Structure, thermodynamic properties and viscosity of silicate melts: development of a model in the Adam and Gibbs theoretical framework

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Abstract

The rheological and thermodynamic properties of silicate melts played a crucial role in the formation and the evolution of the Earth, as well as in the history of human civilisations. For instance, they determined the geologic evolution of the Earth primordial magma ocean, and, thus, influenced the differentiation of the Earth mantle and crust. Nowadays, silicate melt properties control, for example, the dynamic of volcanic eruptions or glass-making processes in the industry. Therefore, predicting silicate melts properties is critical to understand and to solve various problems in Earth and Material sciences.
The Adam and Gibbs theory offers a thermodynamic framework that allows relating the chemical composition of a melt to its structure and its properties. Within this theoretical framework, viscous flow occurs through the cooperative re-arrangement of molecular sub-regions in the melt. From high temperature Nuclear Magnetic Resonance and Raman spectroscopy data, it actually is known that viscous flow occurs because of the cooperative exchange of oxygen atoms between network former polyhedral units, allowing their motions. Therefore, it appears that such structural knowledge can be linked to the melt entropy, heat capacity and viscosity with using the Adam and Gibbs theory.

In this communication, building on our previous work on Na-K silicate glasses (Le Losq and Neuville, 2017), we will show how this idea can be used for modelling the properties of aluminosilicate melts. First, we will highlight how the distribution of network former tetrahedral units can be calculated from the melt chemical composition. Then, this structural knowledge will be linked to the melt thermodynamic properties, which, in turn, will allow calculating the melt viscosity. Such model opens new pathways in order to gain structural, thermodynamic and rheological information about silicate melts and glasses.

References
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