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Thermodynamic Optimization of Critical Metals Processing and Recovery: Part II

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INTRODUCTION

The two conventional metallurgical processing routes for metals extraction from primary resources (mining) and recovery from secondary resources (urban mining and industrial side streams) are pyrometallurgy and hydrometallurgy. A third route combines pyro- and hydrometallurgical processes in a unique way to exploit strengths of the two approaches. In all cases, the selection of the processes to be applied depends mainly on the composition of the feedstock, economic feasibility, and environmental constraints associated with each process.[1] One of the most important pretreatments in the production of metals and chemicals via pyro- and hydrometallurgical processing routes is roasting. Roasting involves gas–solid reactions, and the process valorizes the feedstock for the subsequent metallurgical processing. In addition to dead and partial roasting, decomposition and sulfating roasting are also widely used pyrometallurgical pretreatment processes. Most sulfide ores, concentrates, and tails in general tend to oxidize in air, and these reactions are exothermic. Consequently, heat recovery that contributes to energy efficiency is also an essential part of industrial processes for both complete and partial roasting.

Chukwunwike Iloeje, Fiseha Tesfaye, and Alexandra E. Anderson are guest editors for the Process Technology and Modeling Committee and the Recycling and Environmental Technologies Committee of TMS and coordinated the topic Thermodynamic Optimization of Critical Metals Processing and Recovery in this issue.

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Today, various smelting processes incorporate processing of secondary resources, such as waste electrical and electronic equipment (e-waste). The increasing amount and complexity of e-waste introduce new and additional valuable metals into the conventional metallurgical processes. To efficiently recover these valuable metals, and to define optimal processing parameters, fundamental knowledge regarding the behavior and impact of different (trace) elements and process chemistry is essential.[2] These trends motivate the need to develop systematic thermodynamic optimization theory and techniques, and to conduct detailed materials processing analyses. Such analyses identify optimal parametric relationships, process conditions, and processing strategies that increase resource recovery, improve energy efficiency, and reduce waste generation in metals production from primary and secondary sources. This highlights the value proposition of fundamental research such as determining the phase stability and effect of additives on alloy systems, as well as understanding the effects of composition and processing conditions on material properties and process yield efficiencies.

JOM advisors of the Process Technology and Modeling Committee and the Recycling and Environmental Technologies Committees of TMS organized this special, two-part topic on the "Thermodynamic Optimization of Critical Metals Processing and Recovery," inviting manuscripts that address topics in generalized theory, processing design, and experimental analysis. The first part, published in February 2021, comprised articles that describe experimental and modeling work that investigate material property evolution and thermodynamic optimization approaches for both superalloy development and extractive metallurgy processes.[3] This second part complements the first with articles that employ thermodynamic analysis to elucidate interactions between material properties and processing conditions for both pyro- and hydrometallurgical systems, developing blueprints for novel or improved pretreatment and extractive processes, and supporting results with experimental measurements and pilot process data. After peer review by several experts in the field, seven original research articles were approved for publication.

In the work entitled “Thermodynamics and Reduction of Bi_2O_3 in Waste Tire-Derived Atmosphere,” Atlay and Eroglu investigated the reduction behavior of bismuth oxide in the pyrolysis gas of waste tire. Through thermodynamic analysis carried out in the Bi-O-C-H-S-Ar system, they estimated the temperature range of 427°C to 627°C to be favorable for reduction of Bi_2O_3 to metallic Bi. In their experiments up to 627°C, they observed that the degree of Bi_2O_3 reduction increased with increasing tire pyrolysis. Shekhter et al. developed a FactSage^{TM} software package-based thermodynamic model in their work “Thermodynamic Modeling of Molybdenite Roasting in a Multiple Hearth Furnace” to describe roasting of molybdenite in a multiple hearth furnace. They also compared their results with those of practical data received from Climax Molybdenum plants. According to them, the model allows the prediction of the behavior of impurities and enables the calculation of the content of gaseous species that cause environmental pollution.

