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Origin of the Mixed Alkaline Earth Effect on the Hardness of Silicate Glasses

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Most oxide glasses containing a combination of two (or more) types of alkali or alkaline earth cations tend to exhibit non-additive variations of their properties, when one cation is gradually substituted by the other one. This behavior, known as the mixed alkali effect (MAE), has remained an enigma in glass science. In particular, hardness – a property of primary interest for applications such as protective screens, can exhibit a positive or negative deviation from linearity with respect to the fraction of mixed ions. Here, based on molecular dynamics simulations, we investigate the hardness of mixed calcium/magnesium aluminosilicate glasses. We observe a minimum of hardness for mixed glasses, in agreement with micro-indentation experiments. Such anomalous behavior is found to arise from an increase propensity for shear flow relaxation under load, which is stimulated by the presence of internal stress in the atomic network. Finally, we demonstrate that the internal stress originates from a mismatch between the alkaline earth cations and the rest of the silicate network for mixed compositions. The present results offer a clear atomic picture of the origin of the MAE on hardness and highlight the potential for the nano-engineering of high-performance glasses.

KEYWORDS: Mixed ion effect, hardness, molecular dynamics.