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Machine Learning Approach for Prediction and Understanding of Glass-Forming Ability

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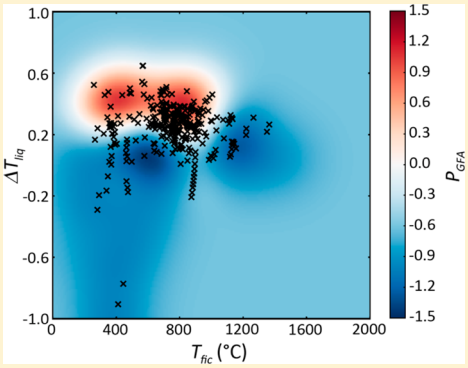
Supporting Information

ABSTRACT: The prediction of the glass-forming ability (GFA) by varying the composition of alloys is a challenging problem in glass physics, as well as a problem for industry, with enormous financial ramifications. Although different empirical guides for the prediction of GFA were established over decades, a comprehensive model or approach that is able to deal with as many variables as possible simultaneously for efficiently predicting good glass formers is still highly desirable. Here, by applying the support vector classification method, we develop models for predicting the GFA of binary metallic alloys from random compositions. The effect of different input descriptors on GFA were evaluated, and the best prediction model was selected, which shows that the information related to liquidus temperatures plays a key role in the GFA of alloys. On the basis of this model, good glass formers can be predicted with high efficiency. The prediction efficiency can be further enhanced by improving larger database and refined input descriptor selection. Our findings suggest that machine learning is very powerful and efficient and has great potential for discovering new metallic glasses with good GFA.



Bulk metallic glasses (MGs), as promising materials with unique mechanical and functional properties, have been drawing attention since they were first discovered over 50 years ago.[1−3] Up to now, one of the biggest problems that hinders the development and applications of MG remains to be the issue of the glass-forming ability (GFA).[4] The GFA of an alloy is most commonly defined as the critical cooling rate above which the liquid undergoes glass transition into the glassy state without the formation of crystals. In principle, glass can be obtained from liquid given a sufficient cooling rate, even for monatomic metal.[5] For industrial purpose, however, most alloys are not able to form MGs at cooling rates of 10^1-10^6 K/s, which severely limits their applications.[4] To design and develop bulk MGs with good GFA (for bulk MGs, the critical cooling rate should be below 10^2 K/s), a lot of effort has been devoted and various empirical criteria have been proposed for predicting the GFA in metallic alloy systems.[6−10] Some simple parameters related to the glass transition temperature T_g, such as a reduced glass transition temperature T_{rg},[11] parameter K_{gl},[12] parameter $T_x/(T_g + T_l)$,[13] and so forth, were proposed to estimate the GFA of metallic alloys. Other works have linked the GFA with geometric packing,[9,14,15] mixing enthalpy,[16] correlation radius,[17] and so forth. Three basic empirical rules had been formulated: multicomponent alloys containing three or more elements, significant atomic size difference, and large negative heat of mixing among the major components.[18] Although these empirical criteria provide useful information in development of MGs, no single empirical criterion is able to satisfactorily explain the GFA of alloys. This is due to the fact that many variables play important roles in the formation of MGs, such as the number of the components, the atomic size of the constituent elements, the composition, chemical interactions, transformation temperatures, and even techniques used to synthesize MGs.[17] However, in each individual criterion, the analysis either deals with a limited number of variables (data) or focuses only on some specific alloy systems. Therefore, it is difficult to determine which of the proposed criteria are really effective in predicting alloy compositions to develop new MGs. Thus, many MGs were developed more or less by trial and error. A recent work by S. Curtarolo[19] showed that the number of possible crystalline phases is an efficient indicator for the GFA of an alloy. These works revealed the possibility to build a better model in which different parameters are considered at the same time. For an ideal model for predicting the formation of MGs, all available variables should be analyzed.

