

Efficient Phase Diagram Information and Computational Thermodynamics

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Industries that process and use metals, from microelectronics to aerospace, can use phase equilibria data for designing and processing complex alloys (three or more components) and diffusion data for controlling the formation and dissolution of precipitate phases within a matrix or at an interface. The number of images or data tables that would be needed for the graphic representation of such data is prohibitively large for systems with a large number of components. Databases that store thermodynamic and diffusion data as analytical functions provide a compact, retrievable storage method. They also permit the extrapolation of properties from binary and ternary systems to higher-order systems based on a physical model. Special task software that allows the nonexpert to extract the required information has been developed for the casting of superalloys and the solidification of Pb-free solders. Examples of user-friendly data representation and data utilization in advanced applications are presented.

Keywords computational thermodynamics, data storage, graphical representation, materials properties, special task software

1. Introduction

The graphic representation of materials properties is the traditional way of visualizing their relationship with internal and external parameters, as well as other properties. Phase diagrams of binary systems are traditionally represented as two-dimensional temperature-concentration (T - x) diagrams for constant pressure, and the pressure dependence of a binary system is frequently represented by a series of T - x diagrams. A ternary system is more complex because the addition of a component adds one more dimension to a graphic representation. Ternary systems at constant pressure are usually represented by a series of projections and sections. Common graphic representations of a ternary system include the liquidus projection, isothermal sections, and isopleths, each of which has its own advantages and disadvantages. For example, an isothermal section provides not only quantitative information of the phase boundaries, but also tie-line and phase amount information. It lacks, however, information on changes as functions of temperature, information that can be provided by an isopleth, that is a T - x diagram in which the concentration of one component or a concentration ratio is kept constant. Because tie-lines rarely coincide with the plane of the isopleth, no tie-line or phase amount information can be obtained from such a diagram.

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Quaternary and higher-component systems are even more difficult to represent by two-dimensional diagrams. As the complexity of the diagrams increases with an increasing number of components, the choice of axis variables becomes crucial and the interpretation of these diagrams becomes more difficult, even for expert users.

Phase diagram information is usually compiled into handbooks that include available diagrams and additional text information. The handbooks that have been published to date can easily fill a bookcase. Although modern storage media, such as CD-ROMs, reduce the amount of physical storage space required, the number of stored diagrams is still enormous and the information is limited to the available diagrams. The representation and compilation of materials property data are faced with the same general problem.

The handbooks *Thermodynamic Properties of Inorganic Materials* [1999SGT] give an example for the use of modern media. These handbooks are accompanied by CD-ROMs that not only contain the book content in electronic format but also software and databases that allow the reproduction of the calculations from the book as well as calculations of additional thermodynamic quantities.

Petzow et al. [1970Pet] noted in their 1970 article that the number of investigated systems is very small compared with the huge number of possible systems, and they suggested computational tools to overcome the limitations of classic representations and experimental methods. Since then, not only have the methods for the computational determination of phase equilibria made enormous progress, but so also has computational power, allowing the customization of phase equilibria calculations for the material problems of interest. Thermodynamic phase equilibria calculations can also provide important data for modeling nonequilibrium processes and other materials properties.

2. Computational Methodology

For the calculation of phase equilibria, the Gibbs energy of each phase is described as a function of composition,

temperature, and (if needed) pressure. This has the significant advantage that the different properties of a system, for example, phase boundaries and enthalpies, are described with one set of functions. Thus, the calculation allows not only a consistent description of the phase thermodynamic properties, but also compact storage of phase equilibria data. The accuracy of the calculated phase boundaries and thermochemical properties is generally of the same order of magnitude as the accuracy of the experimental data on which they are based. The accuracy of the calculated values may be even better than the individual experimental data set if phase boundary and thermochemical data were used for the assessment of the thermodynamic description, thus ensuring that the set of functions consistently describes all properties of the system. An additional advantage of the calculation of phase equilibria is that it allows the prediction of higher-order systems from the extrapolation of the thermodynamic functions of the constituent subsystems and can aid the experimental investigation of such a system with information for the strategic placement of experiments.

The availability of thermodynamic phase descriptions further provides important data that are needed for the modeling of nonequilibrium processes [2000Kat] and other properties, such as diffusion [1982Agr], nanomaterial/interface energies [2001Tan], surface tension of the liquid [1999Tan], and a variety of mechanical properties [2003Sau].

