

Structure of the Mineral-Silicate Melt Interface

JAMES R RUSTAD¹

¹Corning Incorporate, Corning, NY, USA,
rustadjr@corning.com

Predicting the temperature at which a solid phase will nucleate from a silicate melt is a key problem in igneous petrology and also in the industrial production of glass and glass ceramics. Thermodynamic predictions are often not sufficiently accurate in industrial settings. Improved capabilities for prediction of liquidus temperatures, which take into account inhomogeneous aspects of nucleation, and in particular the influence of composition, are needed.

A crucial aspect of nucleation is the atomic-scale structure of the mineral-melt interface. Although a tremendous amount of work has been done on mineral-water interfaces, the mineral-melt interface is much less studied. Despite the great effort has been directed at understanding it, water structure is only perturbed by a small degree when placed in the presence of a surface. This is because of the generally low density of the aqueous phase and because the mineral surface charge can be neutralized by protons, which serve as incredibly versatile charge compensators.

In a silicate melt-mineral interface, surface charge compensation must occur through the cations in the melt. The tendency to accumulate at the interface is balanced against the activities of the cations in the melt, in contrast to mineral-water interfaces which is mostly influenced by pH. In contrast to mineral-water interfaces, which have one or two layers of ordered water, molecular simulations of the melt-mineral systems reveal a highly structured interface, with six-seven ordered oxygen layers extending more than 1 nanometer into the melt. Molecular simulation of a range of mineral-melt pairs reveal highly variable interfacial structures differing significantly from the melt-air interface which tends to accumulate alkali and alkaline earth. Some minerals, such as zircon tend to accumulate alkali ions, while others, such as corundum and spinel are alkali-phobic, accumulating network forming cations such as B^{3+} , Al^{3+} and Mg^{2+} . Thus, depending on the mineral and melt structure and composition a wide variety of charge-compensating strategies may be taken. This will almost certainly have a strong effect on nucleation phenomena and crystal growth in these systems.