Computational Materials Science 155 (2018) 48–54

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Machine leaning aided study of sintered density in Cu-Al alloy

Zhenghua Deng[a], Haiqing Yin[a,b,*], Xue Jiang[a,b], Cong Zhang[a,b], Kaiqi Zhang[a], Tong Zhang[a], Bin Xu[a], Qingjun Zheng[c], Xuanhui Qu[a,b,d]

[a] Collaborative Innovation Center of Steel Technology, University of Science and Technology Beijing, Beijing 100083, PR China
[b] Beijing Advanced Innovation Center for Materials Genome Engineering, Beijing 100083, PR China
[c] Kennametal Inc, 1600 Technology Way, PA 15650, USA
[d] Institute for Advanced Materials and Technology, University of Science and Technology Beijing, Beijing 100083, PR China

ARTICLE INFO

Keywords:
Powder metallurgy
Sintered density
Machine learning
Multilayer perceptron
Cu-Al alloy

ABSTRACT

The mechanical properties of powder metallurgy (PM) materials are closely related to their density. In this case we demonstrate an approach of utilizing machine-learning algorithms trained on experimental data to predict the sintered density of PM materials. Descriptors were selected from the features including processing parameters, chemical composition, property of raw materials and so on. And the training data are collected by the experimental setup in our lab and the literatures on five kinds of P/M alloys. The multilayer perceptron model (MLP) outperformed other four regression and neutral network models with high coefficient of correlation and low error. The sintered density predicted by MLP model agreed well with the experimental data with a tolerable error less than 0.028, which confirms its capability over P/M materials design procedures. Then the obtained MLP model is used for Cu-9Al P/M alloy to guide selecting the processing parameters to reach the expected sintered density of 0.88. The Cu-9Al powders were fabricated with the predicted parameters including the specific shape factor, particle size, pressing pressure and sintering temperature, and the obtained relative sintered density is 0.885.

1. Introduction

Powder metallurgy (PM), with the descriptors of energy-efficient near-net forming and no (less) pollution, plays an irreplaceable role in the materials manufacturing [1,2]. The sintered density is one of the key factors that determine the mechanical properties of powder metallurgy parts [3]. An increase of the porosity from 0 to 5% decreases the tensile strength by 35% [4]. Ductility and resistance to fatigue show higher sensitivity to porosity [5]. At present, most of the sintered density prediction depends on the priori knowledge and trial and error experiments, which greatly decelerate the efficiency of new materials discovery.

Therefore, a more efficient method is urgently needed to predict the sintered density. The Materials Genome Initiative (MGI) [6] and Integrated Computational Materials Engineering [7] (ICME) are deemed to accelerating the materials design process. Xue et al. [8] discovered a new NiTi-based shape memory alloy with targeted transformation temperatures by Support Vector Regression method. Raccuglia [9] used support vector machine methods to predict the viability of untested reactions with experimental failed data collected in the lab and the accuracy of prediction is nearly 90%.

Machine learning methods have been used to predict the sintered density in recent years. Jabar et al. [10] used artificial neural network (ANN) to predict the sintered density of $BaTiO_3$ and the mean error is less than 0.06. Varol et al. [11] used ANN to predict the effect of reinforcement on density, hardness and tensile strength of B_4C_p/Al2024 composites, with the mean absolute percentage error (MAPE) obtained less than 2.15%. Canakci et al. [12] used ANN to predict green density, sintered density and hardness of Al_2O_3/Al metal matrix composites (MMCs) successfully with MAPE less than 5.53%. Azadbeh et al. [13] used response surface methodology models to predict the density, electrical resistivity and hardness of Cr–Mo prealloyed sintered steels, the predicted values agreed well with the experimental ones. The previous investigations, however, focused studies solely on single kind of material for prediction without taking into account of the raw material and the phase transformation, and didn't compare the prediction accuracy of different machine learning methods.

In the present work, machine learning algorithms were used to generate the models to estimate the sintered density of metal compacts by Powder metallurgy. And the obtained model is applied here to predict the sintered density Cu-9Al alloy as well as provide guidance for selection of processing parameters to reach the expected target.

* Corresponding author at: Collaborative Innovation Center of Steel Technology, University of Science and Technology Beijing, Beijing 100083, PR China.
E-mail address: hqyin@ustb.edu.cn (H. Yin).

https://doi.org/10.1016/j.commatsci.2018.07.049
Received 19 June 2018; Received in revised form 22 July 2018; Accepted 25 July 2018

