The 27th Global COE International Frontier Seminar

Title: Mineral/melt element partitioning – How can melt structure help us understand the influence of melt composition?

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Variations in mineral/melt element partition coefficients in natural magmatic systems can be understood via characterization of how compositional variables can be modeled in terms of melt and mineral structure. Relationships to mineral composition and structure are well understood. Significant understanding of the role of silicate melt structure is also becoming available. The solution behavior of major, minor and trace elements can be modeled via the role of nonbridging oxygen in various Q^n-species in the silicate melts. The nonbridging oxygens are, however, not equivalent because the next-nearest neighbor environment around nonbridging oxygen in the different Q^n-species depends on the both the type of Q^n-species and on the distribution of tetrahedrally coordinated cations (in addition to Si^{4+}) between the coexisting Q^n-species. Characterization of how mineral/melt partition coefficients vary with melt compositions is, therefore, essentially a question of determination of Q^n-species type and abundance and ordering of network-modifying cations among the nonbridging oxygen in these Q^n-species. For example, the Fe^{2+}/Mg exchange equilibrium coefficient between olivine melts, often central to assessment of the extent to which natural magmas have been affected by crystal fractionation subsequent to partial melting in the earth's upper mantle is not 0.3 as is often assumed, but varies between 0.17 and 0.45 depending on melt composition (structure). This variation can be understood via characterization of the Fe^{2+}-NBO and Mg-NBO bonding in the melts. Analogous relationships have been developed for other transition metals. Moreover, the competition between the element of interest and other major elements non-equivalent nonbridging oxygens can be used to model the influence of compositional variables such as Al/(A/+Si), alkali/alkaline earth ratio, and abundance of volatiles (especially H_2O and CO_2) can be characterized via their influence on Q^n-species type and abundance in silicate melts. Ultimately, this treatment can be applied to characterization of mineral/melt partitioning in natural magmatic liquids.

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