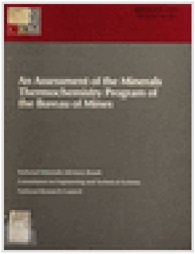

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AN ASSESSMENT OF THE MINERALS THERMOCHEMISTRY PROGRAM OF THE BUREAU OF MINES

Report of the
Committee on Mineral Resources Technology

National Materials Advisory Board
Commission on Engineering and Technical Systems
National Research Council

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1983

NOTICE: The project that is the subject of this report was approved by the Governing Board of the National Research Council, whose members are drawn from the Councils of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine. The members of the committee responsible for the report were chosen for their special competences and with regard for appropriate balance.

The report has been reviewed by a group other than the authors according to procedures approved by a Report Review Committee consisting of members of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine.

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ABSTRACT

This report assesses the Bureau of Mines efforts in thermochemistry, based principally on findings from a visit to the Bureau's Albany Research Center by a working group of the Committee on Mineral Resources Technology. Included are comments on organization, budget, personnel, major experimental methods, data compilation and evaluation, equipment and facilties, and the utility of thermochemical data. The Bureau's program is evaluated through answers to a series of questions: Does a real need exist? Who are the users? Are the current approach and priorities responsive? Is the current level of effort appropriate? Could personnel be used to greater advantage elsewhere? The committee concluded that the program is an extremely valuable one that fills a special need and that the current approach and priorities are responsive to that need. Specific recommendations are also made concerning the support of current research as well as expanding research beyond the present pure substances.

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PREFACE

In 1980, at the request of the Bureau of Mines of the U.S. Department of the Interior, the National Materials Advisory Board established the Committee on Mineral Resources Technology to assess the Bureau's mineral resources technology program. The committee's general objective has been to provide an ongoing assessment of the program's materials aspects, identify gaps, and suggest opportunities to make the program as effective and responsive as possible to national needs.

In a second year's effort, the committee has pursued in greater depth selected portions of the areas covered in the first year, i.e., the Bureau's efforts in minerals thermochemistry and materials substitutes.

This report presents an evaluation of the minerals thermochemistry efforts of the Bureau. The on-site assessment at the Bureau's Albany, Oregon Research Center was performed by a small working group of the committee composed of committee member Herbert H. Kellogg, acting as chairman, and committee technical advisor Reinhardt Schuhmann, Jr., as a working group member. The group was accompanied by liaison representative Kenneth W. Mlynarski and staff officer Richard M. Spriggs. Committee member Milton E. Wadsworth was also slated to be a working group member but was unable to attend. The initial draft of this report was prepared by Professors Kellogg and Schuhmann.

This report has been reviewed by the committee and by outside reviewers. Readers should keep in mind that this report deals only with a limited portion of the total Bureau of Mines effort in mineral resources technology. Reports evaluating other parts of the effort will be published separately, as will the committee's report on the entire mineral resources technology effort.*

On behalf of the committee, I would like to thank the members of the working group, the staff, and the liaison representatives who participated in this project. In addition, thanks are extended to the director and staff of the Bureau of Mines Research Center at Albany, Oregon, which was visited by the working group in conjunction with its evaluation.

Nathaniel Arbiter
Chairman

*As a result of a recent reorganization of the Bureau of Mines, the non-mining portion of the Mineral Resources Technology Program is now identified as the Minerals and Materials Research Program.

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INTRODUCTION

The Committee on Mineral Resources Technology has been charged with providing an ongoing assessment of the mineral resources technology program of the Bureau of Mines, especially to identify gaps and recognize opportunities to make the program as responsive as possible to national needs.

During 1982, the committee was requested to assess selected portions of the program in depth. This report is an assessment of minerals thermochemistry, which is a subelement of the mineral science base. The mineral science base element is designed to provide fundamental scientific information needed to expand the knowledge base from which future mineral processing problems will be solved.

The assessment of the minerals thermochemistry program was performed principally through an on-site visit by a working group of the committee. The group visited the Albany Research Center of the Bureau of Mines on April 19-20, 1982. Visits were made to each laboratory engaged in thermochemical studies. Extensive discussions were held with F. E. Block, Center Research Director; N. A. Gokcen, Supervising Research Chemist, Thermodynamics Group; and other senior research personnel regarding the objectives, methods, resources, management, and output (principally publications) of the Thermochemistry Group of the center.

