Baoji Gold Borui Industry Co., Ltd., Baoji Shaanxi, China) was used as the anodes. The composition of the electrolyte for obtaining electrodeposited Ni–TiN nanocoatings was as follows: 200 g/L nickel sulfate, 50 g/L nickel chloride, 25 g/L boric acid, and 2 g/L to 10 g/L TiN particles (approximately 30 nm). The plating solution temperature was kept at 45 °C and pH 5. The parameters for electrodepositing Ni–TiN nanocoatings are shown in Table 1.

2.2. Sample characterization

The thickness and the surface morphology of the coatings were observed using SEM (JSM-6460LV, JEOL Co., Ltd., Mitaka, Tokyo, Japan). The roughness of the Ni–TiN nanocoatings was quantified using a MicroXAM white light interferometer (KLA-Tencor Co., Ltd., Beaverton, Oregon, USA). The amplitude was characterized by the root-mean-square roughness parameter Rq, which was calculated as the standard deviation of the height of each point on the surface relative to the average value. For each sample, Rq over ten different regions with an area of 900 ± 10 μm × 700 ± 5 μm was measured, and the average value of Rq was calculated. The microstructure of the coatings was observed with a HRTEM (Tecnai-G2-20-S-Twin, FEI Co., Ltd., Columbia, Maryland, USA). Prior to HRTEM observation, the sample was mechanically polished to a 100 μm thickness, sequentially thinned to a 90 nm thickness by using an ion beam thinner, and rinsed with ethyl alcohol. The hardness of the Ni–TiN coating was determined using a standard microhardness tester (HVS–1000, Dongguan Pengzhan Electronic Instrument Co., Ltd., Dongguan Guangdong, China). The Vickers microhardness values were determined in certain intervals (5 mm) from the surface of the coating to the substrate, with a minimum of five measurements for each depth. The crystal structure of the Ni–TiN coating was determined by using X-ray diffraction (XRD, Philips D5000). Scans were recorded over the range of $2\theta = 20–100°$ at an operating target voltage of 40 kV and tube current of 100 mA with a scan step of 0.05°. Using the Scherrer equation, the average grain size could be calculated as follows:

$$D = \frac{180K\lambda}{\pi\sqrt{\beta^2 - \omega\cos\theta}} \tag{1}$$

where D is the diameter of the particles, K is the figure factor of the grains ($K = 0.89$), λ is the wavelength ($\lambda = 0.15418$ nm), β is the width of the diffraction peak at half height, θ is the Bragg angle, and ω is the standard full width at half maximum.

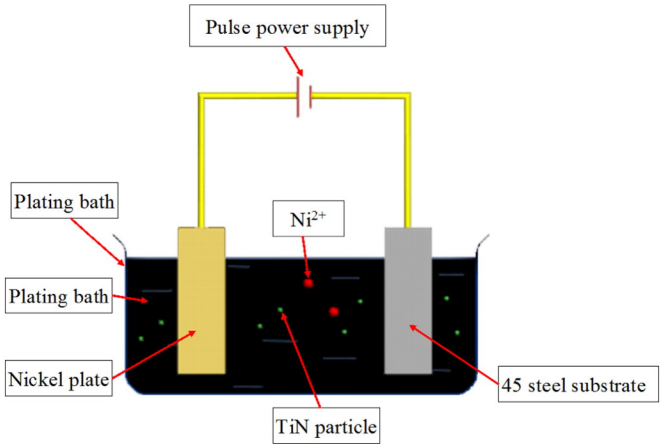

Fig. 2. Schematic of the pulse electrodeposition process.

Table 1
Plating parameters for preparing Ni–TiN nanocoatings.

Parameters	
TiN particle concentration (g/L)	8
Current density (A/dm^2)	5
Pulse frequency (Hz)	80
Duty ratio	0.6
Electroplating time (min)	90

2.3. Artificial neural networks and structure

In this paper, a three-layer BP model is used as the network model. Fig. 3 shows the framework of this model, which comprises input, hidden, and output layers. The basic unit in the network is the neuron; the neurons are connected with each other by weighting factors. TiN particle concentration (c), current density (i), pulse frequency (f), and duty ratio (t) are used as inputs, and the hardness is considered to be the final output of the neural network model. Inputs and outputs are normalized within the range of 0 to 1 [17]. The output y_i produced by neuron i, in layer L, is described as follows:

$$y_i = f\left(\sum_{j=1}^{n} W_{ij} + b\right) \tag{2}$$

where f is the activation function; n is the number of elements in the layer $L-1$; b is the offset or bias of the activation function; and W_{ij} is the weight associated with the connection between neuron i in layer L and neuron j in layer $L-1$, which has an output of w_i.

The error for the BP model is expressed by the following relationship:

$$Error = \frac{1}{NT}\sum_{m=1}^{T}\sum_{n=1}^{N}[x_i(m) - y_i(m)]^2 \tag{3}$$

where N is the number of outputs, T is the number of training sets, x_i is the desired output, and y_i is the network output.

3. Results and discussion

3.1. Microstructure analysis of Ni–TiN nanocoatings

A group of Ni–TiN nanocoating samples was produced at $c = 8$ g/L, $i = 5$ A/dm^2, $f = 80$ Hz, and $t = 0.6$, which are used to observe the microstructure. Fig. 4 shows the cross-sectional SEM image of a Ni–TiN