Application of multinuclear solid-state NMR to structural analysis of slag and glass

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Abstract

Silicate and aluminosilicate melts and glasses are major components in many geological processes in the Earth's mantle and crust. They also are important in the steelmaking process as slag in metal extraction from coals and iron ores, and as mold flux in the continuous casting process to slowly cool molten steel. Since macroscopic properties such as viscous flow are considered to be well related with atomic-scale structure and dynamics, detailed structural analysis of the slags is required.

High-resolution solid-state nuclear magnetic resonance (SSNMR) is one of the best methods for analysis of structure and dynamics. SSNMR is useful for probing the atomic environments of disordered materials such as glasses unlike diffraction techniques. Also, characteristic worth of special mention is that NMR provides structural information on the local structure around a specific kind of atom.

We have been applied to SSNMR to slags and related glasses to obtain information on chemical structure (for example, coordination number and structural role) and dynamics. Our targets are not only glass frameworks (e.g. 29Si, 27Al and 17O) but also network-modifying cations such as 43Ca; some of those nuclei are enriched with isotope to increase NMR sensitivity. In addition, structure and dynamics in molten state of the aluminosilicate system have been investigated using in situ high temperature NMR (˷1500 degC).

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