The following assessment consists of descriptive comments on organization, personnel, budget, major experimental methods, data compilation and evaluation, and laboratory equipment and facilities, and some remarks concerning the utility of thermochemical data. In addition, the Bureau's program in thermochemistry is evaluated in terms of responses to a series of questions raised by the Bureau.

ORGANIZATION, PERSONNEL, AND BUDGET

Thermochemical studies at Albany are principally centered in the Thermodynamics Group, consisting of ten professionals with a budget of $710,000 for FY 82. This group utilizes a variety of precise experimental calorimetric and equilibrium research methods to measure thermodynamic properties of pure substances and also conducts extensive desk studies leading to compilation, critical evaluation, and publication of thermochemical data.

Starting with the current year, the work of the Thermochemical Group is being supplemented by a group of three professionals from the Pyrometallurgy Group, with a budget of $200,000. This group is making thermochemical studies of the systems Al-C-Si and Al-O-C-Si at temperatures near 2000°C.

The Thermodynamics Group's effort is a continuing one that has been in existence at the Bureau for more than 50 years. Until 1966, projects at the Bureau's Thermodynamics Laboratory in Berkeley, California, were generally associated with the works of K. K. Kelley, whose series of data compilations and critical evaluations of thermodynamic data provided an essential data base underlying the great expansion of thermodynamics research and practical metallurgical applications that occurred in the United States during the post-World War II years. The objective of continuously adding new experimental data and critical evaluations of existing data to the accumulated knowledge of thermodynamic properties of materials is an open-ended goal that will never be fully satisfied. In contrast, the smaller thermochemical effort of the Pyrometallurgy Group has a specific goal; presumably this effort will cease when the objective has been reached.

MAJOR EXPERIMENTAL METHODS

To measure thermodynamic properties of mineral and metallurgical substances, the Thermodynamics Group at Albany uses high-temperature, low-temperature, and solution calorimetry as well as other methods.

High-Temperature Calorimetry

A copper-block calorimeter is used to measure the heat content of substances relative to room temperature ($H_T - H_{298}$) by dropping an encapsulated sample from a known high temperature into a copper block of known heat capacity and measuring the temperature rise of the block. Two different furnaces for heating the sample permit measurements up to 1200° and 1800°K, respectively.

The incremental enthalpy and entropy data ($H_T - H_{298}$ and $S_T - S_{298}$) obtained from these measurements are universally used by design engineers for making heat balances on new processes or for predicting the behavior of new feed materials in existing processes. They are also essential, in conjunction with other thermodynamic measurements, for calculating the temperature-dependence of high-temperature chemical equilibria occurring in metallurgical processes. Recent determinations using this procedure have made available high-temperature enthalpy data for the following metallurgically important substances: Cu_2S, Al_2S_3, $KAlO_2$, $Li_2Al_2Si_8O_{20}$, $Na_5Al_3F_{14}$, ZrI_4, K_2SiO_3, $K_2Si_2O_5$, and others.

Low-Temperature Calorimetry

An automated low-temperature adiabatic calorimeter is capable of making precise measurements of the heat capacity of substances between 5° and 300°K. Very few laboratories throughout the world are equipped to make these very sophisticated measurements that are essential to the precise determination of the standard entropy of chemical substances. Standard entropy (S_{298}), along with enthalpy of formation (ΔH_{f298}) and high-temperature enthalpy and entropy increments, constitute one major measurement scheme for predicting chemical equilibria at high temperature. The Bureau laboratory has recently reported entropy measurements for Al_2S_3, Cu_2S, $K_2Si_2O_5$, $FeCl_3$, FeOCl, $Na_5Al_3F_{14}$, TiO, and other substances of metallurgical importance.

