Influence of the alkali modifier on the surface properties of silicate glasses

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Abstract

We have used large-scale molecular dynamics simulations in order to investigate the surface properties of lithium, sodium, and potassium silicate glasses containing 25 mole% of alkali oxide. We have studied two types of surfaces, a melt-formed surface (MS) and a fracture surface (FS), and we have found that the influence of the alkali modifier on the surface properties depends strongly on the nature of the surface. The MS show a saturation of elemental concentration when the alkali is changed from Na to K, while the FS exhibit a monotonic increase of modifier concentration with increasing the alkali size. For the FS we find that larger alkali ions reduce the concentration of under-coordinated Si atoms at the surface and increases the fraction of two-membered rings.
For both types of surfaces, the surface roughness of the surfaces are found to increase with alkali size, with the effect being more pronounced for the FS than for the MS. The height-height correlation function of the surfaces show a scaling behavior that is independent of the alkali species considered: The one for the MS is compatible with the prediction of the frozen capillary wave theory while the ones for the FS shows a logarithmic growth, i.e., on the nanoscale these surfaces are not self-affine fractals. The influence of the modifier on the surface properties are rationalized in terms of the interplay between multiple factors involving the size of the ions, bond strength, and charge balance on the surface.

Keywords: silicate glasses, alkali metals, surface, fracture, roughness

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