To build a model for the prediction of the GFA of an alloy is essentially to find correlation between the GFA and other composition-related parameters that can be obtained prior to experiment.[20] After decades of development, machine learning became a promising method for such a purpose.[21] Materials

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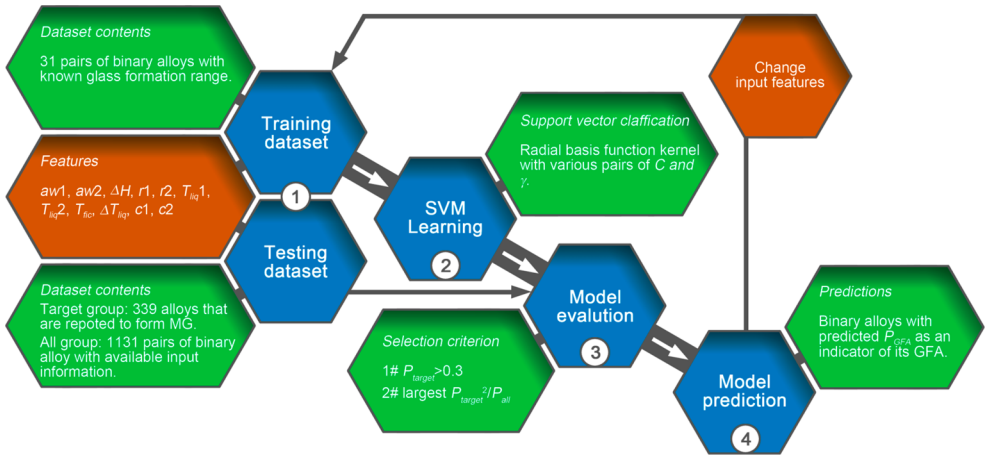

Figure 1. Overall setup for SVM modeling. Our SVM modeling process consists of four major processes, including building of the data set, the learning process, model evaluation, and model prediction. (i) The training data set and testing data set include different alloy compositions with different selected descriptors. (ii) The learning process is SVM with a radial basis function, in which two parameters, C and γ, can be tuned to develop different models. (iii) The best model is selected from (ii) by two criteria: $P_{\mathrm{Target}} > 0.3$ and largest E. (iv) The best model is used for prediction to find new glass formers. Input descriptors are changed to start a new process to assess the effect of different groups of descriptors.

design that involves machine learning has been used successfully in various research fields.[22−27] Norquist's work,[23] especially, sheds light on the valuable but long-neglected information concealed in failed experiments. The powerfulness of machine learning, in these cases, lies in its ability to analyze large volume and (/or) multidimensional data, which is perfectly matched for the prediction of the GFA of an alloy.

In this work, we aimed to develop models, using machine learning, to predict the GFA of an alloy by its composition. Our results indicate the possibility to pick out alloys with good GFA from all possible alloy compositions based on pre-existing data. We started on binary alloys because there is more available information, most importantly the phase diagrams, for us to analyze. We performed learning and testing processes and found that models with different prediction efficiencies can be developed from different input descriptors. Our results show that there is a deep and important link between the liquidus temperature and the prediction of GFA. The work has the potential to boost the speed of MG research fundamentally and provide implications for solving the challenging and elusive issue of GFA.

There are various machine learning approaches to develop models with the ability to recognize patterns from a data set and to have predictions over new data.[21] In this study, we use the support vector machine (SVM) method, which is one of the most popular and powerful techniques for data classification.[28,29] The SVM method constructs a hyperspace and solves the classification problem by constructing a flat or curved surface to best classify data points from different categories. As a typical supervised learning process, we divided the modeling process into four sections, that is, database preparation, SVM learning, model evaluation, and model prediction. Figure 1 is a flowchart illustrating the whole modeling process.

Studies on the GFA of alloys have continued for decades, and many MGs have been experimentally synthesized. In order to build a proper database for SVM, we must have information on both good glass formers and bad glass formers, so that the machine can learn the differences to separate them. Unfortunately, the bad ones are not always reported. Here, we found, from published papers, 31 binary alloys with known compositional range to form MG or not to form MG. For each binary alloy, we collected 91 data points with composition ranges from 5 to 95% (with an increment of 1%). These data are used as the training data set.

