JOM, Vol. 73, No. 5, 2021
https://doi.org/10.1007/s11837-021-04634-w

THERMODYNAMIC CONSIDERATIONS FOR IMPROVED RENEWABLE ENERGY PRODUCTION

Thermodynamic Considerations for Improved Renewable Energy Production

FISEHA TESFAYE [1,3] and CHUKWUNWIKE O. ILOEJE [2,4]

1.—Johan Gadolin Process Chemistry Centre, Åbo Akademi University, Piispankatu 8, 20500 Turku, Finland. 2.—Energy Systems Division, Argonne National Laboratory, 9700 South Cass Avenue, Lemont, IL 60439-6903, USA. 3.—e-mail: fiseha.tesfaye@abo.fi. 4.—e-mail: ciloeje@anl.gov

Developing technologies essential to the transition towards a decarbonized energy future require discovery of new energy materials with unique properties and wider thermal and chemical stability ranges. To facilitate this discovery, comprehensive databases of inorganic materials critical to advanced clean energy technologies need to be developed. Recent efforts in advanced energy materials research have made progress in identifying and optimizing promising materials for high-performance energy applications. For instance, Bi-Te-based alloys with high *ZT* (figure-of-merit) values at room temperature are competitive options for thermoelectric applications in refrigeration and green power conversion from low-temperature waste heat.[1]

The search for these high-performance energy storage and conversion materials involves the determination of thermal stabilities, phase transformations, phase equilibria with coexisting phases, and other application-relevant thermodynamic properties. The availability of such data also enables efficient and cost-effective materials processing. Figure 1 illustrates the relationship of experimental techniques, computational tools, and materials design that facilitates materials discoveries with unique properties.

The *JOM* advisors of the Recycling and Environmental Technologies and Process Technology and Modeling technical committees of The Minerals, Metals & Materials Society have organized special topics focused on improved extractions and recoveries of the strategic metals including those important components of energy materials. The most recent publications are summarized in "Thermodynamic Modeling of Sustainable Non-Ferrous Metals Production: Part II".[2] This special topic complements the series by inviting original research papers focusing on the research of energy materials and energy efficiency processes. After peer-review by several experts in the field, six original research articles were selected for publication.

In the work entitled "Synthesis and Thermodynamic Investigation of Energy Materials in the Ag–Te–Cl System by the Solid-State Galvanic Cells", Moroz et al. have reviewed and experimentally investigated phase stabilities and thermodynamic properties of potential energy materials in the Ag–Te–Cl system. They presented new thermodynamic data of the candidate energy materials, $Ag_{19}Te_6Cl_7$, $Ag_{10}Te_4Cl_3$, Ag_5Te_2Cl, and $Ag_{23}Te_{12}Cl$, below 500 K. Hasanova et al. optimized the phase diagram of the Bi-Te system in their work "Refinement of the Phase Diagram of The Bi-Te System and the Thermodynamic Properties of Lower Bismuth Tellurides". Their optimization of the phase diagram incorporating Bi_2Te_3, Bi_4Te_5, Bi_8Te_9, BiTe, Bi_4Te_3, Bi_2Te, and Bi_7Te_3 compounds was based on high-temperature synthesis, differential thermal analysis (DTA), X-ray diffraction (XRD), and scanning electron microscopic analyses, as well as electromotive force (EMF) measurements of the samples. The paper "Solid-Phase Equilibria in the Cu-Sb-S System and Thermodynamic Properties of Copper-Antimony Sulfides" by Mashadiyeva et al. investigated the solid-phase equilibria and thermodynamics in the system Cu-Sb-S by means of powder X-ray diffraction (PXRD), DTA, and EMF techniques. Their proposed phase diagram suggests that the chalcogenide functional compounds, Cu_3SbS_4, $CuSbS_2$, Cu_3SbS_3, $Cu_{12}Sb_4S_{13}$, and $Cu_{14}Sb_4S_{13}$, are thermodynamically stable at 300 K. The fourth

Fiseha Tesfaye and Chukwunwike O. Iloeje are guest editors for the Recycling and Environmental Technologies Committee and Process Technology and Modeling Committee of TMS, respectively, and coordinated the topic Thermodynamic Considerations for Improved Renewable Energy Production in this issue.

(Received March 1, 2021; accepted March 3, 2021; published online March 22, 2021)

