B10: Formation of critical compounds in recycling slags – a study of the melt chemistry with MD simulations and of the solidified compounds in a micro preparation approach

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Our objective is to understand the solidifying processes of potential EnAMs in the system Al_2O_3, MgO, CaO, Li_2O, SiO_2 in the presence of Mn on a molecular level. Especially Li, Mn, and Al species in the solid products and their polytopes in the melt are of interest. *Our rationale* is that when we study the molecular structure of the melt and the solid with respect to micro structuring (phase separation) as a function of concentration and temperature, we will understand the processes decisive for the formation of EnAMs. In the melt simulation Li, Al and Mg are mainly considered as their potentials are known to be very reliable and $LiAlO_2$ is a potential EnAM for Li recovery. The influence of the following parameters on melt structure and solidification will initially be considered: concentrations of the components as well as the O_2 partial pressure, temperature, and viscosity (all derived from simulation and/or) experiments.

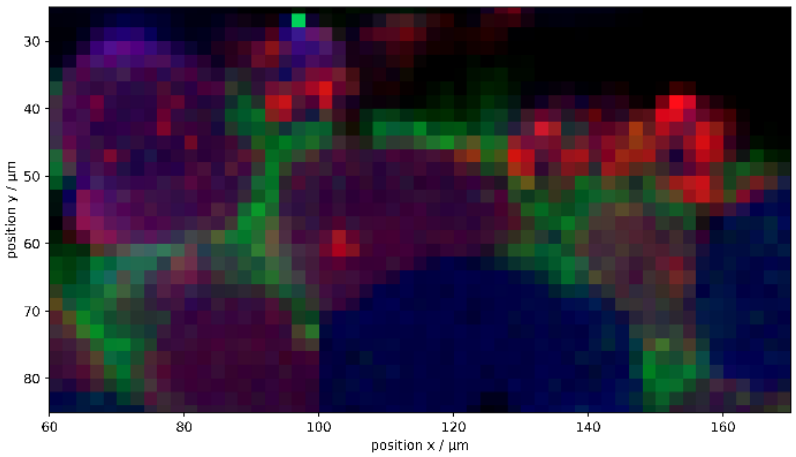

Figure 1 Elemental distribution (red Mn, blue Ca, green Pt as contamination) in a fast solidified CaO, Li_2O, SiO_2, MnO slag analogue; separation of $Li_xMn_yO_z$ and $Ca_mSi_nO_o$ rich phases.

We developed a micro preparation and a bulk synthesis to produce melts and solids of defined composition. The approach allows to study the solidification of many components as a function of concentration and temperature. The results from the molecular dynamics simulations and the experimental microscopic and chemical characterization combined contribute to the

products' genesis hypothesis. Phase separations in fast cooled slag analogues are studied, the components are determined, and the species identified (*e.g.,* oxidation state of Mn). The influence of melt structure, composition and viscosity on the species formation is evaluated.

First results show a phase separation in CaO, Li_2O, SiO_2, MnO slag analogues subjected to fast cooling (see Figure 1). Species determination shows Mn species being mostly $LiMnO_2$. Though viscosities for these phases are yet not be modelled because of refining of potentials, $LiAlO_2$ viscosity was successfully modelled over a wide temperature range matching literature data (see Figure 2).

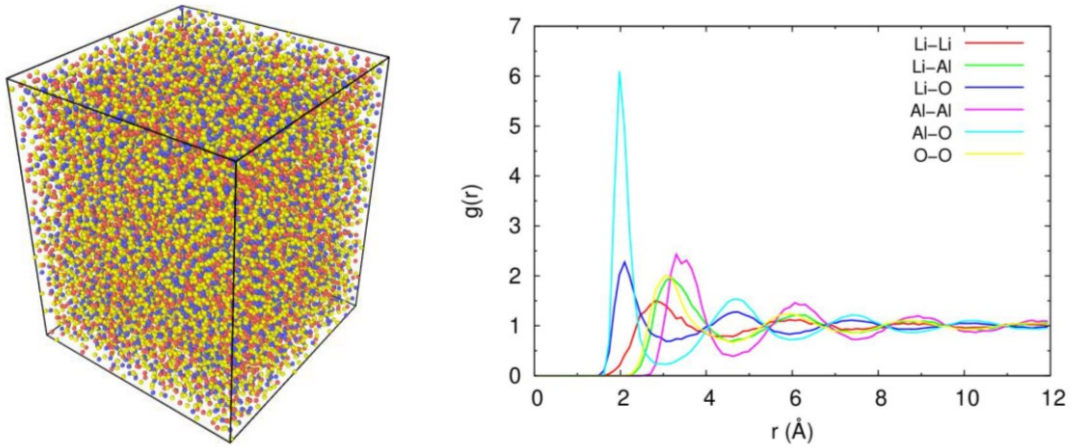

Figure 2 a) MD simulation of $LiAlO_2$ at T: 1900 K. b) pair correlation function from MD simulation for $LiAlO_2$ at T: 1900 K.