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Original Research Paper

Simulation of structural features on mechanochemical synthesis of Al_2O_3–TiB_2 nanocomposite by optimized artificial neural network

Ali Ghafari Nazari [a,*], Masoud Mozafari [b]

[a] Materials Engineering Department, Islamic Azad University, Southern Branch, Tehran, Iran
[b] Biomaterials Group, Faculty of Biomedical Engineering (Center of Excellence), Amirkabir University of Technology, P.O. Box 15875-4413, Tehran, Iran

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ABSTRACT

In this study, structural features of alumina–titanium diboride nanocomposite (Al_2O_3–TiB_2) were simulated from the mixture of titanium dioxide, boric acid and pure aluminum as raw materials via mechanochemical process using the optimized artificial neural network. The phase transformation and structural evolutions during the mechanochemical process were characterized using X-ray powder diffractometry (XRD). For better understanding the refining crystallite size and amorphization phenomena during the milling, XRD data were modeled and simulated by artificial neural network (ANN). An ANN consisting of three layers of neurons was trained using a back-propagation learning rule. Also, the ANN was optimized by Taguchi method. Additionally, the crystallite size, interplanar distance, amorphization degree and lattice strain were compared for the simulated values and experimental results.

1. Introduction

Titanium diboride (TiB_2) is an attractive combination of high Vickers hardness, electrical conductivity, excellent chemical resistance to molten nonferrous metals and relatively low specific gravity [1,2]. Owing to the fact that TiB_2 is mechanically poor, such as fracture toughness and impact strength, these properties are improved by making composite. Therefore, TiB_2–Al_2O_3 composite is useful for a variety of applications like cutting tools, wear-resistant substrates and lightweight armor [3–5]. Recently, mechanical activation and mechanical milling have been extensively implemented for preparing and synthesizing composite powders and advanced materials [6].

Mechanochemistry is concerned with the physical and chemical change of materials caused by mechanical energy. During the milling repeated welding and fracturing of powder particles increases the area of contact between the reactant powder particles due to a reduction in particle size and allow fresh surfaces to repeatedly come into contact; this causes the reaction to proceed without the necessary diffusion through the product layer which enhances the formation of new compounds, amorphization of the crystalline structures, phase transformation and formation of chemical reaction [7–9]. There is a complicated and non-linear relationship among the operational parameters such as time and speed of milling, ball-to-powder weight ratio (BPR), raw materials, number and diameter of balls, and atmosphere of milling on the properties of product [7].

X-ray diffractometry (XRD) is a powerful technique for characterizing solids which is widely applied in the identifying the crystalline solid phases and offers a unique advantage in the quantitative analysis of mixtures [10]. Every change in the operational parameters of mechanochemistry process has an influence on the XRD pattern of milling product. The experimental studies have been conducted to examine the effects of significant parameters on the mechanochemistry synthesis in TiB_2–Al_2O_3 nanocomposite. This research evaluated the feasibility of using artificial neural networks (ANN) in recognize peak-shaped signals in the analytical data. It was concluded that ANN is superior to conventional classifiers (e.g., multiple linear regressions) in classifying patterns in which the input is noisy and the system is not well defined. Besides, ANNs are non-linear estimators which can establish more sophisticated responses [11]. They can store large amounts of pattern information with relatively few neurons and connections [10]. For optimizing ANN, Taguchi method was used in which non-numerical parameters, such as kind of function, are optimized as the opposite of other statistical methods, like: response surface methodology or mixture design [12].

This paper tries to implement of optimized network (OANN) for modeling and predicting XRD patterns in producing Al_2O_3–TiB_2 nanocomposite by milling boric acid, titanium dioxide, and aluminum powders. The crystallite size, interplanar distance, amorph-

* Corresponding author. Tel.: +98 912 3383264; fax: +98 21 26550055.
E-mail address: alighafarinazari@yahoo.de (A.G. Nazari).

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