In their work entitled “$PbSO_4$ Reduction Mechanism and Gas Composition from 600 to 1000°C,” Yun Li et al. performed thermodynamic modelling and experimental work to better understand the reduction pathways of $PbSO_4$, a common feed constituent in lead-containing waste materials. The study used various techniques to determine the influence of time, temperature, and CO/CO_2 ratio on the decomposition and reduction of $PbSO_4$ species. The authors proposed three different transformation sequences based on the thermodynamic and experimental results, one of which showed the direct reduction of $PbSO_4$ to PbS, eliminating the need to process SO_2- and/or SO_3-bearing off-gas. - Tao Chen et al. also coupled thermodynamic modeling and experimental work in their study “Effect of Mn Addition on Melt Purification and Fe Tolerance in Mg Alloys” to investigate the influence of manganese addition, temperature, and settling time on iron removal and the resulting precipitate phases in magnesium-rich melts. The thermodynamic calculations and experimental results, which were in close agreement, showed that all three variables studied influenced the type of precipitate formed as well as the elemental distribution within the melt. The authors note that both types of results generated from this study can provide practical operational guidelines for the purification and casting of these types of melts.

In the next three papers, Zekavat et al. in “Leaching of Antimony from Stibnite Ore in KOH Solution for Sodium Pyroantimonate Production: Systematic Optimization and Kinetic Study,” Xu et al. in “High-Efficiency and Oxidant-Free Leaching of Rhenium from Arsenic–Rhenium Filter Cake,” and Celep et al. in “Extraction of Metals from Scrap Marble Cutting Segments in Nitric Acid Solutions” investigated novel approaches and optimal processing conditions for efficient leaching. All three studies investigated the impact of process parameters, including concentration, temperature, solid-to-liquid ratio, and residence time, on the efficiency of the leaching process, elucidated the leaching mechanism for their respective systems, and proposed correlations for the leaching kinetics based on thermodynamic and experimental analyses. In the first study, Zekavat et al. characterized the relationship between the leaching mechanism for antimony and process conditions, identified diffusion through the ash layer as the rate-limiting step, and showed that residence time and leaching temperature were key drivers for leaching efficiency. These outcomes describe optimal process conditions for antimony recovery that can inform new hydrometallurgical mineral processing. In the second study, Xu et al. described an approach for leaching rhenium via displacement reaction in copper sulfate solution, which can avoid the negative impact of residual oxides on downstream extraction performance seen with traditional processes that use oxidizing agents. Their study identified distinct temporal phases for the leaching process and proposed a composite mechanism that captures the transition from kinetic- to diffusion-controlled leaching rates. They also identified optimal process conditions for efficient leaching. Celep et al. in the third study employed the response surface method to describe and compare respective leaching rate and extents for cobalt, copper, and silver from scrap using nitric acid. Besides demonstrating the efficacy of nitric acid as a leaching agent, their study also identified chemical kinetics as the rate-controlling process, and derived correlations that describe the leaching rate and the impact of process parameters on recovery efficiency.

The papers published in this special topic should be of interest to a broad readership including those planning to meet the strict environmental regulations while promoting sustainable production of the critical metals. All titles and authors of the articles published under the topic “Thermodynamic Optimization of Critical Metals Processing and Recovery” in the March 2021 issue (vol. 73, no. 3) of *JOM* are listed below. The articles can be accessed fully via the journal’s page at: http://link.springer.com/journal/11837/73/3/page/1.

- “Thermodynamics and Reduction of Bi_2O_3 in Waste Tire-Derived Atmosphere” by M.C. Atlay and S. Eroglu

- "Thermodynamic Modeling of Molybdenite Roasting in a Multiple Hearth Furnace" by L. Shekhter, J. Litz, N. Shah, and L. McHugh.
- "$PbSO_4$ Reduction Mechanism and Gas Composition from 600 to 1000°C" by Y. Li, P. Taskinen, Y. Wang, S. Yang, Y. Chen, and A. Jokilaaskso.
- "Effect of Mn Addition on Melt Purification and Fe Tolerance in Mg Alloys" by T. Chen, Y. Yuan, T. Liu, D. Li, A. Tang, X. Chen, R. Schmid-Fetzer, and F. Pan.
- "Leaching of Antimony from Stibnite Ore in KOH Solution for Sodium Pyroantimonate Production: Systematic Optimization and Kinetic Study" by M. Zekavat, H. Yoozbashizadeh, and A. Khodaei.
- "High-Efficiency and Oxidant-Free Leaching of Rhenium from Arsenic–Rhenium Filter Cake" by S. Xu, Y. Shen, T. Yu, H. Zhang, H. Cao, and G. Zheng.
- "Extraction of Metals from Scrap Marble Cutting Segments in Nitric Acid Solutions" by O. Celep, M. Orak, E. Y. Yazici, and H. Deveci.

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CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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