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Understanding Glass Hardness from Constraint Theory

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Understanding the composition dependence of glass properties is of critical importance for the quantitative design of new glassy materials. Hardness is an important mechanical property of glasses, but a theoretical prediction of glass hardness has hitherto been impossible. In this work, we present a topological approach for quantitative prediction of hardness of inorganic glasses, taking the ternary soda-lime-borate glassy system as an example. 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. By comparison of the hardness prediction with that of the glass transition temperature, we demonstrate the importance of accounting for the temperature dependence of the network constraints. The predicted values of hardness are in excellent agreement with experimental data, and we are also able to account quantitatively for changes in hardness that occur when the surface composition changes.

Keywords: topological constraint model; hardness; network topology; borate glasses