



NITheP cordially invites you to a seminar by

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Date: Monday, 24 April 2019 Time: 15h15 -16h15

Venue: NITheP Seminar Room, 3rd Floor, H-Block

Title: Computational Modelling of Structural and Transport Properties of Molten Slag System

Abstract: The DC Arc Furnace in the Pyrometallurgy Division at Mintek is used for smelting metal ores to obtain pure metals or alloys. Any improvement in the smelting process is most desirable, such as increasing efficiency as well as reducing waste material and environmental impact. Conditions such as electrical power, temperature, heating and cooling rates, composition of components, and smelting sequence may be varied to optimize the process. Hence, an understanding of the system is invaluable and Molecular Dynamics (MD) modelling can yield such information. An understanding of electrical conductivity (resistivity) is vital in terms of both furnace operation as well as design, especially for electrical furnaces.

Knowledge of other transport properties such viscosity and thermal conductivity are also invaluable. Transport properties can be predicted from correlation functions of MD trajectory data (from the atomic displacements, velocities and forces). Other useful properties such as density, linear expansion coefficient, enthalpy and heat capacity can be more directly obtained from MD. MD predictions [1, 2] of some of these properties will be presented.

A range of CMAS slags ($\text{CaO-MgO-Al}_2\text{O}_3\text{-SiO}_2$) have been studied[3] using MD in order to determine their electrical conductivities and structural properties including coordination number, relative numbers of bridging and non-bridging oxygens, relative numbers of Si-O-Si and Si-O-Al bridges, and the degree of polymerisation.

Artificial neural networks (ANN) have been employed to study the possible structure-conductivity relationship for CMAS slag systems. Various combinations of structural properties were used as ANN inputs in order to determine which are most effective in predicting conductivities as outputs, while ANN settings or conditions were also tested.

- [1] I.T. Todorov; W. Smith; K. Trachenko and M.T. Dove, “ *DL_POLY_3: new dimensions in molecular dynamics simulations via massive parallelism.*” *J. Mat. Chem.*, 2006, **16**, 1911-1918.
- [2] A. Pedone, G. Malavasi, M.C. Menziani, Alastair N. Cormack and U. Segre, “*A New Self-Consistent Empirical Interatomic Potential Model for Oxides, Silicates, and Silica-Based Glasses*”, *J. Phys. Chem. B*, 2006, **110**, 11780-11795.
- [3] L. Mongalo; A.S. Lopus and G.A. Venter, “*Molecular Dynamics Simulations of the Structural Properties and Electrical Conductivities of Cao-MgO-Al₂O₃-SiO₂ Melts*”, *J. Non-Cryst. Sol.*, 2016, **452**, 194-202.