Master Thesis / PFE offer – Material Science

Thermodynamics of residual elements in steel matrix in the frame of new decarbonised metallurgical routes

Decarbonization of steel production will be partially done with mixed optimized scraps / Direct Reduced Iron (DRI) loading in Electrical Arc Furnace. This steelmaking solution for CO_2 neutral steel production will introduce higher quantities of residual elements in the liquid steel (Sn, Sb, P, Mo, As) which cannot be eliminated by classical refining operation. In order to develop metallurgical solutions to manage these impurities in the steel, a state of the art of the thermodynamics must be proposed to define knowledge gaps.
In this study, a literature survey will first be carried out to collect existing data on thermodynamic quantities (e.g. solubility, enthalpy, activity, etc.), in Fe solid solution (austenite or ferrite), for a number of selected systems (e.g. binary systems such as Fe-Mo, Fe-Sn...). Machine learning approaches will then be used, fed by these bibliographic data. A few targeted experiments (typically thermal analysis) could also be carried out. The aim is to obtain a model for predicting the solubility of residual elements (in the ppm range) in steels.

Keywords: Metallurgy - Thermodynamics - Phase transformation

Starting time: February/March 2025, duration 6 months

Location: SIMAP Laboratory (Univ. Grenoble Alpes, CNRS, Grenoble INP) 1130 Rue de la Piscine, BP 75, 38402 Saint Martin d'Hères, France.
In the framework of a program associating SIMaP laboratory and ArcelorMittal Research Center, Maizières-les-Metz.

Requirements: Master student (M2 Master thesis) or engineer student (PFE) with a background in material science and solid knowledge in metallurgy, thermodynamics and phase diagrams, and an interest in exploratory research and machine learning.
The candidate will receive the legal internship allowance.

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References:
Y.M. Zhang *et al.*, Revisiting Hume-Rothery's Rules with artificial neural networks, Acta Materialia 56 (2008) 1094–1105. https://doi.org/10.1016/j.actamat.2007.10.059.

Chen *et al.*, Coupling physics in machine learning to investigate the solution behavior of binary Mg alloys, Journal of Magnesium and Alloys 10 (2022) 2817-2832. In open access at https://doi.org/10.1016/j.jma.2021.06.014.