For a common machine learning process, a subset is partitioned from these data as an independent testing data set for evaluation purpose. However, the size of the training data set here is not large enough for such a procedure. Any reduction of the training data set is very likely to largely change the model performance; hence, we have to find another way to evaluate models. In this work, we use a testing data set that consists of two groups of data. Group "Target" is a group of 339 binary alloys that are reported to form MG by the melt-spun technique. These data are all collected from a review paper by Miracle.[30] The other group is named "All" as this group consists of all possible binary compositions (1131 pairs with atomic number smaller than 82) with available input data. In this way, the prediction efficiency of a model is assessed by its ability to separate data from group Target and group All.

Another part in building a database for machine learning is to select proper input and output parameters. There are several GFA-related parameters that could be used as output parameters. The critical cooling rate is one of the most precise parameters to characterize the GFA of an alloy; however, it is very difficult to obtain these data experimentally, especially for binary glass formers due to their generally worse GFA. On the basis of this fact, we simplified the problem into a classification problem by using a criterion to separate alloys into two categories: good glass formers and bad glass formers. The criterion is whether the alloy is able to form MG by the melt-spun technique. There is no information on the margin of error for this matter. For input descriptors, we selected a total of 11 parameters including 2 atomic weights (aw1, aw2), the mixing enthalpy (ΔH), 2 atomic radii ($r1$, $r2$), 2 liquidus temperatures for each element ($T_{\mathrm{liq}}1$, $T_{\mathrm{liq}}2$), the fictive liquidus temperature (T_{fic}), the difference in liquidus temperature (ΔT_{liq}), and 2 contents of each element ($c1$, $c2$). The fictive liquidus temperature is defined as $T_{\mathrm{fic}} = T_{\mathrm{liq}}1 \cdot c1 + T_{\mathrm{liq}}2 \cdot c2$, and the difference in liquidus temperature is defined as $\Delta T_{\mathrm{liq}} = (T_{\mathrm{fic}} - T_{\mathrm{liq}})/T_{\mathrm{fic}}$, where T_{liq} is the actual liquidus temperature obtained from the binary phase diagram. See Supporting Information section S1 for detailed information on the database.

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SVM with a radial basis function kernel (Scikit-Learn python[31]) is used to develop models for prediction. Two SVM parameters, C and γ, can be adjusted to yield different models. After the machine learning process with the training data set (see Supporting Information section S2 for training set accuracy), the model is applied to the testing data set to obtain P_{Target} and P_{All}, which are the probability of finding good glass formers in the Target group and All group, respectively. P_{Target}/P_{All} indicates the ability to pick out good glass formers from all possible compositions. However, this parameter does not work well for situations when both P_{Target} and P_{All} are very small, which might yield large P_{Target}/P_{All}. These models are not ideal for prediction; we also would like the model to cover a larger amount of data from group Target, which means that the model captures more characteristics of good glass formers. Hence, we defined parameter $E = P_{Target}^2/P_{All}$ to be the indicator of model performance. The best SVM model is selected based on two criteria: (1) $P_{Target} > 0.3$ and (2) largest E. Grid searches are run for every training data set to obtain the best SVM model.

Model predictions of P_{Target}, P_{All}, and E with different SVM parameters are shown in Figure 2a–c for a training data set with nine input descriptors (without $c1$ and $c2$). The evolution of P_{Target} and P_{All} shares a similar trend with the change of C and γ, and they both become larger with the increase of C and the decrease of γ. Parameter E, on the contrary, is found to have a maximum value of 3.96 when $C = 2^{-6}$ and $\gamma = 2^2$ (marked with a check mark in Figure 2c). For each training data set, we are able to select the best SVM model in this way.

