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Modeling glass-forming ability of bulk metallic glasses using computational intelligent techniques

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ABSTRACT

Modeling the glass-forming ability (GFA) of bulk metallic glasses (BMGs) is one of the hot issues ever since bulk metallic glasses (BMGs) are discovered. It is very useful for the development of new BMGs for various engineering applications, if GFA criterion modeled precisely. In this paper, we have proposed support vector regression (SVR), artificial neural network (ANN), general regression neural network (GRNN), and multiple linear regression (MLR) based computational intelligent (CI) techniques that model the maximum section thickness (D_{max}) parameter for glass forming alloys. For this study, a reasonable large number of BMGs alloys are collected from the current literature of material science. CI models are developed using three thermal characteristics of glass forming alloys i.e., glass transition temperature (T_g), the onset crystallization temperature (T_x), and liquidus temperature (T_l). The R^2-values of GRNN, SVR, ANN, and MLR models are computed to be 0.5779, 0.5606, 0.4879, and 0.2611 for 349 BMGs alloys, respectively. We have investigated that GRNN model is performing better than SVR, ANN, and MLR models. The performance of proposed models is compared to the existing physical modeling and statistical modeling based techniques. In this study, we have investigated that proposed CI approaches are more accurate in modeling the experimental D_{max} than the conventional GFA criteria of BMGs alloys.

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1. Introduction

Due to the superior physical and chemical properties compared to their crystalline counterparts, bulk metallic glasses (BMGs) have attracted a lot of attention of the researchers and engineers. Owing to their excellent properties, BMGs find a number of important and exciting applications in sporting goods, jewelry, medical, surgical instruments, electronics, defense, and aerospace [1]. In the last two decades, different families of amorphous alloys with excellent glass forming ability have been presented in the literature. For example, La-, Zr-, Pd-, Mg-, Cu-, Fe-, Ti-, Pr-, Co-, Ca-, Y-, Au-, Hf- and Gd-based metallic glasses have shown superb glass-forming ability [2]. However, there exist no scientific rules or justified theories to design bulk metallic alloys with excellent GFA. To date, GFA is one of the hot issues ever since metallic glasses are discovered [3]. In the past few years, the glass-forming ability (GFA) of these alloy systems, which is often described in terms of maximum section thickness (D_{max}), has been increased from 1 mm to several centimeters. The accurate estimation of D_{max} highly depends on the fabrication conditions. The critical cooling rate (R_c) is another quantitative measure of GFA, which is the minimum cooling rate to get completely amorphous solid from melts. The larger GFA of alloys can be expected for the smaller R_c or higher D_{max}. In other words, the accurate values of D_{max} and R_c of each metallic glass could only be obtained after the fabrication of metallic glass through the laborious experimentation. Therefore, it is imperative to uncover a more effective criterion for evaluating the GFA of BMGs. In order to make BMGs cost effective for various engineering and industrial applications, it would be very useful if we could model D_{max} prior to its fabrication [4].

The scientist and engineers have proposed various physical and statistical modeling based approaches to predict GFA. They developed various GFA criteria using thermal parameters which highly effect the GFA of metallic glasses [2]. These criteria are mostly based on three thermal characteristics of glass forming alloys i.e., glass transition temperature T_g, the onset crystallization temperature T_x, and liquidus temperature T_l. These parameters can easily be determined from differential thermal analysis (DTA) and differential scanning calorimetry (DSC). These physical and statistical techniques model experimental D_{max} with

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thermal parameters/characteristics of the glass-forming alloys. For example, the reduced glass transition temperature $T_{rg} = T_g/T_l$ [5], the supercooled liquid range $\Delta T_x = T_x - T_g$ [6], $\gamma = T_x/(T_g + T_l)$ [7], $\gamma_m = (2T_x - T_g)/T_l$ [8], $\Delta T_{rg} = (T_x - T_g)/(T_l - T_g)$ [9], $\delta = T_x/(T_l - T_g)$ [10], $\Phi = T_{rg}(\Delta T_x/T_g)^{0.143}$ [11], $\alpha = T_x/T_l$ [12], $\beta = T_x/T_g + T_g/T_l$ [13], $\beta_1 = T_x \times T_g/(T_l - T_x)^2$, and $\omega = T_g/T_x - 2T_g/(T_g + T_l)$ [14]. However, due to the simple foundation of physical/statistical models [5–14], it is difficult to model D_{max} accurately for the synthesized glass-forming alloy. In fact, there exists a complex nonlinear relationship between the GFA and its thermal parameters. These models compromise on accuracy for correlating D_{max} of BMGs. Keeping in view this fact, there is ever increasing demand for the advanced computational intelligent (CI) techniques. We have employed these CI techniques to model the experimental D_{max} (instead of R_c) in terms of thermal parameters. Because the values of R_c are difficult to be measured. The measurement of R_c involve a series of continuous cooling experiments involving heat transfer calculations that makes it quite tedious and a costly job. On the other hand, the values of D_{max} can be measured easily. It is most widely used indicator of glass forming-ability of metallic glasses. We have prepared a dataset of thermal parameters of BMGs alloys along with D_{max} values from the literature of material science. CI techniques can model a complex function, like D_{max}, by selecting useful information from the input training alloys, and then predict D_{max} for novel alloys.

