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Topological Model of the Dissolution Kinetics of Silicate Glasses

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Understanding and predicting the dissolution rate of silicate glasses is of primary importance for various applications, including bioactive glasses and borosilicate wasteforms. However, the mechanism of silicates' dissolution – and its rate-limiting step – remains poorly understood. In particular, present models linking the composition and structure of silicate glasses to their dissolution rate in a given solvent have remained largely empirical thus far. Here, based on vertical scanning interferometry (VSI), we study the dissolution of a family of borosilicate glasses under several values of pH. In addition, we parametrized a new transferable inter-atomic potential to assess the structure of these glasses from molecular dynamics (MD) simulations. From a detailed analysis of the simulated structures, we demonstrate that the kinetics of the dissolution is controlled by the topology of the atomic network. Finally, we propose a new topological model of the dissolution, which is shown to offer realistic predictions of the activation energy of dissolution for a wide selection range of silicate glasses and crystals.

KEYWORDS: Dissolution, Borosilicate glasses, Topological constraint theory, Vertical scanning Interferometry, Molecular Dynamics.