Following the training and evaluation protocol, as we discussed above, models were developed using data sets with different input descriptors. Model prediction efficiency differs largely with different input descriptors, as shown in Figure 3. In Figure 3, All represents the nine input descriptors: aw1, aw2, ΔH, $r1$, $r2$, $T_{liq}1$, $T_{liq}2$, T_{fic}, and ΔT_{liq}. We can see that poorer performance is obtained if we add $c1$ and $c2$ into the data sets. Our interpretation is that although the content of each element is, of course, very important in designing MGs it might not directly correlate with GFA. Using these descriptors is misleading for the machine learning process. We also noticed that ΔT_{liq} served as the most important descriptor in the learning process. It is surprising that the SVM model has very good performance with only ΔT_{liq} as an input descriptor, but the performance is much worse if all descriptors except ΔT_{liq} ("All − ΔT_{liq}") were considered as input. We then tested different groups of input descriptors and found that the best SVM model is the one that was trained with two input descriptors: ΔT_{liq} and T_{fic}.

Model predictions on each alloy composition are measured by the decision function P_{GFA}. The larger the P_{GFA}, the better the GFA of the alloy. The model considers an alloy to be a good glass former if $P_{GFA} > 0$. Figure 4 shows the prediction result from the best SVM model on the testing data set. The distribution of P_{GFA} on different groups of data is shown in Figure 4a. We can see that the distribution of predicted P_{GFA} values on group Target significantly differs from that of the predicted P_{GFA} values on group All. Such a difference indicates the ability of the model to pick out good glass formers from all possible compositions. Figure 4b shows the predicted P_{GFA} with different input of ΔT_{liq} and T_{fic}. The best glass formers, based on model prediction, are the ones located in the red region with T_{fic} from 300 to 1000 °C and ΔT_{liq} from 0.2 to 0.6. Data from group Target are marked as "×" in Figure 4b. It is clear that the distribution of × and the red region are well correlated.

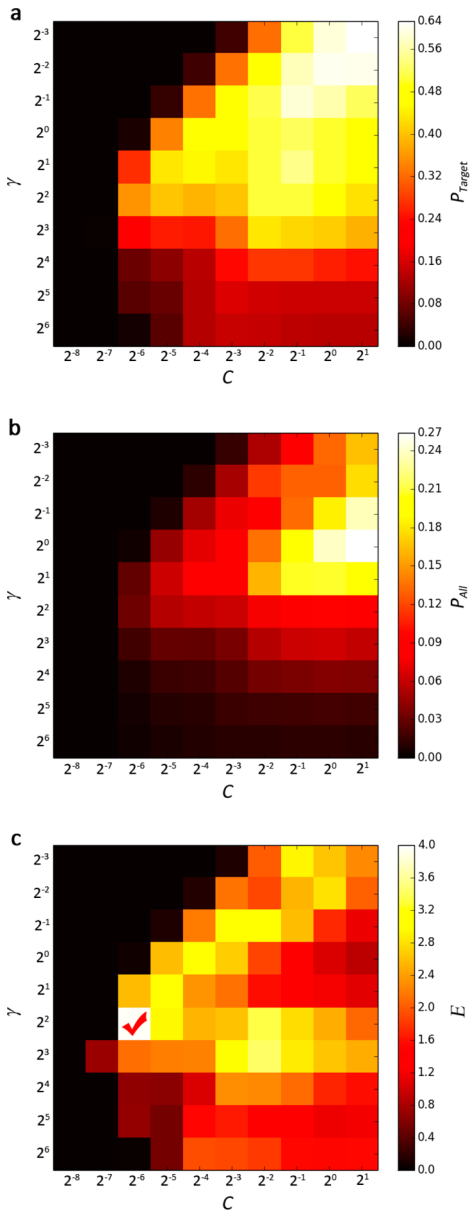

Figure 2. Predictions from models trained with different parameters. (a–c) Model predictions of P_{Target}, P_{All}, and E. The best model is identified to be the one with the largest E, which is marked with check mark in (c).

However, some exceptions are also observed, meaning that the model is still far from perfect. Although only a small portion of alloys is predicted to be good glass formers, there are still many of them not reported yet. Using the SVM model, we obtained a list of alloys with large predicted GFA that are not included in our database. Alloys like $Fe_{24}Lu_{76}$, $Ti_{73}Ni_{27}$, $Co_{90}Mo_{10}$, $Co_{26}Lu_{74}$, and so forth are predicted to be good glass formers. One hundred of these alloys are summarized in Figure 5, in which larger sized words indicate better GFA.

