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Learning the indentation size effect in hardness of glasses through symbolic reasoning-informed machine learning

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Abstract Body: The hardness of glasses is not an intrinsic property as it depends on the indenter material, geometry, and loading conditions. Apart from composition, the hardness also varies non-linearly with the load, a phenomenon called indentation size effect (ISE), which remains poorly understood. To this extent, we used a symbolic reasoning-informed ML (SRIML) to develop a model that can learn from the existing composition and load data extracted from the INTERGLAD database and scientific literature. A purely data-driven model was also trained aside from the SRIML model. Although the data-driven model successfully predicted the composition dependence within the training dataset, it failed for data outside the training dataset and could not capture the load dependency. In contrast, the SRIML model performed reasonably well predicting the hardness and also captured the load dependency. Furthermore, to explain the dependence of composition and load on the glass hardness, we employed Shapley Additive Explanations (SHAP) theory-based game technique. The analysis reveals that few elements, such as N, Si, and La, contribute significantly to the hardness, whereas others, like Na, P, and Te, were found to influence the hardness of oxide glasses negatively. The derived composition-property relationships can aid in designing glasses with tuned hardness for varied applications.