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Assessment of Nano-Imprinting Process in CuZr Amorphous Films Through Combination of Machine Learning and Molecular Dynamics

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Abstract

The current study aimed to establish a machine learning (ML) framework to predict key parameters, namely the degree of strain localization (ϕ), elastic recovery (E_{rec}), and maximum force needed (F_{max}), in the nano-imprinting process of CuZr metallic glasses (MGs). The ML model incorporated both structural features and imprinting process parameters as inputs. An extreme learning procedure was employed to develop the ML model, resulting in rapid data convergence, a short computational training time, and high

predictive performance. Regression analysis demonstrated that the ML model achieved impressive predictive accuracy, with R^2 coefficient values of 0.976, 0.959, and 0.971 for φ , E_{rec} , and F_{max} , respectively. The findings indicated that the prediction of φ and F_{max} heavily relied on inputs related to structural defects, such as free volume, while E_{rec} prediction was primarily influenced by inputs describing densely packed regions within the MGs. Additionally, the imprinting temperature and rate of filling displacement were identified as crucial factors in predicting the output targets. Consequently, the proposed ML model is believed to serve as a promising tool for predicting and characterizing output parameters that determine the feasibility and quality of the nano-imprinting process in MGs. In summary, this study successfully developed an ML framework that integrates structural features and process parameters to accurately predict important outcomes in the nano-imprinting of CuZr metallic glasses. The proposed model has the potential to enhance the understanding and optimization of the nano-imprinting process, contributing to advancements in the field.

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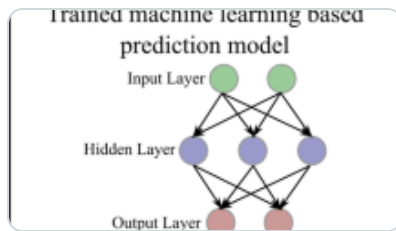
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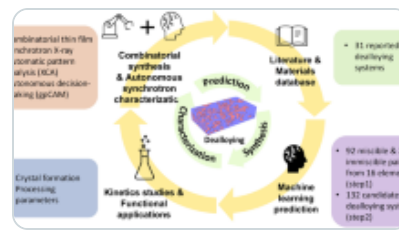
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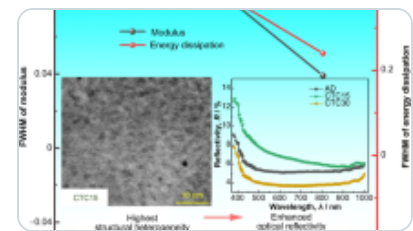
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Ethics declarations

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The authors declare that they have no conflict of interest.

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