

Acid-base properties and structons: towards a structural model for predicting the thermodynamic properties of silicate melts

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Abstract

Phase equilibrium relationships in igneous systems can be estimated using empirical mathematical models based on multi-component regular solution formulae. Although these provide useable results within the fitted region, they can give very misleading values outside the compositional range of curve fitting. Moreover, they usually give poor estimates of the well-characterized melting relations of simple systems and do not relate to the large body of thermodynamic activity data available in the metallurgical literature, nor to spectroscopic, diffraction or computational models of silicate melt properties. The aim of this paper is to extend previous acid-base models of silicate melts and to use a quasi-chemical model to calculate the activities of quasi-chemical silicate mixing units, or structons, from combinations of the oxo-species used in quasi-chemical and polymer models to calculate oxide activities in metallurgy.

Keywords

silicate melt;acid-base;oxide melt;thermodynamic properties

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References

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
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