Industrial Materials For The Future

Project Fact Sheet

Thermochemical Models and Databases for High-Temperature Materials Processing and Corrosion

Benefits

Improved thermochemical understanding of glass and refractory systems will lead to substantial economic, energy, and environmental benefits.

- The availability of thermodynamic data for various glass systems could lead to improved, higher-strength glass and thus lighter glass.
- Improved refractories that result from a better understanding of chemical behavior would lead to improved furnace designs, which are estimated to yield a 12.5 % improvement over conventional furnaces.
- Estimated savings would be in the vicinity of 12 trillion Btu/year for a 50% market introduction.

Applications

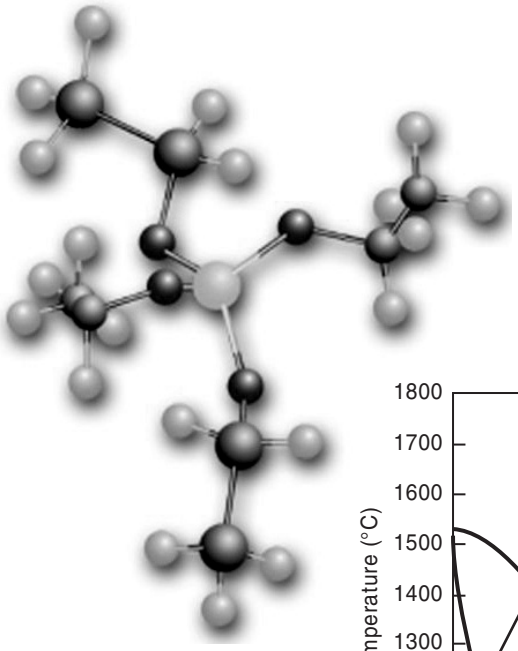
This project has applications throughout the IOF and supporting industries:

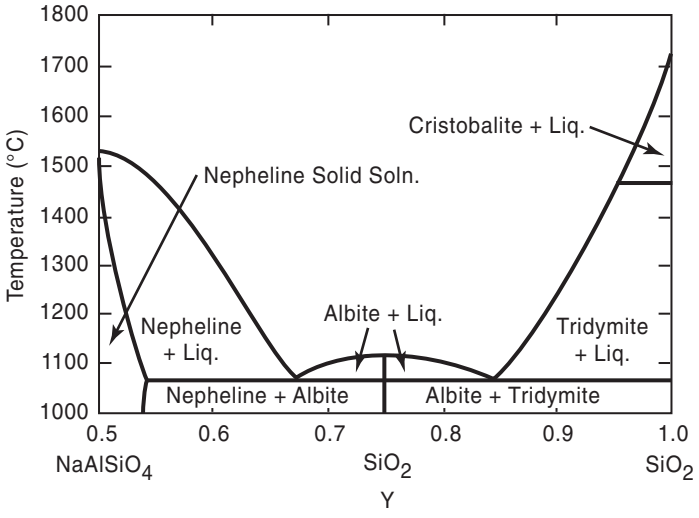
- **Agriculture,**
- **Aluminum,**
- **Chemical,**
- **Forest Products,**
- **Glass,**
- **Heat Treating,**
- **Metalcasting,**
- **Mining,**
- **Petroleum,**
- **Process Heating,** and
- **Steel.**

- Prediction of melting temperatures and the formation of flaws in glass formulations for the glass industry.
- Enabling computational models to predict corrosion of refractories and other materials for the glass and heat-treating industries.
- Heat-transfer modeling of furnaces and molten phases of glasses and metals for the glass and heat-treating industries.
- Modeling of high-temperature chemical reactions occurring in material synthesis.
- Prediction of process energy efficiency and pollutant formation for combustion and other high-temperature manufacturing processes for the furnace-manufacturing industries.

An internally consistent thermochemical database for refractory oxide materials will enable the prediction of the behavior of materials at high temperatures.

The objective of this project is to employ advanced computational techniques to develop a coherent database of thermochemical values and sets of models for gas and condensed-phase systems of importance to the processing of glass and to the industrial use of refractories. The product will be a web-based database/model information site that will provide the necessary input for commercial application.





Calculated phase diagram.

Project Description

Goal: The goal of the project is to greatly improve the availability, accuracy, and accessibility of thermochemical property data required to understand, simulate, and optimize industrial processes involving glass and refractory materials at high temperatures.

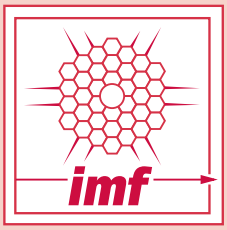
Issue: Even though accurate thermodynamic data are critical to modeling high-temperature processes, industry has been unable to invest in the measurement or prediction of such data. As a result, industry is forced to rely on the incomplete and inaccurate data currently available or resort to methods of estimation.

Approach: The present project will employ the latest theoretical and computational concepts to address the need for improved and expanded thermochemical data in modeling high-temperature glass and refractories. This basic information will be available for use in global thermochemical calculations for predicting behavior in high-temperature systems.

Potential payoff: (1) The models and thermochemical data generated by this project will enable the development of new classes of ceramic and composite materials needed to improve component lifetimes, increase energy efficiency, and reduce waste in furnaces and other high-temperature processes. (2) The data can also be used in the development of functionalized coating systems for improving refractory longevity or increasing the energy efficiency of glass. (3) Modeling of combustion and materials synthesis processes (e.g., on-line coating of glass) will be greatly facilitated by the availability of a large-scale, self-consistent database of thermodynamic properties, which are key inputs to any model of a high-temperature process. The results of this work, if introduced to 50% of the potential market, could lead to as much as 12 trillion Btu/year in energy savings.

Progress and Milestones

- Develop and validate critical subcomponents for glass model.
- Establish method for predicting gas-phase thermochemistry of transition-metal compounds.
- Make go/no-go decision to build comprehensive glass thermochemical model.
- Complete web site design for distribution of project results.
- Complete integrated (gas+solid-phase) web-based thermochemical information system.
- Complete thermochemical database for gas-phase compounds.



Primary

Sandia National Laboratories
Livermore, CA

Oak Ridge National Laboratory
Oak Ridge, TN

Project Partners

American Air Liquide
Countryside, IL

Atofina Chemicals, Inc.
King of Prussia, PA

Lawrence Livermore National Laboratory
Livermore, CA

Monofrax, Inc.
Falconer, NY

Pilkington North America
Toledo, OH

PPG Industries, Inc.
Pittsburgh, PA

Reaction Design
San Diego, CA

RHI Refractories (formerly Harbison-Walker)
West Mifflin, PA

Shell Oil Products Company, LLC
Houston, TX

SRI International
Menlo Park, CA

For Additional Information, Please Contact

EERE Information Center
Phone: (877) 337-3463
Fax: (360) 236-2023
eereic@ee.doe.gov

Visit our home page at
http://www.eere.energy.gov/industry/

Office of Industrial Technologies
Energy Efficiency
And Renewable Energy
U.S. Department of Energy
Washington, DC 20585
http://www.oit.doe.gov

January 2002

ORNL 2002-01489/chj