The SVM process handles data in a way that we are not able to understand the results directly, especially when dealing with multidimensional data sets. Different input descriptors contribute to the learning process in a complex way. Given the current database, which is not ideally large, it is incautious to draw conclusions by simply comparing results from two different groups of descriptors. Here, we only stress two main

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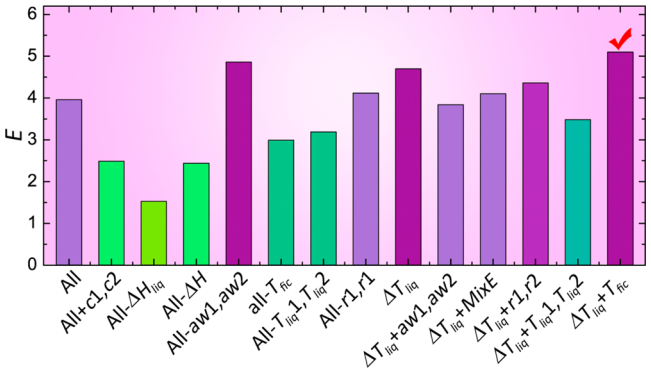

Figure 3. Input descriptors' assessment. Prediction efficiency, indicated by E, of SVM models trained from different input descriptors. Parameter ΔT_{liq} shows the strongest connection with GFA, and the combination of ΔT_{liq} and T_{fic} yields the best model (marked with a check mark).

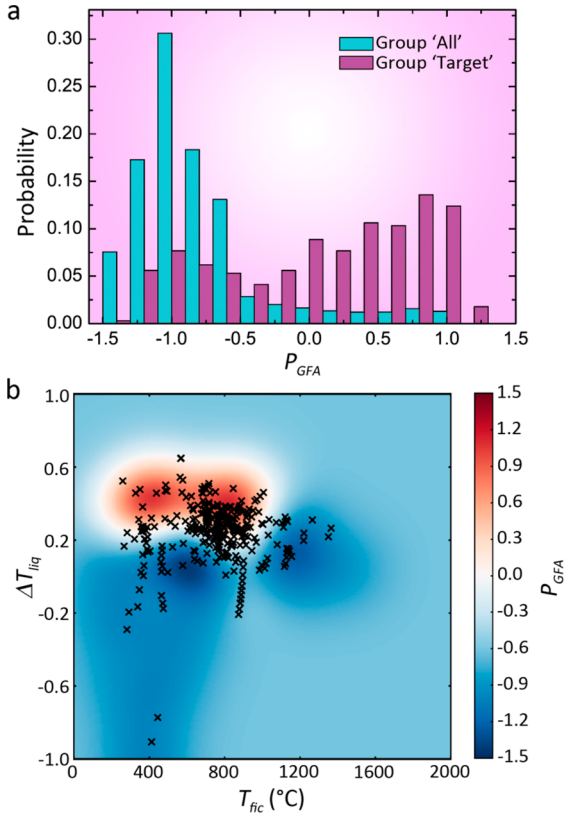

Figure 4. SVM model predictions. (a) Probability distributions of P_{GFA} from the prediction of the best SVM model in different data groups. $P_{GFA} > 0$ indicates a good glass former. A clear difference in the distributions indicates the high prediction efficiency of the SVM model. (b) The mesh grid, colored red and blue, indicates the model prediction with different values of ΔT_{liq} and T_{fic}, and the data of group Target are marked with "×". It is clear that the data of group Target are distributed mostly in the red region, indicating the very good prediction efficiency.

interpretations: (1) parameter ΔT_{liq} is the most relevant descriptor; (2) parameters ΔT_{liq} and T_{fic} together yield the best SVM model. The prediction result from our best model is obviously efficient, as shown in Figure 4. Compared with traditional analysis of GFA, our model collects information

Figure 5. Word cloud depiction of the best glass formers from SVM model prediction. These alloys are all predicted by our model and not in our training data set or group Target in the testing data set. Words in larger font indicate better GFA of the alloy.

from as many sources as possible and is capable of exploiting the information simultaneously.

