ScienceDirect

Journal of Non-Crystalline Solids

Volume 625, 1 February 2024, 122733

A micromechanical nested machine learning model for characterizing materials behaviors of bulk metallic glasses

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https://doi.org/10.1016/j.jnoncrysol.2023.122733

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Abstract

In the present work, a novel micromechanical data-driven Machine Learning (ML) framework was proposed to characterize material parameters in bulk metallic glasses (BMGs) using nanoindentation simulations with Berkovich and spherical tips. A vast collection of data on material behavior in BMGs during nanoindentation was compiled, utilizing a series of Drucker-Prager model coefficients. The predictive model was constructed using a nested machine learning algorithm, which incorporated hyper-parameters tuning and a principal model. This nested configuration optimized the architecture of a deep neural network, acting as the key estimator for BMG material properties. The outcomes indicated that the ML model proficiently predicted critical material properties, including compressive yield strength, elastic modulus, flow stress ratio, and Poisson ratio. Notably, the ML model exhibited superior accuracy in predicting elastic modulus and compressive strength, suggesting a robust correlation with flexural elasticity and compressive strength. Furthermore, the study highlighted the significance of input

feature weight functions, as they strongly influenced the ML model's performance. Each output target's dependence on the individual proportion of input features contributed to the model's adaptability in handling variations in material properties. Finally, the findings of this work contribute to a deeper understanding of the relationships between input features and material properties, facilitating improved predictions of BMG behavior.

Introduction

Bulk metallic glasses (BMGs) have gained significant attention in materials science due to their unique combination of high strength, excellent corrosion resistance, and remarkable thermal stability [1], [2], [3], [4]. However, understanding and predicting the mechanical features of BMGs, such as elastic modulus, yield strength, and hardness, is a complex task due to their amorphous nature and intricate atomic structure [5,6]. Traditional experimental and computational methods face limitations in accurately characterizing and predicting MG properties. Recently, the application of ML methods has emerged as a promising approach for predicting and understanding the physical and mechanical behaviors of BMGs [7], [8], [9], [10]. Various ML techniques have also been successfully applied to predict the plasticity characteristics and mechanical properties of BMGs, providing valuable tools for accelerating materials design and development. For instance, Zhao et al. [11] formulated an LSTM (Long Short-Term Memory) model with the aim of predicting the serrated flow behaviors observed in BMGs during indentation process. The investigation unveiled a self-organized critical event within the serrated flow, which exhibited greater prominence at lower loading rates. Another study showed the potential of combining atomistic simulations and ML models for predicting the plastic behavior of BMGs in different conditions [12].

Peng et al. [13] proposed an ML strategy using neural networks to predict the atomic stiffness of metallic glass based on the radial distribution function. Li et al. [14] utilized an ML framework to investigate the impact of minor element additions on the elastic modulus of CuZrAl MGs. The outcomes highlighted the importance of element interactions with the base composition. In another study, several ML models were employed to model the Vickers hardness of amorphous alloys. The Light Gradient Boosting Machine (LightGBM) model

demonstrated superior performance with determination coefficients of 0.981 [15]. The model's interpretability was also enhanced by applying the Shapley additive explanations (SHAP) theory. Sarker et al. [16] made a significant discovery of new wear-resistant MGs in the Fe-Nb-B alloys by the combination of ML predictions and high-throughput (HiTp) experimentation. The synergistic approach leads to the identification of MG alloys with exceptional hardness, exceeding that of hardened stainless steel and rivaling diamond-like carbon. Xiong et al. [17] applied an ML model to predict the elastic moduli BMGs. The ML model demonstrated good agreement with experimental measurements, including the identification of errors reported in the literature, highlighting its potential for accelerating the design of advanced materials with specific mechanical behaviors. In another work, An inverse analysis method based on an artificial neural network (ANN) was presented by Han et al. [18]. The purpose was to determine the free-volume-model parameters of thin film metallic glasses using nanoindentation. The ANN model was trained using systematic finite element analyses (FEA) data and successfully validated by predicting the mechanical features of thin films on different substrates. Park et al. [19] utilized the ANN model in combination with FE nanoindentation to determine the free volume model parameters for BMGs. A material database was generated through FE analysis, and the ANN was trained and tested using this database to establish correlations between FVM and indentation parameters.

Nanoindentation has emerged as a promising approach in materials science, known for its capability to generate extensive datasets suitable for training ML models. Therefore, this study introduces an innovative methodology that amalgamates deep neural networks with nanoindentation techniques to comprehensively assess the material behaviors of amorphous alloys. To achieve this, we conducted FE simulations to delineate the pressure-dependent characteristics of BMGs. These simulations were based on the Drucker-Prager model (DPM) [20,21], providing crucial insights into BMGs' responses under varying pressures. Furthermore, to optimize the model's performance, a hyper-parameter tuning procedure was meticulously implemented during the model training phase. To validate the accuracy and robustness of our trained model, experimental nanoindentation tests were conducted on a diverse range of MG samples. By combining simulation-based insights with empirical nanoindentation results, this study offers a comprehensive and well-rounded evaluation of the MG material behaviors, contributing to the advancement of both materials science and machine learning applications in this field.

Section snippets

FEM simulation

The FE modeling was employed to simulate nanoindentation tests on a diverse set of material characteristics for BMGs. In order to address the issue of uniqueness in indentation responses, two distinct indenters, namely spherical and Berkovich, were utilized. The FE model, implemented using Abaqus/Standard, was designed with an axisymmetric configuration and had dimensions of 200×200 μm^2 (See Fig.1). A conical indenter was utilized in the FE model to precisely depict the non-axisymmetric…

Model validation and accuracy assessment

The first stage of evaluating the model's predictive capability is through regression analysis, which determines how accurately the model can forecast output targets. The parity plots in Fig.5a illustrate the results of the regression analysis for the m, ν, E, σ_c targets. It is evident that the ML model performs exceptionally well for all targets. However, considering the MBE and R^2 calculations, the ML model demonstrates superior accuracy in predicting the elastic modulus (E) and compressive…

Conclusions

This study presented a novel micromechanical data-driven ML approach for characterizing material parameters in BMGs through nanoindentation simulations with Berkovich and spherical tips. The generation of a comprehensive database of BMG material behavior under nanoindentation, utilizing a set of DPM variables, provided a robust foundation for the predictive model. The important findings are as follow:

- The application of a nested machine learning algorithm, integrating hyper-parameters tuning and …

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Credit author statement

The study was conceived and designed by Moustafa Sahnoune Chaouche. Experimental work was conducted by Moustafa Sahnoune Chaouche, and simulations and data analysis were performed by Hani K. Al-Mohair. The study was managed by Shavan Askar, who also contributed to data analysis. Data collection and literature review were carried out by Barno Sayfutdinovna Abdullaeva, while Naseer Ali Hussien participated in simulations and modeling. Data analysis and interpretation were further contributed by…

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.…

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