

The power of computational thermochemistry in high-temperature process design and optimization: Part 1 - Unit operations

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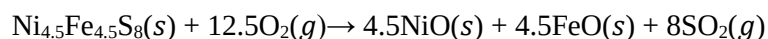
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Supplementary Material

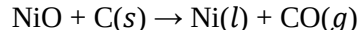
This file provides an overview of reactions related to each case study presented in the main manuscript. These reactions are simplified approximations based on stoichiometric compounds, *i.e.*, multicomponent phases are not considered.

Case study #1:

- Roasting of pentlandite ($\text{Ni}_{4.5}\text{Fe}_{4.5}\text{S}_8$) [1]:

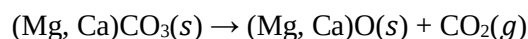


- Carboreduction of nickel monoxide:



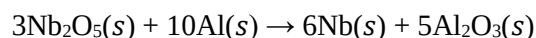
Case study #2:

- Example of thermal decomposition of carbonates:

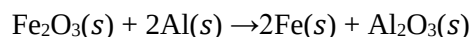


Case study #3:

- Aluminothermic processing of niobium oxide [2]:

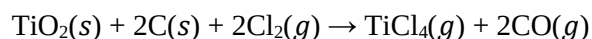


- Aluminothermic processing of iron oxide [2]:

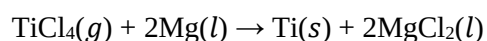


Case study #4:

- Carbochlorination of titanium dioxide [3]:



- Magnesiothermic reduction of TiCl_4 [3]:



Rererences

- [1] M. S. Moats, W. G. Davenport, Nickel and cobalt production, in: Treatise on Process Metallurgy, Elsevier, 2014, pp. 625–669.
- [2] J. Yang, F. Bourgeois, K. Bru, A. Hakkinen, E. Andreiadis, D. Meyer, Q. Bellier, H. BArt, S. Virolainen, J. Lambert, et al., State of the art on the recovery of refractory metals from primary resources, msp-refram, european union's horizon 2020 research & innovation programme under grant agreement no. 688993, accessed march 20th, 2020, 2016.
- [3] Y. Xia, H. D. Lefler, Z. Z. Fang, Y. Zhang, P. Sun, Energy consumption of the kroll and hamr processes for titanium production, in: Extractive Metallurgy of Titanium, Elsevier, 2020, pp. 389–410.