The principal concepts that are used for the thermodynamic calculation of phase equilibria can also be applied for the calculation of other properties. For example, the representation and storage of diffusion data face an even worse dilemma than that for phase equilibria data. The description of multicomponent diffusion at a given temperature, pressure, and composition requires n^2 diffusion coefficients, where n is the number of independent concentration variables. Because the treatment of diffusion is of the most interest for dynamic processes, such a set of diffusion coefficients is needed for each point in the concentration profile and thus for each time step in the treatment of a diffusion problem, requiring a huge amount of data. For the computational treatment of diffusion processes, the diffusion coefficients can be calculated from the thermodynamic factor and the mobility of the elemental species in the phases of interest. The thermodynamic factor is obtained from the phase equilibrium calculation, and the mobility is calculated from an auxiliary database, which is constructed in a fashion similar to the thermodynamic database, but from distinctly different data.

2.1 General Database Development Strategy

The basic strategy for the assessment of the thermodynamic description of a multicomponent system is shown in Fig. 1. First, the thermodynamic descriptions of the constituent binary systems are derived. Thermodynamic extrapolation methods are then used to extend the thermodynamic functions of the binaries into ternary and higher-order systems. The extrapolation is then compared with experimental results and, if necessary, ternary interaction func-

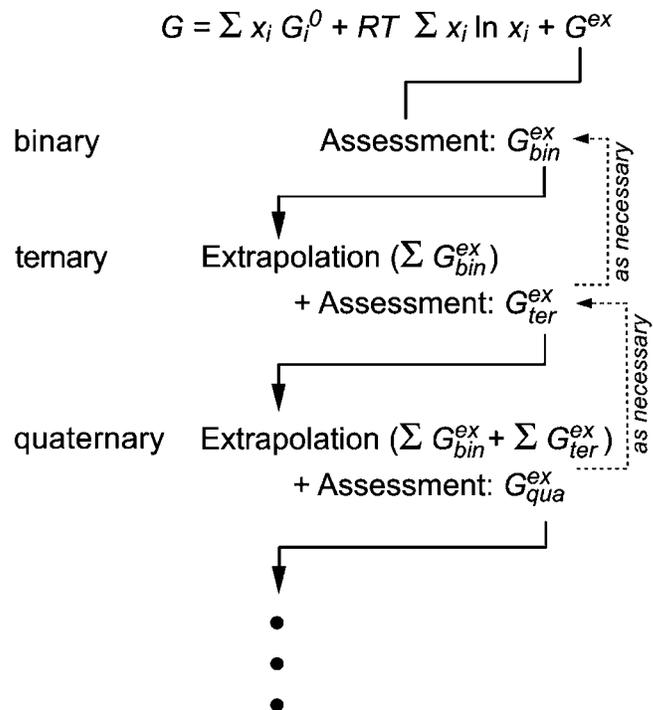


Fig. 1 CALPHAD methodology. The assessed excess quantities of the constituent subsystems are used for the extrapolation to a higher-component system. The example is given for the Gibbs energy.

tions are added to the thermodynamic description of the higher-order system. However, in cases in which satisfactory agreement between experimental and calculated data cannot be obtained after introducing and adjusting ternary parameters, it may become necessary to reevaluate the description of the constituent binary systems to determine whether a particular system needs to be reassessed. In principle, this strategy is followed until all 2, 3, . . . j constituent systems of a j -component system have been assessed. However, experience has shown that, in most cases, no corrections, or very minor corrections, are necessary for the reasonable prediction of quaternary or higher-component systems. Because true quaternary phases are rare in metallic systems, the assessment of the ternary constituent systems is often sufficient to describe a j -component system. For the construction of a thermodynamic database for a multicomponent system, however, this strategy still requires the assessment of a large number of systems. It is, therefore, highly desirable to make use of assessments that have already been published in the literature.

Whether the database is built from scratch or assessments from the literature are used, the first step in the construction of such a database should be the compilation of the crystal structures and homogeneity ranges of all phases that occur in the constituent systems because they form the basis for selecting an appropriate model description. The model description of a phase is an important choice because it is directly related to the requirement that the descriptions of phases with the same or similar crystal structure in all pos-

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sible systems must be compatible for the description of this phase in the multicomponent system. Even when the crystal structures of the phases are identified to be identical, compatibility problems can still arise from the choices of different models for the same crystal structure in different systems [1997Ans]. In the case in which a model description of a phase from an assessment from the literature is not compatible with the selected model, the description of this phase must be remodeled. Ferro et al. [2002Fer] provide guidelines for the model description of ordered intermetallic compounds.