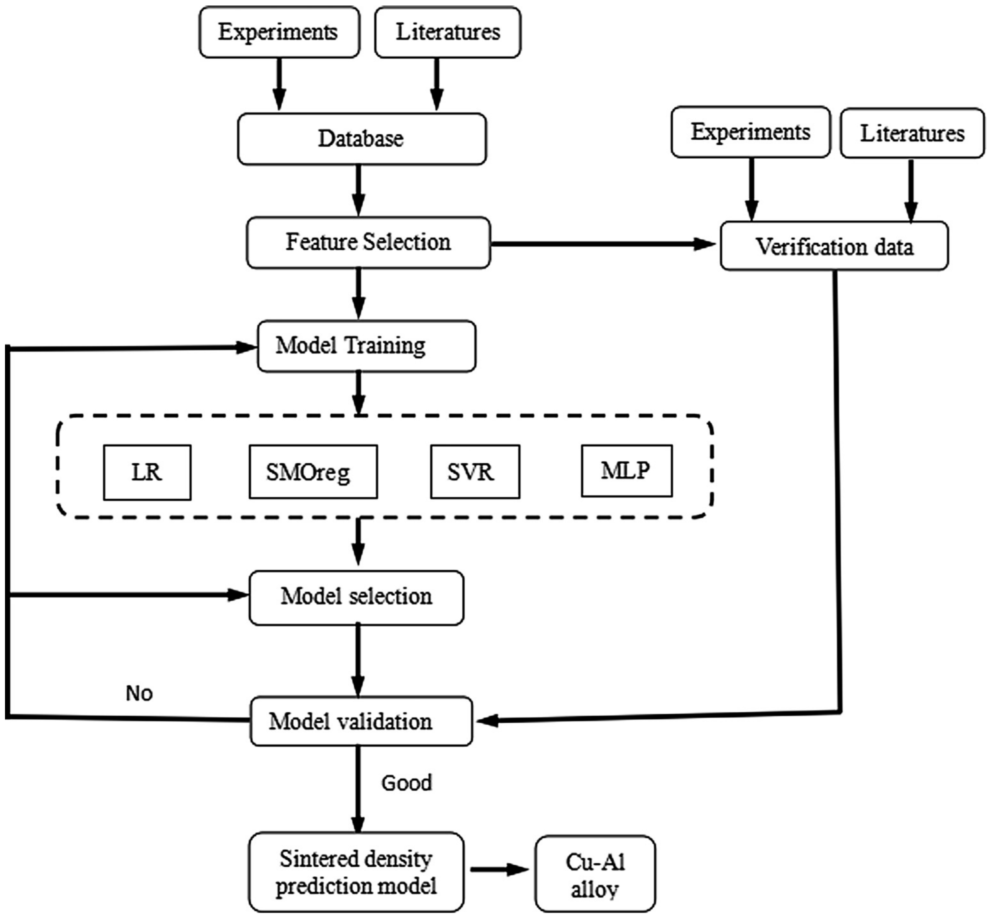

Fig. 1. Schematic Diagram of machine learning model generation and sintering density optimization.

2. Procedure of modeling

The feedback mechanism of the machine learning modeling and sintering optimization process are described in Fig. 1. Machine-learning models generated from experimental data are used to guide selection of processing parameters to reach the expected sintered density.

2.1. The database and descriptor selection

The data used in this work were collected by two means, one from the experiments in our laboratory and the other from literatures [14–22]. The dataset consists of 197 items of data from iron alloys, copper alloys, aluminum alloys, and molybdenum alloys, magnesium alloy, which is listed in Appendix 1.

The powder metallurgy generally consists of three basic steps: powder blending, die pressing, and sintering. As shown in Fig. 2, we choose the relevant descriptors as form the input of the statistical learning model depends on this process and literatures[23]. And the sintered density is the target value.

To further screen descriptors, the principal component analysis (PCA) was utilized, which achieved dimensionality reduction by select important principal components as new independent variables and discard some insignificant independent variables [24].

Through screening the descriptors, 14 descriptors are selected in the dataset. they are classified into three groups including material chemical composition, processing parameter and raw material, as shown in Table 1.

V is the volume fraction of each kind of powder, n represents the element of the materials, E is the Young's modulus of each element, HB is the hardness of each element, f/k is the specific shape factor of each

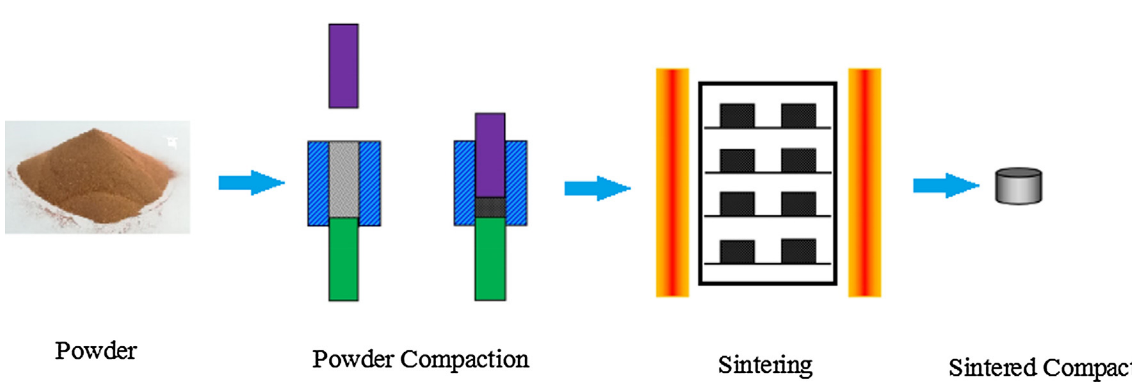

Fig. 2. Powder metallurgy production method.