

**A MODEL DESCRIBING THE COMPONENT ACTIVITIES OF MOLTEN SLAG
BASED ON HTRS MEASUREMENT AND MD SIMULATION**

G.C. Jiang, J. L. You and S.P. Huang

It is intended to deduce the component activities of molten slag from the informations of its bonding structure, which results from high temperature Raman spectroscopy (HTRS) and MD simulation. The model is called as SELF-BoSS. This paper takes the CaO-SiO₂ system melted under 1873 K as example to illustrate the model. As generally accepted concept, the microstructure unit of the mentioned silicate is Si-O tetrahedron. There are 5 tetrahedral Q_n (Q₄, Q₃, Q₂, Q₁, Q₀). Here, n denotes the number of the bridging oxygen around a Si⁴⁺. Under molten state the Raman spectroscopy is an envelope. By means of HTRS the envelopes of several samples under 1873 K were registered.