Although the availability of thermodynamic descriptions of the constituent binary systems is crucial for the construction of a multicomponent database, complete thermodynamic descriptions of the ternary systems are also highly desirable. However, the number of ternary systems for which thermodynamic descriptions have been developed is small compared with that of assessed binary systems. The assessment of a ternary system is frequently hampered by the lack of sufficient experimental data for the refinement of the thermodynamic functions for the entire temperature and composition regimen. Even when sufficient data are available, the development of a complete thermodynamic description can be time-consuming and can result in delays for the development of the multicomponent database. Therefore, higher priority can be given to those ternary systems that include the base element for the alloys of interest. Finally, the sequence by which elements are added can be guided by their importance as an alloying element.

The above strategy has been used to construct a number of thermodynamic databases for technical alloy systems, as well as a few mobility databases for diffusion simulations. The same strategy can be applied for the development of other property databases. Models for properties, such as molar volume, thermal conductivity, Young's modulus, and Poisson's ratio are similar to those used for the thermodynamic and diffusion functions [2003Sau].

2.2 Basic Types of Phase Equilibria Calculations

The calculation of a single equilibrium is the basic tool for obtaining phase equilibrium information from thermodynamic data. This kind of calculation is carried out by setting the degrees of freedom to zero. In the most common case, the total composition of the system, and its temperature and pressure are fixed to allow the minimization of the Gibbs energy of the system. Single-point equilibrium calculations are the core of any kind of calculation that involves the stepping of one variable or the mapping of two or more variables. Single-point calculations can provide the derivatives that are needed to evaluate the effects of changes in the conditions.

In one-dimensional stepping calculations, one of the variables that was fixed for the single-point equilibrium calculation is stepped. At each step, a single-point equilibrium calculation is carried out. The most common application of the stepping formalism is to step the temperature variable. The graphic representation of the results is not a phase diagram but a property diagram displaying, for instance, phase fractions, phase compositions, and enthalpies

as a function of the step variable. A well-known example of this kind of calculation is the lever-rule calculation of equilibrium solidification. However, stepping calculations can be used for many other applications by using another variable for stepping, such as the concentration or activity (partial pressure) of a component or the overall pressure.

Other types of stepping calculations are actually single equilibrium calculations that are connected by special conditions. Examples are the solidification calculation of the Scheil path or the solidification calculation incorporating diffusion in the solid phase. The special conditions for the Scheil path calculation are derived from the assumptions of a local equilibrium existing between the (uniform) liquid and the increment of solid formed at each temperature step, and that no diffusion occurs in the solid phase. Solidification calculations that consider diffusion in the solid phase are most easily performed if the slopes of the liquidus surface and the partition coefficients are obtained from the phase equilibria calculation at each temperature step.

Mapping calculations are the basic tool for generating traditional phase diagrams. Most commonly, the mapping is carried out for a T - x or concentration-concentration diagram. While other quantities may be chosen for the mapping, the usefulness of the resulting diagram depends on the selected mapping variables. Hillert [1997Hil] discussed reasonable choices for mapping variables.

3. Software Tools

A series of software tools is available for the calculation of phase equilibria and phase equilibria-related properties. Although these software tools have some features in common, their versatility and input requirements vary. In general, the input requirements for a versatile software package will be more complex, in that the equilibrium conditions must be defined by the user. By comparison, task-specific software tools, where the equilibrium conditions are predefined and only the alloy composition must be specified by the user, are simpler.

3.1 General Phase Equilibria Calculation Tools

General, fully integrated software packages, such as FactSage [2002Bal], MTDATA [2002Dav], PANDAT [2002Che1], or Thermo-Calc [2002And], offer great versatility with a suite of modules for data input, different types of calculations, and graphic output of the results. (Commercial products are referenced in this article as examples; such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology.)

Graphic user interface-based versions of the software provide user-friendly interfaces. A general calculation module allows the user to specify the equilibrium conditions for the calculation, while other modules offer predefined types of calculations. Although the features offered by the individual software packages differ, some modules, such as those for the calculation of binary and ternary phase dia-

grams, are common to all software packages. The software packages allow a choice of thermodynamic databases, including user-specified databases. Some of the software packages also include an assessment module for the refinement of the thermodynamic functions of the phases with respect to experimental data; this is a valuable tool for the development of thermodynamic databases. In addition, the software packages provide code libraries that can be linked with user-written applications. For example, DICTRA [2002And], a program for the simulation of diffusion-controlled phase transformations, is linked with ThermoCalc [2002And], which supplies the needed thermodynamic information.

