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Predicting the Composition Dependence of Glass Hardness

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Hardness is an important mechanical property of glasses, but direct calculation of hardness from first principles has shown to be too complex. Temperature-dependent constraint theory has recently been successfully applied to predict the composition dependence of dynamic properties such as glass transition temperature and liquid fragility index. Here, we extend this theory to quantitatively predict hardness of glasses, taking the ternary soda-lime-borate glassy system as an example. By comparison of modeling results with experimental data, we show that hardness is governed by the number of network constraints at room temperature and that a critical number of constraints is required for a material to display mechanical resistance. Furthermore, by applying a surface diffusion process, we have modified the surface composition of the borate glasses. We show that the resulting change in hardness can be predicted by considering the number of room temperature constraints in the modified surface layer. Our result implies that constraint theory may be used as a tool for predicting the composition dependence of other mechanical properties.