Solution Calorimetry

The Bureau laboratory operates three solution calorimeters for the determination of the standard enthalpy of formation of chemical substances (ΔH_{f298}). The hydrochloric acid solution calorimeter is used for substances soluble in this medium, such as AlCl, $Mn(OH)_2$, and $CuCl_2$. The hydrofluoric acid calorimeter is used primarily for measurements on silicates ($NaFeSi_2O_6$, $Li_2Al_2Si_8O_{20}$, etc.). A newly devised bromine-hydrobromic acid calorimeter is used for determining the heat of formation of metal sulfides.

Values of ΔH_{f298} for chemical and mineral substances are basic to heat balance and chemical equilibrium calculations, yet knowledge of this property is lacking for many substances, and is very inexact for many others. The Bureau research on this subject continues to fill gaps in the data base for this essential quantity.

Other Experimental Methods

The Bureau is developing a specially modified and automated differential scanning calorimeter/thermogravimetric analyzer (DSC/TGA). When operative, this device should make it possible to accumulate data very rapidly on the heat capacity and enthalpy of transition for a wide variety of metal oxides, chlorides, sulfates, and sulfides. The data obtained will not be as precise as those determined by the copper block calorimeter, but they can be determined much more rapidly and they should be of adequate accuracy for many purposes.

Direct measurement of high-temperature chemical equilibria involving mixtures of M/MO (metal/metal oxides) or MO/MS (metal oxide/metal sulfides) are made by means of electrochemical cells employing stabilized zirconia as a solid electrolyte. This well-established technique is capable of much better precision than most other means for studying high-temperature equilibria. Analysis of equilibrium data as a function of temperature also permits calculation of reaction entropy and enthalpy as a check on other methods for obtaining these quantities. This method has recently been used by the Bureau to determine the standard free energy of formation of ZnS(β), MoS_2, WS_2, MnS, and $Fe_{0.9}S$. Other galvanic cells have been used to study the standard free energy of FeF_2 and FeF_3, and the thermodynamic properties of liquid Al-Ni and Al-Si alloys.

The thermodynamic activity of aqueous solutes, knowledge of which is essential to quantitative application of thermochemical calculations to hydrometallurgical systems, is being measured by a novel apparatus for the measurement of the partial pressure of water vapor over the solution. The method is capable of yielding values of activity for the concentrated, multicomponent aqueous solutions that are of practical interest in hydrometallurgical processes. Solutions of $CoCl_2$, $CuSO_4$, $MnSO_4$, and $ZnSO_4$ are currently being studied.

The Pyrometallurgy Group is engaged in studies of the phase equilibria in the systems Al-C-Si and Al-O-C-Si at temperatures near 2000°C. These very difficult studies are needed to better understand recent unsuccessful attempts to produce aluminum or aluminum-silicon alloys by carbothermic reduction of aluminum-bearing raw materials (clays and/or bauxite).

DATA COMPILATION AND CRITICAL EVALUATION

The Thermodynamics Group at Albany is maintaining an active effort in compilation and critical evaluation of thermochemical data, continuing the program carried on for many years by Dr. K. K. Kelley, who is best known to two generations of chemical metallurgists for his classic series of Bureau of Mines Bulletins entitled "Contributions to the Data on Theoretical Metallurgy." The continued updating of compilations such as these, the labor involved in searching the literature, the critical evaluation of conflicting data, and the extrapolations and interpolations are all done by researchers with special expertise. Thus, the user of the published compilation, whether in academic research, industrial process engineering, or new process development, has readily available the best thermodynamic information needed for a particular problem.

The current compilation effort at the Bureau has been improved by a computer-assisted data bank as well as computerized calculation, graphics, and word processing. Despite these aids, however, data evaluation depends heavily on highly experienced personal judgment, and the Bureau has recently lost (by retirement) one of its two researchers assigned to this work.

A major compilation of thermochemical properties of the elements and their oxides will soon be issued, but a companion volume on the critically important metal sulfides is only partly completed, and work on it has been temporarily discontinued because of the retirement mentioned. The Bureau should give a high priority to filling the vacancy in the data evaluation staff because of the special value of the data compilations to the metallurgical industry.

