MACHINE LEARNING METHODS FOR DESIGNING MECHANICAL MATERIALS.

Objective

To create a model which will be able to predict new material designs and discover new mechanisms.

Description

Artificial intelligence, especially machine learning (ML) and deep learning (DL) algorithms, is becoming an important tool in the fields of materials and mechanical engineering, attributed to its power to predict materials properties, design materials and discover new mechanisms beyond intuitions. As the structural complexity of novel materials soars, the material design problem to optimize mechanical behaviors can involve massive design spaces that are intractable for conventional methods. Addressing this challenge, ML models trained from large material datasets that relate structure, properties and function at multiple hierarchical levels have offered new avenues for fast exploration of the design spaces. The performance of a ML-based materials design approach relies on the collection or generation of a large dataset that is properly preprocessed using the domain knowledge of materials science underlying chemical and physical concepts, and a suitable selection of the applied ML model. Recent breakthroughs in ML techniques have created vast opportunities for not only overcoming long-standing mechanics problems but also for developing unprecedented materials design strategies.

REVIEW OF LITERATURE

2.1"Artificial intelligence and machine learning in design of mechanical materials." Authors: Kai Guo, Zhenze Yang, Chi-Hua Yu and Markus J. Buehler. Published on: 17th December 2020.

In this review, they first present a brief introduction of state-of-the-art ML models, algorithms and structures. Then, they discuss the importance of data collection, generation and preprocessing. The applications in mechanical property prediction, materials design and computational methods using ML-based approaches are summarized, followed by perspectives on opportunities and open challenges in this emerging and exciting field.

2.2 "High strength aluminum alloys design via explainable artificial intelligence." Authors: Seobin Parka, Saif Haider Kayanib, Kwangjun Euhc,

Eunhyeok Seo, Hayeol Kima, Sangeun Park, Bishnu Nand Yadava, Seong Jin Park, Hyokyung Sungb, Im Doo Junga; Published on: Journal of Alloys and Compounds, 15 May 2022.

Here, they have approached to discover new aluminum (Al) alloys with the assistance of artificial intelligence (A.I.) for the enhanced mechanical property. With the guide of A.I.-based recommendation algorithm, new Al alloys were designed that had an excellent combination of strength and ductility with a yield strength (YS) of 712 MPa and elongation (EL) of 19%, exhibiting a homogeneous distribution of nanoscale precipitates hindering dislocation movement during deformation. So this A.I. assistant system can accelerate the search for high-strength alloys for both experts and non-experts in the field of Aluminium alloy design.

2.3"Bayesian Machine Learning in Metamaterial Design: Fragile Becomes Supercompressible" Authors: Miguel A. Bessa, Piotr Glowacki, and Michael Houlder; Published on:2019.

Here, a computational data-driven approach is followed for exploring a new metamaterial concept and adapting it to different target properties, choice of base materials, length scales, and manufacturing processes. Guided by Bayesian machine learning, two designs are fabricated at different length scales that transform brittle polymers into lightweight, recoverable, and supercompressible metamaterials. The macroscale design is tuned for maximum compressibility, achieving strains beyond 94% and recoverable strengths around 0.1 kPa, while the microscale design reaches recoverable strengths beyond 100 kPa and strains around 80%.

2.4"Prediction of Physical and Mechanical Properties for Metallic Materials Selection Using Big Data and Artificial Neural Networks." Authors: D. Merayo , A. Rodríguez-Prieto , And A. M. Camacho; Published on: IEEE Access, January 22, 2020.

In this work, a computer-aided tool is developed to predict relevant physical and mechanical properties that are involved in the selection tasks of metallic materials. The system is based on the use of artificial neural networks supported by big data collection of information about the technological characteristics of thousands of materials. Thus, the volume of data exceeds 43k. An artificial neural network (ANN) is built with thousands of perceptrons, whose topology and connections have been optimised to accelerate the training and predictive capacity of the ANN. After the corresponding training, the system is able to make predictions about the material density and Young's modulus with average confidences greater than 99% and 98%, respectively.

2.5 “LSTM Neural Network based Tensile Stress Prediction of Rubber Streching” Authors: Dazi Li; Mingjie Yan; Zhiwen Miao; Yue Fang; Jun Liu; Published in: 2020 IEEE International Conference on Networking, Sensing and Control.

