Data-Driven Prediction of Metallic Glass Forming Ability via Bayesian Inference

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Metallic glasses (MGs) are a class of non-crystalline alloys characterized by the absence of long-range order while often exhibiting pronounced short-range ordering [1–3]. This atomic arrangement yields materials with unique combination of physical properties, including high specific strength, large elastic limits [4], good corrosion and wear resistance [5]. These properties make MGs attractive for a range of structural and functional applications.

The formation of an amorphous structure in metal alloys is a non-equilibrium process, in which the liquid is rapidly cooled to bypass crystallization. A key metric in this context is the glass forming ability (GFA), which describes the ease with which a metallic alloy can form a glass. GFA is commonly evaluated by the critical cooling rate required to suppress crystallization or by the maximum casting diameter achievable under a given cooling rate [6].

At present, there is no universal rule to design MGs, and conventional experimental screening is costly. Identifying alloy compositions suitable for metallic glass formation from the vast and multi-dimensional space of elemental combinations remains a significant challenge.

In the present study, we develop - using literature data - a Bayesian machine learning model based on Gaussian processes for predicting the GFA of metal-alloy compositions.

First, as shown in Fig. 1, starting with the thin-film metallic glasses, a Gaussian Process Classification (GPC) model was trained using a dataset containing 6835 thin-film alloys to predict the composition-dependent probability of glass formation. With the optimal descriptor set, the model achieves a prediction accuracy of 87% on an independent test set. Our analysis shows that predicting glass formation under thin-film deposition conditions involves a complex mixture of compositional disorder, thermodynamic properties, electronic structure properties, atomic radii, and other bonding parameters. To validate the predictive capacity of the model, we experimentally synthesize Cu–Zr–Al alloy films by magnetron sputtering and compare their structure to the model predictions. The results confirm the compositional dependence of GFA and demonstrate the effectiveness of our combined computational–experimental approach for guiding TFMG and amorphous alloy discovery [7].

Subsequently, the GFA of bulk metallic glasses (BMGs) was further investigated. In this context, the maximum critical casting diameter (D_{max}) was adopted as the quantitative metric for GFA. A dataset containing approximately 1,300 BMG compositions with reported D_{max} values are collected from the published literature. A clear empirical observation is that D_{max} differs across different elemental systems. Therefore, the samples were grouped according to their dominant element (i.e., the element with the highest atomic fraction), and a hierarchical Gaussian process regression (HGPR) model was introduced to investigate this families effect. HGPR updates both the group-specific parameters and the global parameters in a partially pooled manner. Small-sample groups tend to shrink toward the global population, while large-sample groups are able to preserve their own characteristics, reducing posterior uncertainty. The current results indicate that the hierarchical effect can significantly reduce model uncertainty, and the overall predictive performance reaches an R^2 *(true Dmax, predicted Dmax)* of 0.82.

References

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Figures

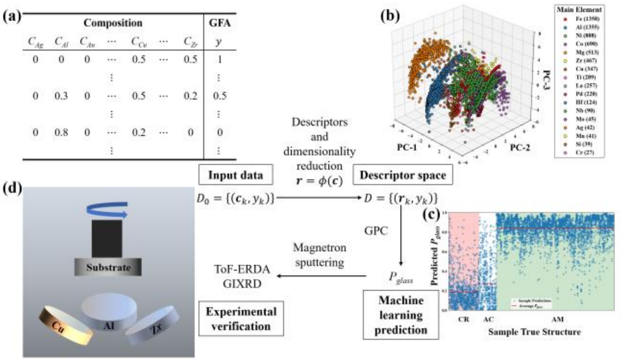

Figure 1. The workflow of GPC process