LABORATORY EQUIPMENT AND FACILITIES

The various calorimeters with their associated control and measurement instrumentation at Albany constitute a unique and probably irreplaceable facility for measuring thermodynamic properties. Several of the units clearly evolved from, and even included original parts from, the precision units developed at Berkeley. However, the replacement of old-fashioned instrumentation with modern electronic instrumentation, data processing, and automation appears to substantially increase the data productivity of the classical methods.

Other experimental requirements of the thermochemistry program for materials preparation, analysis, and structural characterization are well met in facilities that appear to have been fully modernized in the last year or two.

THE UTILITY OF THERMOCHEMICAL DATA

Thermochemistry employs the fundamental relations of thermodynamics, along with measured thermochemical properties of substances, to yield quantitative predictions of the energy flows into (or out of) chemical reaction systems and the equilibrium or rest state of the system. To cite a simple example: if 107 m^3 (S.T.P.) of air at 25°C are blown through a bath consisting of 159 kg of molten Cu_2S maintained at 1227°C, the equilibrium state of the resulting system and the heat release can be predicted from a knowledge of the thermochemical properties of the system Cu-O-S-N without the necessity of costly and time-consuming experiments. In this example it can be shown that the oxygen from the air will react quantitatively with the copper sulfide to yield about 127 kg of molten copper containing predictably small amounts of dissolved oxygen and sulfur, and 107 m^3 (S.T.P.) of a gas consisting of 21 percent SO_2 and 79 percent N_2. The reaction will release 8270 kcal of heat to the surroundings if the temperature of liquid and product gas is maintained at 1227°C. Other possible reaction products, such as Cu_2O, CuO, $CuSO_4$, CuS, SO_3, SO, S_2, NO, and NS, can be shown to be either absent or negligible in amount.

Calculations such as this consume only minutes or hours of one person's time, whereas performance of the experiment with any degree of accuracy would require costly equipment and the work of several people over a period of weeks. Essential to the calculation, however, is an accurate knowledge of the thermochemical properties of all possible species in the system Cu-O-S-N, and these data require considerable time and effort for determination. The overriding advantage of the thermochemical approach comes from the fact that, once the properties of a substance like Cu_2S have been determined, its behavior can be predicted in <u>any</u> reaction system--i.e., time-consuming determinations of thermochemical properties for a chemical substance serve to predict the behavior of that substance in a wide variety of practical systems.

The knowledge of thermochemical properties of chemical substances that has accumulated during the 20th century is now sufficiently comprehensive for process design and development laboratories throughout the world to use thermochemical calculations on a routine basis. This applies equally well to the chemical and petrochemical industries, the plastics industries, the biological and drug industries, the electronics industries, the fuels and power industries, as well as to metals production and use industries. Equilibrium calculations involving enthalpy, entropy, and free energy are used to predict the direction and extent of reaction, yields, and even estimated costs. Heat-balance calculations involving enthalpy are used to predict fuel requirements and heat recovery from products. The rapid escalation of fuel prices over the past 10 years has focused attention on redesign of processes to conserve energy, and thermochemical calculations are indispensable for this purpose.

Particularly when confronted by a new problem or novel process, application of thermochemical calculations is usually the first step towards a quantitative understanding of the system behavior. Unfortunately, lack of thermochemical data usually precludes full use of what the chemical substance has to offer. The expansion of our knowledge of thermochemical data is a continuing need that is essential to technological progress in many diverse fields.

EVALUATION OF THE PROGRAM IN THERMOCHEMISTRY

The committee was asked to evaluate the Bureau's thermochemical program with respect to four criteria. They are discussed in the following sections.

Need for the Information

The committee was asked whether a real need for the information generated by this research exists in the mineral community. Who are the users?

The users are industrial laboratories and process development teams, offices of design and construction companies engaged in metallurgical projects, contract research organizations, and academic laboratories. Any researcher or laboratory called on to make the most basic evaluation of a metallurgical process--namely, a heat balance--must employ thermochemical data (ΔH_{f298} and $H_T - H_{298}$). In addition, more sophisticated metallurgical calculations that attempt to predict the chemical equilibria that determine the feasibility of an untried metallurgical process must use free energy calculations (a combination of data for ΔH_{f298}, $H_t - H_{298}$, S_{298}, and $S_T - S_{298}$ as well as activity data for solution systems).

