Molecular dynamics simulation of viscosity of selected pure oxide melts

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ABSTRACT

Viscosity of oxide melts is one of the fundamental physicochemical properties that plays a crucial role in important technological and natural processes like slag flow, slag/metal separation, volcano eruptions etc. However, many oxides melt at extremely high temperatures and are highly corrosive in the liquid state, which makes experimental measurement of melt viscosity by traditional experimental techniques a difficult and expensive, if not unachievable, task. In this case it might be useful to employ other methods of viscosity determination such as modelling or simulation. In the present paper the shear viscosity coefficients of selected pure refractory oxides (CaO, MgO, Al_2O_3 and others) have been simulated at temperatures above their melting points via the classical molecular dynamics and compared to the available viscosity data (e.g. experimental viscosities, other model predictions) collected by the authors. The simulation has been carried out using the non-commercial molecular dynamics simulation package LAMMPS and the Born-Mayer-Huggins potential, which parameters for the selected oxides were taken from the literature. Several viscosity calculation techniques (the Stokes-Einstein & Green-Kubo equations, the so called Einstein relations, and the non-equilibrium molecular dynamics methods) have been applied to ensure a more reliable viscosity calculation. It has been demonstrated that the simulated viscosity of the selected melts agrees with the available experimental data. It has also been shown that the simulated viscosity of a number of the oxide melts investigated is close to that calculated by phenomenological viscosity models, which supports viscosity extrapolation from the corresponding binaries and ternaries, if no experimental data is present for unary systems. In general, it has been demonstrated that the molecular dynamics simulation could provide a reasonable estimation of viscosity if no other viscosity data is available.