3.2 Semispecific Calculation Tools

MALT [2002Yok] is a pure substance database that is bundled with programs for the calculation of chemical equilibria and chemical potential diagrams. This package allows the user to create a supplemental database and provides a special function for use as an interface to user-written programs. ThermoSuite [2002Che2] consists of modules for the tabulation and graphic display of the thermochemical properties of pure substances and reactions, and the calculation of complex equilibria, and a module for drawing binary and ternary phase diagrams. Several databases are available for ThermoSuite.

3.3 Task-Specific Calculation Tools

The advantage of task-specific calculation tools, such as JMatPro [2003Sau] and SolCalc, is that equilibrium conditions are prescribed by the task, and the user is only required to enter an alloy composition and the temperature range of interest. However, because many task-specific calculations not only provide information on phase formation, but also compute a specific property of the material, such as enthalpy, thermal expansion or stress, additional input, supplied either by auxiliary databases or by the user, may be needed. In the latter case, the software usually provides guidance for the required quantities. The results are displayed in graphic form but can also be obtained in tabular form.

4. The SolCalc Program

The coupling of macroscopic and microscopic models is important for the accurate description of the casting process and the resulting microstructure [1989Rap]. Macroscopic modeling involves heat and fluid flow in the casting, and these models are coupled to the micromodels through the details of the latent heat release. Although the level of complexity of micromodels varies considerably, all require phase diagram information such as the concentrations at the liquid-solid interface, the liquidus slopes, and the partition coefficients. Even though phase diagrams represent thermodynamic equilibrium, it is well established that the phase diagram can be applied locally (local equilibrium) to describe the solidification path in which only the concentrations at the liquid-solid interface are assumed to obey the requirements of thermodynamic equilibrium, permitting the

description of nonequilibrium situations that can be found in solidification.

A set of subroutines for calculating phase equilibrium, the liquidus slope, the enthalpies of phases, and the effect of back-diffusion has been developed for solidification calculations [1995Boe, 1998Boe, 2001Ban]. The Gibbs energy minimizer that was used was originally developed by Lukas et al. [1982Luk] and was expanded by Kattner et al. [1996Kat]. The subroutines have been implemented for a number of solidification simulations [1997Ban, 1997Sch]. Four programs based on the subroutines *Liquidus*, *Lever*, *Scheil*, and *Backdiff* have been written. The first three of these require only the overall alloy composition, the start temperature, and the end temperature, as well as the temperature step as input, while *Backdiff* requires additional input for the kinetic and geometric (dendrite spacing) parameters. These four programs, along with the NIST-Ni [2002Kat] and NIST-Sn [2003Kat] thermodynamic databases and a user-friendly interface, are bundled under the name *SolCalc*. Figure 2 gives an example for the *SolCalc* input for a lever rule solidification calculation of a superalloy.

4.1 The Liquidus Program

This program calculates the liquidus temperature for a given composition. In addition, it calculates the partition coefficients:

$$k_i = \frac{C_i^{solid}}{C_i^{liquid}}$$

and the slopes of the liquidus

$$m_i = \frac{\partial T}{\partial C_i^{liquid}}$$

where C_i^{phase} is the concentration of solute i in phase. The results are presented in tabular form.

4.2 The Lever Program

For solidification obeying the lever rule, complete diffusion is assumed in the solid as well as in the liquid at each temperature during cooling. Thus, all phases are assumed to be in thermodynamic equilibrium at all temperatures during solidification. The program performs a stepping calculation for the given alloy composition, temperature range, and temperature step. The total fraction solid and total enthalpy content of the alloy are displayed in graphic form as the default output (Fig. 3). The results are also available in tabular form, with columns for the temperature, total fraction solid, total enthalpy, and columns with phase fraction, enthalpy content, and composition for each phase that is formed during solidification.

