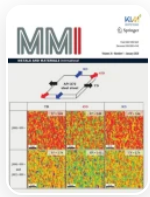


Tribological Properties Assessment of Metallic Glasses Through a Genetic Algorithm-Optimized Machine Learning Model

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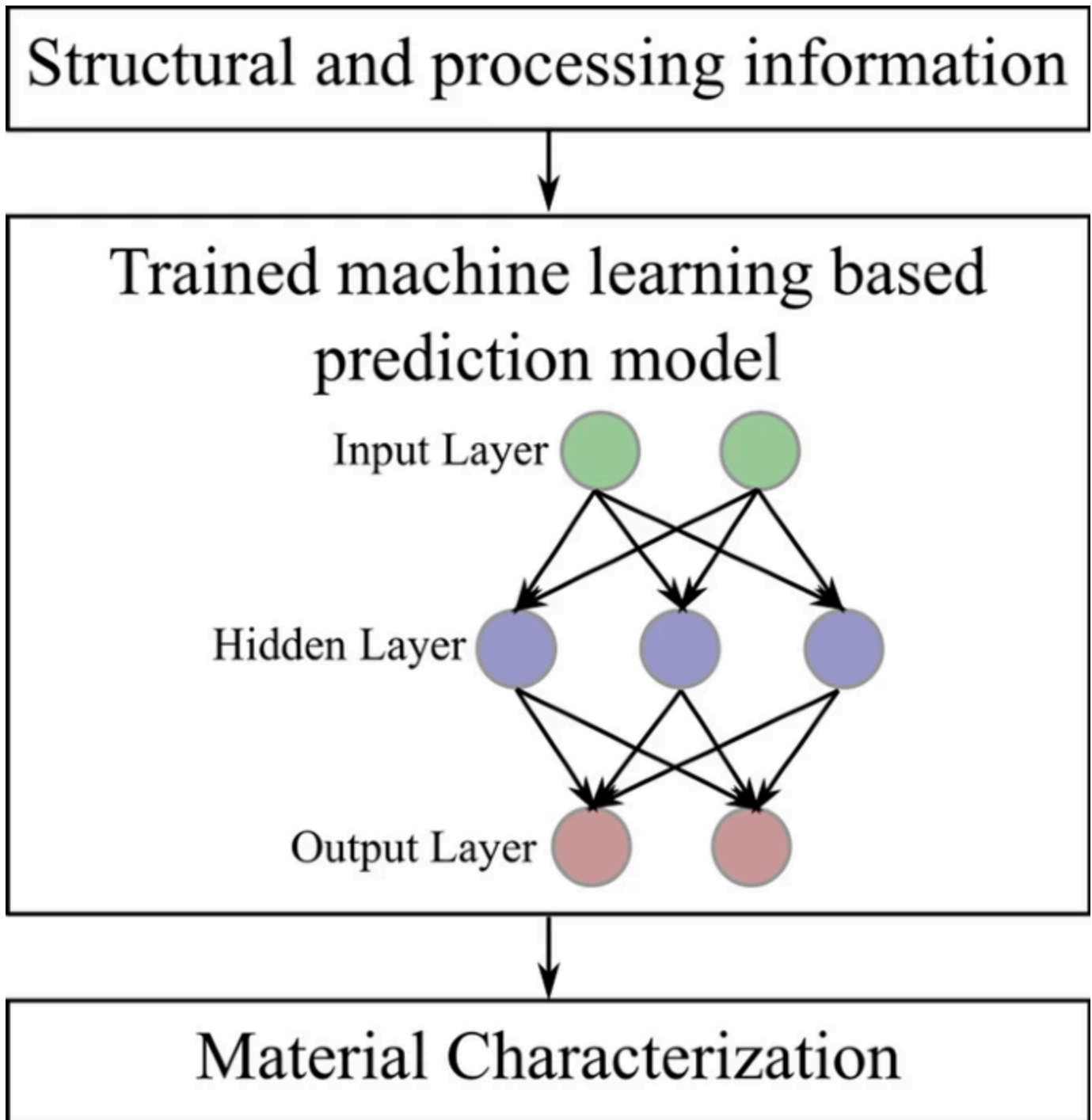
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Abstract

In this work, a machine learning (ML) model, optimized by genetic algorithm, was established to predict and characterize the tribological behavior of CuZr metallic glasses (MGs). By optimizing initial weight and bias coefficients through the genetic algorithm, the convergence of training process is expedited while keeping high performance of ML model. In the present study, the initial dataset was obtained through the molecular dynamics (MD) simulation of nanoscratching with a broad range of processing parameters and CuZr alloying

compositions. The structural features of MGs along with the nanoscratching parameters were selected as the inputs while the pile-up index (Pi) and coefficient of friction (COF) were the targets. The results indicate that the Pi (COF) targets can be predicted with determination coefficient and mean absolute percentage error of 0.95 (0.97) and 3.3% (2.9%), respectively. Moreover, it is found that the Pi output strongly depends on the structural input features, while COF target is significantly affected by the processing input features. The ML model is also able to identify CuZr MGs with various alloying compositions but the same tribological behavior, facilitating the materials design with preferred properties.

Graphical Abstract



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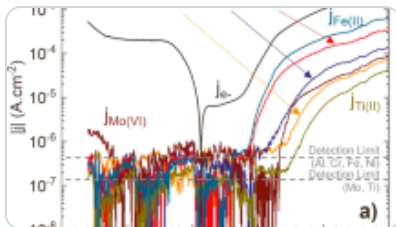
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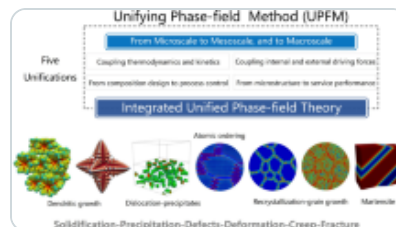
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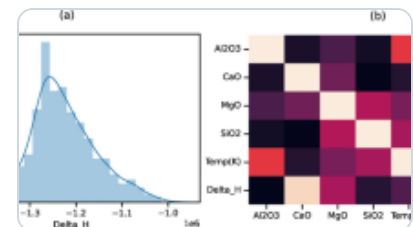
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Ethics declarations

Conflict of interest

The authors declare no conflict of interest.

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