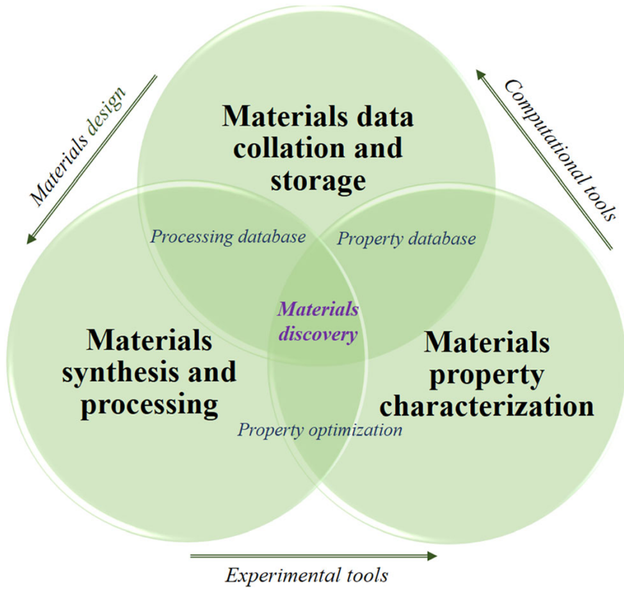

Fig. 1. Schematic of components of a comprehensive framework for materials discovery.

paper "Solid-Phase Relations in the Tl_2Te-Tl_2Te_3-$TlTbTe_2$ System and Thermodynamic Properties of Thallium-Terbium Tellurides" by Imamaliyeva et al. presents phase equilibria and thermodynamic data of phases in the Tl–Tb–Te ternary system. According to them, one of the objectives of studying such systems was to explore improved performance and additional functionality of materials because of the introduction of rare-earth elements. They applied the EMF and PXRD analysis techniques to investigate the thermodynamic properties of the equilibrium phases and their relationships in the system.

The last two papers in this topic, "Production of High Purity TiO_2 Powder from $FeTiO_3$ via High Temperature Sulfurization" by Shin et al. and "A Study on the Roasting Process for Efficient Selective Chlorination of Ilmenite Ores" by Kim et al., present interesting thermodynamic considerations for efficient titanium production through high-temperature processes. Titanium is used in various applications ranging from aerospace parts, power plants, and automotive parts to the medical and steel industries owing to its lightweight and excellent corrosion resistance. In particular, its light weight combined with the other important properties make titanium the choice as an alloying element for energy-efficient applications.

The peer-reviewed articles in this special topic could be of interest to a broad readership, including those promoting efficient recovery of low-temperature waste heat. All the titles and authors of the articles published in the May issue of *JOM* (volume 73, issue 5) under the special topic "Thermodynamic Considerations for Improved Renewable Energy Production" are listed below. The articles can be fully accessed on the journal's web page at: http://link.springer.com/journal/11837/73/5/page/1.

- "Synthesis and Thermodynamic Investigation of Energy Materials in the Ag–Te–Cl System by the Solid-State Galvanic Cells" by M. Moroz, F. Tesfaye, P. Demchenko, M. Prokhorenko, S. Prokhorenko, D. Lindberg, O. Reshetnyak, and L. Hupa.
- "Refinement of the Phase Diagram of the Bi-Te System and the Thermodynamic Properties of Lower Bismuth Tellurides" by G. Hasanova, A. Aghazade, S. Imamaliyeva, Y. Yusibov, and M. Babanly.
- "Solid-Phase Equilibria in the Cu-Sb-S System and Thermodynamic Properties of Copper-Antimony Sulfides" by L.F. Mashadiyeva, P.R. Mammadli, D.M. Babanly, G.M. Ashirov, A.V. Shevelkov, and Y.A. Yusibov.
- "Solid-Phase Relations in the Tl_2Te-Tl_2Te_3-$TlTbTe_2$ System and Thermodynamic Properties of Thallium-Terbium Tellurides" by S. Imamaliyeva, D. Babanly, V. Qasymov, and M. Babanly.
- "Production of High Purity TiO_2 Powder from $FeTiO_3$ via High Temperature Sulfurization" by S.-H. Shin and S.-J. Kim.
- "A Study on the Roasting Process for Efficient Selective Chlorination of Ilmenite Ores" by J. Kim, Y.R. Lee, and E.J. Jung.

ACKNOWLEDGEMENTS

The organizers of this topic would like to thank all the authors and reviewers who have contributed to the successful publication of this special issue. The authors of this editorial article are grateful to the Academy of Finland (decision number 311537) for financial support as part of the activities of the Johan Gadolin Process Chemistry Centre at Åbo Akademi University. We acknowledge support from UChicago Argonne LLC, Operator of Argonne National Laboratory ("Argonne"). Argonne National Laboratory's work was supported by the U.S. Department of Energy, Office of Energy Efficiency and Renewable Energy, under contract DE-AC02-06CH11357. The U.S. Government retains for itself, and others acting on its behalf, a paid-up nonexclusive, irrevocable worldwide license in said article to reproduce, prepare derivative works, distribute copies to the public, and perform publicly and display publicly, by or on behalf of the Government. The Department of Energy will provide public access to these results of federally sponsored research in accordance with the *DOE Public Access Plan*.

CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

REFERENCES

1. Ch. Wang, Mh. Li, Cw.Chiu, and X.-H. Wang, *JOM* 72, 3558–3566 (2020). https://doi.org/10.1007/s11837-020-04288-0.
2. C.O. Iloeje, F. Tesfaye, and A.E. Anderson, *JOM* 73, (2021). https://doi.org/10.1007/s11837-020-04561-2.