4.3 The Scheil Program

Solidification following the Scheil path, in which diffusion in the solid is forbidden, produces the worst case of

Solidification Calculation Type

Lever (Equilibrium)

Back Diffusion (Intermediate Segregation)

Scheil (Worst Case Segregation)

Liquidus (Liquidus Temperature Only)

Database

NIST Ni

NIST Sn

User Defined

Composition Units

Atomic Percent

Mass Percent

Atomic Fraction

Mass Fraction

Calculation Temperatures

Celsius Kelvin Fahrenheit

Start Temperature: 1400

Stop Temperature: 1100

Temperature Step: 1

NIST-Ni Database Elements

Back Diffusion Data

	Concentration	D0 [m ² /s]	Q [kJ/mol]
Al	5.75	1.87E-04	268.0
Co	12.5	2.2E-05	256.2
Cr	4.2	5.0E-05	260.0
Hf		8.6E-05	257.1
Mo	1.4	3.0E-04	288.5
Re	5.4	9.0E-05	278.7
Ta	7.2	9.0E-05	278.7
Ti		8.6E-05	257.1
W	6.	8.6E-05	295.0
Ni	Balance		

Cooling Rate [C/s]: 1

Secondary Dendrite Arm Spacing [µm]: 50

Estimate Dendrite Arm Spacing

Calculate Exit

Fig. 2 Graphic user interface of *SolCalc*. If a back-diffusion calculation is selected, the interface provides guidance for the additional needed input quantities.

microsegregation with the lowest final freezing temperature. The Scheil solidification path is usually approximated by stepping through the temperature interval of interest and assuming that the thermodynamic equilibrium exists only as a local equilibrium at the liquid-solid interface for each temperature step. At each temperature step, the fraction of the solid phases formed is removed from the calculation, and the composition of the remaining liquid phase is used as the liquid composition for the next temperature step.

Simultaneously, the fractions of the solid phases that have been removed are summed to give the total fraction of the solid formed during solidification. The average composition of each solid phase and the accumulated phase fractions are used for the enthalpy calculation. After solidification is complete, usually when the fraction of the liquid phase has dropped below a small, preset number, calculation of the enthalpy is continued until the final temperature is reached with no further adjustments in phase fractions or average phase compositions. The output is similar to that of the *Lever* program, except that the quantities tabulated for the individual phases are the accumulated phase fraction,

enthalpy for the average composition, and the average composition.

4.4 The Backdiff Program

The lever rule and the Scheil solidification form the two limiting cases of solidification. The modeling of real solidification behavior requires a kinetic and a geometric analysis of microsegregation and back-diffusion. Instead of solving the diffusion equations in the solid, Boettinger et al. [1998Boe] suggested the use of an approximation following the approach of Wang et al. [1993Wan] that estimates the solid concentration gradient. The resulting equations guarantee overall solute conservation, flux balance at the solid-liquid interface, and liquid concentrations that remain on the liquidus. This approximation is used only for the solidification of the primary phase and reproduces the Scheil path for small amounts of solid diffusion but fails to reproduce the lever rule path for large amounts of diffusion. The complete treatment of solid diffusion during multiphase solidification is quite complex; therefore, the simplifying as-

