Machine learning based prediction of dissolution kinetics in silicate glasses

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Publication date:
2018

(GOMD-S1-024-2018) Machine learning based prediction of dissolution kinetics in silicate glasses

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Silicate glasses, due to the exposure to water during service life, undergo corrosion and dissolution. Accurate predictions of dissolution kinetics in these glasses are hindered by the lack of fundamental understanding and the large number of intrinsic and extrinsic factors controlling the process. To address this issue, we use a data-driven approach to predict the dissolution kinetics of glasses. To this extent, we use high fidelity experimental measurements on the dissolution rates of aluminosilicate glasses. Glasses with varying compositions exposed to a wide range of pH values, ranging from acidic to basic, are considered. We investigate the efficiency of four classes of machine learning methods namely, linear regression, support vector regression, random forest and artificial neural network. We observe that, while linear methods fail in predicting the dissolution rates, artificial neural network provides accurate predictions exhibiting an excellent match with the experimental results. Through a detailed study, we show that the machine learning techniques can be used to identify the input-output relationship of the data, that is, linear vs. non-linear and ultimately, to predict accurately the dissolution kinetics of glasses. Overall, such data-driven approaches can be useful in glass science to understand the governing mechanisms, and to accelerate the design of commercial glasses.