Fracture surface energy of glasses obtained from crystalline structure and bond energy data

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Abstract

The search for strong and tough oxide glasses is important for making safer, more environmentally friendly, thinner glasses (1). As fracture toughness experiments in brittle materials are complicated and time-consuming (2), modelling glass fracture surface energy, (g), and fracture toughness, KIc, is of interest for screening promising candidates. Inspired by Rouxel's idea of preferred crack growth along cutting weakest bonds within a glass structure (2) and a study by Tielemann et al. (3), which indicates a correlation between crystal fracture surface and glass-crystal interfacial energies, we present a new approach for predicting (g). Combining both ideas, we used diatomic bond energies and readily available crystallographic structure data for estimating (g). The proposed model assumes that fracture surface energy of a glass equals the fracture surface energy of the cleavage plane in its respective isochemical crystal. We calculated (g) - values for more than 25 iso-chemical silicate systems and compared them to calculated values from Rouxel's model (2) that applies well using glass densities and chemical bond energies. Not only does our model yield good agreement with (2), but it also enables an estimation for glasses with unknown density and can therefore contribute to broaden the data basis for glass property modelling tools. Most interestingly, however, this agreement indicates a remarkable equivalence between fracture cleavage planes in a crystal and its corresponding glassy structure.
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