The use of thermochemical calculations by all sectors of the metallurgical industry and academia is now so common as to be comparable to the use of computers. In fact, the use of computers and the use of thermochemical calculations have much in common. Both provide means to arrive at useful answers as quickly as possible. When combined--thermochemical calculations made with the aid of computer--they form a powerful team that has become a necessity for modern metallurgical and chemical process research and development.

The Bureau's work on thermochemistry fills the special need of providing data on important mineral and metallurgical materials. Other laboratories engaged in thermochemical research are mostly academic laboratories in departments of chemistry and metallurgy. Their choice of substances to study is dictated by goals of theoretical chemistry rather than practical metallurgical problems. As a result, they have little interest in mineral materials, and only a dedicated laboratory such as the Bureau's can be relied on to fill the gaps in knowledge of metallurgically important substances.

The Bureau is to be specially commended for recognizing the importance of thermochemistry as long ago as 1930. At that time, thermochemistry was in its infancy, and some legitimate doubts of its utility might have been raised. Today, all metallurgists recognize its importance, and its value will increase as the properties of more and more substances of metallurgical interest are determined.

Responsiveness to the Need

The committee was asked if such a need exists, whether the current approach and priorities are responsive to that need.

The Albany Research Center Laboratory is probably the only one in the world that continuously produces such a wide spectrum of thermochemical measurements. No one of the experimental techniques used by the Laboratory can be singled out as less important than the others. Each contributes vital data to the bank of thermochemical knowledge. The data evaluation and compilation of work should perhaps be singled out as having special importance. That work deserves the effort of at least two full-time, experienced researchers. It should be brought back to that level as soon as possible.

The Bureau's work is more valuable to some researchers than to others. For example, recent studies of the properties of $FeCl_3$ and $FeOCl_2$ should prove valuable for research on chlorination of ilmenite or ferric chloride leaching of copper concentrates, but other researchers may wish that the Bureau had studied the unknown properties of pentlandite (Ni(Fe)S) in order to better understand smelting of nickel concentrates. However, the Thermodynamics Group systematically maintains a list of "Compounds for Which Thermodynamic Data Are Needed," and sets priorities, taking into account potential applications of the data to problems in mineral extraction. The committee believes that, within the limitations of budget and personnel under which the thermochemistry program operates, the priorities assigned to the various projects properly reflect the needs of the metallurgical industry.

Another measure of the responsiveness of the program to need is the number of publications, which place new thermochemical data promptly into the hands of the users. Measured solely by number of publications per dollar funding, figures supplied to the committee indicated that the Thermodynamics Group generated at least 9 times as many publications per dollar as all the rest of the Bureau's field research activities.

Level of Effort

The committee was asked whether the current level of effort is appropriate, in terms of both manpower and funding.

During the more than 50 years that the Bureau's thermochemical research program has operated, it has made landmark contributions that are cited and used throughout the world--in the chemical industry, the metallurgical industry, and academia. Probably no other Bureau research can rival that of thermochemistry in value generated per dollar spent, in the permanency of that value, and in the recognition it has brought to the Bureau's work.

Thermochemical research is no longer fashionable in academic departments of chemistry. It is viewed as routine and painstaking application of known methods of measurement and not attractive for most graduate research. A few academic metallurgy or chemistry departments engage in thermochemical studies, but their numbers are small and their budgets severely limited. As a result, the output of new thermochemical data from academia is quite limited. Industrial laboratories, with one or two exceptions like Dow Chemical Company and U.S. Steel Company, seldom engage in thermochemical research; the metallurgical industry has always looked to government and academic laboratories for basic thermochemical data.

The committee's familiarity with the thermochemical work of other laboratories in government (U.S. Geological Survey, National Bureau of Standards, other agencies), industry, or academia is general rather than specific in nature. There are indications, however, that a study should be made on a national (or even international) scale and that such a study could conceivably reveal some serious deficiencies that should be rectified by expansion of thermochemical research funding by the Bureau of Mines, other government agencies, or by government funding of academic research. In any event, such a study would provide a better basis for decisions on what changes in the level of effort are needed.