Previously, support vector regression (SVR), general regression neural network (GRNN), artificial neural network (ANN), and multiple linear regression (MLR) based CI techniques are used in predicting the lattice structure of perovskites compounds [15,16]. These techniques provide an efficient alternative in modeling material [17], monitoring structures [18], fabrication [19], chip designing [20], and vibration modeling [21]. For example, ANN based computing approach is tried to model undercooled liquid region of metallic glasses [4]. ANN approach is used to model the crystallization temperatures of Ni–P based amorphous alloys. Promising good results are obtained for the crystallization peak temperature [22]. The main advantage of CI techniques is that once an efficient model is built for training samples then they can be successfully used to predict the structure of novel samples. It is of practical interest to employ CI techniques in less resources/skill environment.

These techniques have gained much importance in predicting various structural properties of materials [15,16]. These approaches have ability to reduce the experimental and temporal cost. ANN based computational models are inspired from the functional aspects of the biological neural networks. Sometimes, ANN based models are trapped in local minima [16,22] and their performance may be degraded as compared to statistical learning theory based SVR models. SVR models use the Lagrange constraints optimization and Mercer theorem to extract useful information from input data [23,24]. Due to simplicity, GRNN approach can extract suitable information for developing regression model.

During model developing phase, the optimal parameters values are computed using the training data. Next, the developed model is used to predict D_{max} of novel glass alloys of the same family. The performance of CI models is reported in terms of percentage relative absolute difference (PAD) error and correlation coefficient R. GRNN model has revealed an excellent tendency in modeling the current GFA problem. The mean PAD errors are computed to be 1.971% and 3.681% for training and novel BMGs, respectively. However, SVR model has given the mean PAD errors of 2.700% and 4.525% for training and novel BMGs, respectively. ANN model has given mean PAD values of 3.817% and 3.676% for training and novel alloys, respectively. MLR models have developed linear relationship of thermal parameters with experimental D_{max}. This model has given relatively higher mean PAD error of 3.656% and 4.895% for training and novel alloys, respectively. The overall performance in terms of PAD error for GRNN, SVR, ANN, and MLR models are found to be 2.750, 3.531, 3.753, and 4.220, respectively. This highlights the best correlation of GRNN models among CI models. We also underlines improved performance of GRNN model in comparison to existing models based on the physical/statistical techniques.

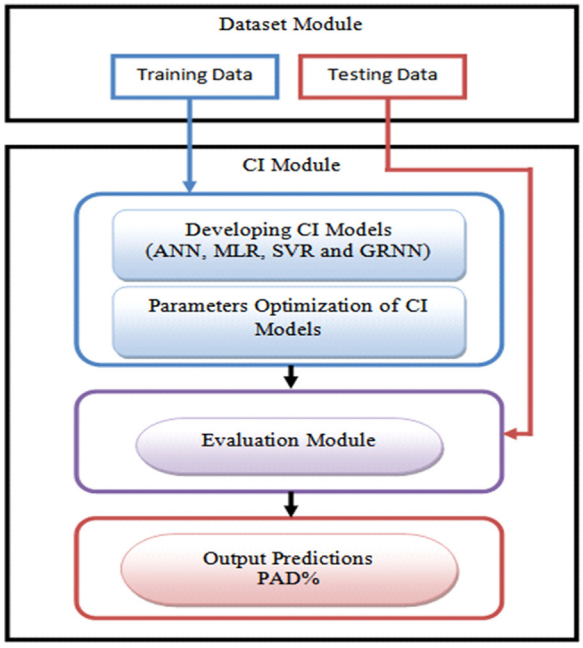

Fig. 1. Block diagram of the proposed CI models.

The rest of paper is organized such that in Section 2, a brief description of input data collection is given. In this section, it is explained how CI models are developed. In Section 3, simulated results of the proposed models are described and analyzed with the conventional GFA approaches. Finally, conclusions are provided in Section 4.

2. Materials and methods

Glass formation is a competing process between liquid phase and the resulting crystalline phases. The glass formation of the molten alloy would be favored if the liquid phase is stabilized on cooling and the competing crystalline phases become difficult to precipitate out. Since it is quite hard to study the cooling process of metallic glasses, few characteristic temperatures upon heating are often used for predicting GFA. These temperatures include the glass transition temperature T_g, crystallization temperature T_x and liquidus temperature T_l which reflect both thermodynamic as well as kinetic aspects of the alloy. It is well known that the glass transition and the crystallization procedure are strongly related to characteristic temperatures T_g, T_x and T_l. These thermal parameters are building blocks almost all the mathematically driven GFA criteria. The functional dependency of D_{max} is developed using three thermal characteristics T_g, T_x, and T_l of metallic glass compounds. The experimental values of D_{max} are used as dependent variables along with three independent variables as follows:

$$D_{max-pred} = f_{CI}(T_g, T_x, T_l) \quad (1)$$

Block diagram for developing CI models is shown in Fig. 1. Detail description of developing CI models is given in Section 2.2. The performance of models is measured in terms of percentage relative

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