As shown above, the SVM model that we developed exhibits promising ability to capture the characteristics of good glass formers, although only data of binary alloys with good GFA (they all form MG in a certain composition range) were used for training. There are still many element pairs that were not predicted to form MG in any composition. Also, it is worth pointing out that the training data set consists of data from only 31 pairs of elements. This number could be largely increased if more experimental data, whether alloys could form MGs or not, were collected and shared in standard format. A more abundant database should significantly improve the performance of machine learning for much better prediction of GFA of alloys. The improvement in our ways of dealing with data has the potential to boost material research speed fundamentally.[23,32]

Our results indicate the strong correlation between ΔT_{liq} and the GFA of an alloy, which is in accordance with our expectations. ΔT_{liq} is an indicator of the liquid line in a binary phase diagram, which includes information on the formation of crystals from liquid. Because the GFA of an alloy is essentially its ability to avoid crystallization, ΔT_{liq} should be strongly related to GFA because it describes the temperature that it can reach without crystallization. A larger ΔT_{liq} means that the alloy can be cooled to a lower temperature without crystallizing in equilibrium states. The correlation between ΔT_{liq} and GFA has been previously discussed by Donald and Davies[33] with a similar parameter ΔT^*.

Although multidimensional data analysis is one of the strong points of SVM, the best model that we obtained is trained by only two input descriptors. The fact that input descriptors except for ΔT_{liq} show no obvious correlation with model performance does not necessarily mean that these descriptors are not important in the glass formation process. As we mentioned above, the formation of glass is a complex process that involves different parameters in complicated ways. Miracle studied the GFA of MGs from the perspective of particle packing and developed a predictive model using multiple structural constraints.[34] Recent work by Curtarolo[19] suggested that a larger number of possible crystalline phases could introduce structural and energetic "confusion" that obstructs crystalline growth. However, it could also increase the possibility of finding one stable phase that lowers the GFA of an alloy. These results indicate that simple parameters like the ones that we used in this work might not be good enough for the SVM method to capture the characteristics of good glass formers, but they might be if they were modified into something that relates to GFA in a more direct way. Although our model was developed to predict the GFA of binary alloys, it

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has the potential to be generalized to not only predict GFA of multicomponent metallic alloys, such as Fe-based alloys, but also get more insight into the underlying mechanism of the GFA of metallic alloys.

Ward et al. developed predictive models using mainly decision trees for predicting the band gap energy of crystalline materials and the GFA of inorganic materials.[27] As another typical example of using machine learning to make predictions of material properties, Ward et al. built data sets using 145 attributes, and 10-fold cross-validation was employed to create a model with high accuracy. Here, we did not perform 10-fold cross-validation because of unlabeled data in group All. Instead, we used parameter E as an indicator of model efficiency. The above results indicate that our algorithm is valid and efficient. Moreover, in our work, much a smaller number of input features was considered, and the correlation between different input features and results were analyzed for better understanding of the physical origin of the GFA of metallic alloys. Although the method and models are different between our works, both works demonstrate that machine learning is quite promising for future material discovery and there is still large space for improvement.

The use of machine learning enabled us to discover the characteristics of good glass formers through multidimensional data analysis. Our results indicate the importance of parameter ΔT_{liq} in the GFA of an alloy, which is in accordance with our understanding of the glass formation process. Using the SVM model, new binary alloys with good predicted GFA is suggested. With improvement of the database, the machine learning technique has the potential to revolutionize the discovery of new glass formers. A well-developed predictive model not only provides us with suggestions for real experiments but also helps us gain physical insights on the challenging issue of the GFA.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jpclett.7b01046.

Detailed information on the data source and database, the support vector machine (SVM) method and parameter selection, model evaluation process, and model prediction process (PDF)

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Notes

The authors declare no competing financial interest.

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