

Coal ash chemistry by experiments and theoretical calculation

Jin Bai, Lingxue Kong, Huaizhu Li, Wen Li

State Key Laboratory of Coal Chemistry, Institute of Coal Chemistry, Chinese

Academy of Sciences

Email: stone@sxicc.ac.cn (Jin Bai)

Silicates melts widely exist in the earth and also other planets such as Mars et al. Coal mineral is just one of the silicates. Coal ash chemistry is the interdisciplinary of coal chemistry, silicate chemistry, physical chemistry and chemical engineering. It plays the key role for stable and long term operation of coal gasifiers, especially for the slagging gasifiers. We combined in-situ experiments, thermodynamic calculation (FactSage) and molecular simulation to investigate the properties of coal ash transformation at high temperatures. The process from solid to liquid phase in ash sintering and fusion process has been detailed interpreted through TMA and FactSage calculation, and the new method for liquidus temperature is also built based on FactSage data. The crystallization of minerals is regarded to manipulate the slag flow behavior at cooling condition during slag tapping. The crystallization kinetics of typical minerals in coal ash slag including anorthite, spinel, mullite were established. Combining with thermodynamic data, then it is possible to predict the slag flow behavior following the physical laws.