Challenges in the thermodynamic determination of sulphur activity and solubility in iron melt

Anže Bajželj[1,2], Tilen Balaško[2] Jaka Burja[1,2]

[1] *Institute of Metals and Technology, Ljubljana, Slovenia.*
[2]*University of Ljubljana, Faculty of Natural Sciences and Engineering, Department of Materials and Metallurgy, Ljubljana, Slovenia.*
E-mail: anze.bajzelj@imt.si

Sulphur is an important element in iron melt, often viewed in a negative light, as even in small quantities, it can cause problems during steel casting, lead to hot shortness during hot forming, degrade mechanical properties, and create various other issues. Despite its negative attributes, sulphur plays a crucial role in steel welding capabilities, and forms non-metallic inclusions which can promote good chip formation, thereby accelerating steel machinability.

Sulphur is a surface-active element, meaning it preferentially occupies phase boundary sites and thus significantly affects the system's surface energy and Gibbs free energy, even at low concentrations. This means that even at low dissolved sulphur concentrations in the melt, changes in the surface energy of the steel melt occur, along with the formation of more non-metallic inclusions. In the presence of sulphur in iron melt, a greater number of both sulphide and other non-metallic inclusions form.

The solubility of sulphur in molten iron is high, but determining the concentration of dissolved sulphur is extremely challenging. In practice, a multiphase high-temperature equilibrium system exists, comprising iron melt, a gas phase, and slag. Each phase contains a certain amount of dissolved sulphur, which cannot be accurately determined at a given moment, temperature, and pressure. Therefore, it is neither simple nor precise to estimate the amount of dissolved sulphur in the melt, which would serve as a basis for further evaluation of the number of non-metallic inclusions.

The present research will focus on methods for determining the solubility of sulphur in iron melt. The literature provides several examples used for assessing sulphur solubility in iron melts. In steelmaking practice, slag also enters the system, significantly influencing sulphur solubility in the melt. Various empirical models are used to estimate the distribution of sulphur between the melt and slag, with these models being based on empirical data due to the system's complexity.