To improve the accuracy of stress prediction under low strain rate, a stress prediction method based on a hybrid model of convolutional neural network (CNN) and long short-term memory (LSTM) network is proposed for the temporal characteristics and non-linearity of stress data. Firstly, feature vectors are extracted by CNN, constructed in the manner of sequence and used as input data of LSTM network. Then the LSTM network is employed to predict the stress. Stress data obtained in the process of rubber stretching are divided into two parts: training data and test data. The model is trained by training data and test data are used for validation of the proposed model. Experimental results show that the proposed prediction method has higher prediction accuracy than the standard LSTM network.

2.6 “Elevating Prediction Performance for Mechanical Properties of Hot-Rolled Strips by Using Semi-Supervised Regression and Deep Learning” Authors: Siwei Wu; Jian Yang; Guangming Cao; Yunlong Qiu; Guoguang Cheng; Meiyi Yao; Jianxin Dong; Published in: IEEE Access; 20 July 2020.

In this work, to solve the problem of the lacking enough labeled training data for deep learning, a safe semi-supervised regression supporting Bayesian optimization deep neural network (SAFER-BODNN) model was proposed to establish mechanical property prediction model of hot-rolled strips. The results show that this model achieves good performance for mechanical property prediction of hot-rolled strips with correlation coefficient of; 0.9610 for yield strength, 0.9682 for tensile strength, and 0.8619 for elongation, respectively. Compared with the deep neural network trained on the labeled dataset, the SAFER-BODNN model obtains stable smaller predicted errors and among all the variables, C content and Mn content have large influence on the yield strength and tensile strength. The investigation makes full use of unlabeled data to elevate the prediction performance of the deep neural network, and also provides a way for deep learning modeling when the data are insufficient.

2.7 “Utilizing computer vision and artificial intelligence algorithms to predict and design the mechanical compression response of direct ink write 3D printed foam replacement structures” Authors: Devin J. Roach, Andrew

Rohskopf, Craig M. Hamel, William D. Reinholtz, Robert Bernstein, H. Jerry Qi, Adam W. Cook; Published in: IEEE Access; 20 July 2020.

Current approaches for designing foam replacement structures are based on intuitive understanding of their properties or an extensive number of finite element method (FEM) simulations. These approaches, however, are computationally expensive and time consuming. In this work, a novel methodology for determining the mechanical compression response of direct ink write (DIW) 3D printed foam replacement structures using a simple cross-sectional image is being proposed. By obtaining measurement data for a relatively small number of samples, an artificial neural network (ANN) was trained, and a computer vision algorithm was used to make inferences about foam compression characteristics from a single cross-sectional image. Finally, a genetic algorithm (GA) was used to solve the inverse design problem, generating the Additive Manufacture printing parameters that an engineer should use to achieve a desired compression response from a DIW printed FRS.

2.8 "Predicting the Young's Modulus of Silicate Glasses using High-Throughput Molecular Dynamics Simulations and Machine Learning" Authors: Kai Yang, Xinyi Xu, Benjamin Yang, Brian Cook, Herbert Ramos, N. M. Anoop Krishnan, Morten M. Smedskjaer, Christian Hoover & Mathieu Bauchy.

The application of machine learning to predict materials properties usually requires a large number of consistent data for training. However, experimental datasets of high quality are not always available or self-consistent. Here, as an alternative route, they combine machine learning with high-throughput molecular dynamics simulations to predict the Young's modulus of silicate glasses. This combined approach offers good and reliable predictions over the entire compositional domain. By comparing the performances of select machine learning algorithms, they also discuss the nature of the balance between accuracy, simplicity, and interpretability in machine learning.

2.9 "Machine learning-assisted discovery of strong and conductive Cu alloys: Data mining from discarded experiments and physical features" Authors: QingkunZhao, HuiyaYanga, Jiabin Liu, Haofei Zhou, Hongtao Wang, Wei Yang; Published in: Materials & Design, 1 January 2021.

Here they propose a method of material design based on ML to discover high-performance Cu alloys. The ML models are trained from "discarded" experimental data that show undesirable hardness and/or electrical conductivity. They constructed effective Gaussian process regression-based models from limited training data by engaging additional

features. The predicted Cu alloys were experimentally synthesized and characterized, exhibiting superior hardness or electrical conductivity with respect to original training data. The impact of physical features on ML models was further evaluated by a genetic algorithm. Atlast there findings suggest that ML holds great potential for developing high-performance Cu alloys.

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