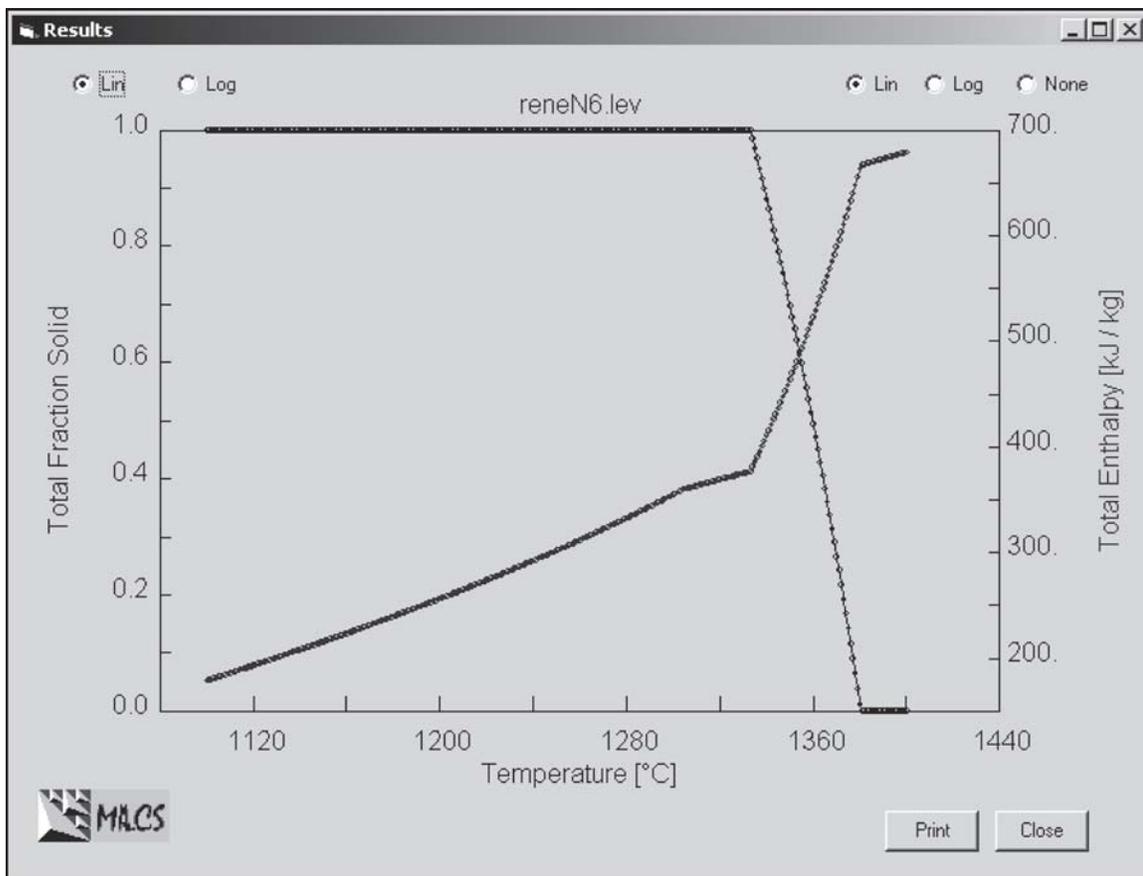


Fig. 3 Default graphic output of *SolCalc*. The results are from a lever rule calculation of the René N6 superalloy. The curve touching the temperature axis at 1400 °C is the total fraction solid, the other curve is the total enthalpy. The two curves are distinguished by different colors on the computer screen.

sumption was made that additional phases solidify according to the lever rule. After solidification of the primary phase is complete, its average composition is fixed. Lever rule calculations are then carried out for the remaining phases until no liquid phase is left. At this point, all phase concentrations are fixed, and the calculation of the enthalpy is continued until the final temperature is reached.

The *Backdiff* program requires additional input: the Arrhenius parameters for binary interdiffusion coefficients; the secondary dendrite arm spacing as a measure of diffusion length; and the cooling rate. The suggested quantities for these values are provided by the *SolCalc* user interface. The output is similar to those of the *Lever* and *Scheil* programs.

4.5 Applications of the Results

The results of these programs have been used for solidification calculations of superalloys [1995Boe, 1998Boe, 2001Ban] and solders [2001Kat, 2001Moo], and for the modeling of differential thermal analysis (DTA) [2002Boe].

The programs have been incorporated into a finite-element package for modeling the solidification of castings [1997Ban], and subroutines of the code were used for the simulation of freckle formation and macrosegregation in directional solidified Ni-base superalloys [1997Sch].

The solidification calculations of the solder alloys were also used to evaluate the effect of Pb contamination of a variety of Pb-free solders. This contamination occurs when Pb-free solder is used to solder components that have been pretinned with a Pb-containing solder. Moon et al. [2001Moo] used Scheil solidification calculations to create a ternary diagram with the lowest final freezing temperatures as a function of Pb contamination and composition of an Sn-Bi solder.

The heat-flow model for DTA requires variation of the enthalpy with the temperature of the analyzed material as input. For a pure substance, this quantity can be readily obtained from an equation in which the enthalpy is given as a function of temperature, while for multicomponent materials the enthalpy-temperature relationship also depends on the freezing range and segregation in the material. The output tables generated by the *SolCalc* programs were used by Boettinger et al. [2002Boe] to simulate the DTA curves for multicomponent alloys.

5. Conclusions

A wide spectrum of software for the calculation of phase equilibria is available. Within this spectrum, task-specific software has made phase diagram-related information more

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accessible to the nonexpert user. The examples given in this article are just a few examples of the applications available for phase equilibria information. Model linkage among thermodynamic, kinetic, and mechanical properties is available, and is constantly being improved, increasing the sophistication level of the software tools for the calculation of phase equilibria and related properties. With the increased availability of software tools, the need for thermodynamic and auxiliary property databases that cover the wide spectrum of materials becomes apparent. Current thermodynamic and auxiliary databases are usually tailored with respect to a base element or a major solid phase. The most general thermodynamic database for alloys currently contains the descriptions of 298 binary and 59 ternary systems. However, the number of databases that are available for thermodynamic assessments and the assessment of auxiliary properties is steadily increasing.

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