Bureau research should be expanded on a modest scale by providing several new personnel and the corresponding budget to conduct the types of measurement and data evaluation currently performed at Albany. The committee reiterates its belief that strengthening the effort on data evaluation should be given top priority. It is important for all the specialized areas of thermochemical research to hire and train new scientists so that the program will not suffer major disruption with the retirement or loss of a single key individual. Another manpower need to be considered is the strengthening of the metallurgical and mineral technology component of the staff to broaden the present strong chemical orientation.

A vigorous case can be made, in addition, for a significant increase in thermochemical funding to expand thermochemical research beyond the limitations of current Bureau studies. The majority of current Bureau research is limited to determinations of the properties of pure substances, usually stoichiometric compounds. Although this information is of vital importance, it goes only part way toward thermochemical description of the phase encountered in practical metallurgy--the slags, mattes, molten salts, alloys, and concentrated aqueous solutions. The thermochemical behavior of these complex solution phases requires special measurement techniques and painstaking data evaluation. With the exception of the recent Bureau work on measurement of activity in concentrated aqueous solutions, and the newly initiated studies of phase equilibria in the systems Al-C-Si and Al-O-C-Si, this vital area has been neglected by Bureau research. With its present budget limitation, the Bureau laboratory could engage in these new areas only at the expense of its current work; the committee doubts the wisdom of that course. With a significantly increased budget, however, the Bureau should expand into this new area.

Use of Personnel

The committee was asked whether the personnel with the training and skills of those assigned to this research could be used to greater advantage in pursuit of other research objectives.

As should be obvious from its response to the first three items in this evaluation, the committee believes that the personnel are properly assigned and that their capabilities are being effectively used.

FURTHER OBSERVATIONS

The committee was favorably impressed with the value of Bureau thermochemical work, with the quality of the experimental equipment, and with the qualifications of the senior personnel. However, the members sensed that the Thermodynamics Group as a whole does not feel secure and confident in its identity. The group has a unique and important mission on the national scene in mineral and metallurgical thermochemistry. Its director has promoted and participated in various activities to put the program "on the map," and his efforts deserve the fullest support. In the committee's view, the senior personnel should interact more vigorously with other laboratories in universities, industry, and government to exchange ideas and information. The senior personnel at the Bureau, who are mostly chemists by training, need to understand better the mineral and metallurgical industries they serve and the nature of industrial problems. In turn, industrial and academic laboratories need a better acquaintance with the capabilities and work of the Bureau laboratory. As an example, one of the committee members, although well experienced in academic thermochemistry, was unaware that the Bureau laboratory maintains a computer file of thermodynamic data that can be used to supply information on request to the public.

This report is not the place for detailed suggestions on how to improve the sense of mission and outside interactions that the committee believes should be strengthened, but the matter needs to be given serious consideration within the Bureau of Mines.

SUMMARY

It is concluded that the minerals thermochemistry program of the Bureau of Mines is an extremely valuable one that fills the special need of providing data on important mineral and metallurgical materials to many users. The current approach and priorities are judged to be responsive to that need.

The committee recommends that support of current Bureau research be expanded on a modest scale and that there be a significant increase in funding to expand thermochemical research beyond pure substances to include the complex phases encountered in practical metallurgy. It is also recommended that the Bureau give high priority to filling a vacancy in the data evaluation staff. It is also suggested that the senior personnel interact more vigorously with other laboratories to exchange ideas and information.

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16. Abstracts
This report assesses the Bureau of Mines efforts in thermochemistry, based principally on findings from a visit to the Bureau's Albany Research Center by a working group of the Committee on Mineral Resources Technology. Included are comments on organization, budget, personnel, major experimental methods, data compilation and evaluation, equipment and facilities, and the utility of thermochemical data. The Bureau's program is evaluated through a series of questions: Does a real need exist? Who are the users? Are the current approach and priorities responsive? Is the current level of effort appropriate? etc. The committee concluded that the program is extremely valuable and fills a special need, and that the current approach and priorities are responsive to that need. Specific recommendations are also made concerning the support of current research as well as expanding research beyond the present pure substances.

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17c. COSATI Field/Group

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