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The first two terms correspond to G0, and the third term corresponds to Gideal in Equation 4. The remaining terms are the excess Gibbs energy term, Gxs, in Equation 4. The coefficients , and can be visualized as the Gibbs energies of the end-member phases. The end-member phases are formed when each sublattice is occupied only by one kind of species and can be either real: A atoms on sublattice 1 and B atoms on sublattice 2 or hypothetical , and. The remaining terms of Gxs describe interactions between the atoms on one sublattice similar to regular-solution type models for disordered solution phases. For example, Ansara et al. This model was later modified by Ansara et al. It should be noted that Equations 5 and 6 are, in fact, special cases of Equation 7. Equation 7 reduces to Equation 6 if only one sublattice is considered or to Equation 5 if only one species is considered on each of the two sublattices. The generality of the sublattice description allows the formulation of a general description for multicomponent phases that can easily be computerized. From the condition that the Gibbs energy at thermodynamic equilibrium reveals a minimum for given temperature, pressure, and composition, J. Gibbs derived the well-known equilibrium conditions that the chemical potential, , of each component, n, is the same in all phases, 8 The chemical potentials are related to the Gibbs energy by the well known equation 9 Equation 8 results in n nonlinear equations that can be used in numerical calculations. The equations obtained from these methods are usually nonlinear and are solved numerically using a Newton-Raphson technique. In order to obtain an optimized set of coefficients, it is desirable to take into account all types of experimental data e. The coefficients can be determined from the experimental data by a trial-and-error method or mathematical methods. The trial-and-error method is only feasible if few different data types are available. In this case, mathematical methods, such as the least squares method of Gauss, 42 the Marquardt method, 43 or Bayesian estimation method, 44 are more efficient. The determination of the coefficients is frequently called assessment or optimization of a system. Several methods exist to determine the weighting terms used in such an extrapolation formula. The usual strategy for assessment of a multicomponent system is shown in Figure 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 results of such extrapolations can then be used to design critical experiments. The results of the experiments are compared to the extrapolation, and if necessary, interaction functions are added to the thermodynamic description of the higher order system. As mentioned previously, the coefficients of the interaction functions are optimized on the basis of these data. In principle, this strategy is followed until all 2, 3, However, experience has shown that, in most cases, no corrections or very minor corrections are necessary for reasonable prediction of quaternary or higher component systems. Since true quaternary phases are rare in metallic systems, assessment of most of the ternary constituent systems is often sufficient to describe an n-component system. Thermodynamic databases of multicomponent systems require consistency in the model descriptions and the parameters used. With the constant improvement of computational technology, the use of more realistic models, such as the sublattice model description, becomes feasible. This allows more accurate descriptions of complex systems and makes it desirable to reassess systems that have been previously assessed. The progress that has been made with these reassessments is shown in Figure 2 for the Al-Ni system, a basic system for superalloys. The Al and Ni phases were described as one phase since they both have the fcc structure. Although the general topology of the experimentally determined phase diagram 48 is reproduced, major differences occur for the equilibria involving the Al3Ni2 and AlNi phases. These differences are at least partially a result of ignoring the homogeneity range of the Al3Ni2 phase and not considering the fact that AlNi is an ordered phase with CsCl structure. In the second assessment by Ansara et al. While the phase diagram calculated from these improved

analytical descriptions shows better agreement with the observed diagram, some noticeable disagreement still remains. The range of the Al solid solution is overestimated, and the region of single-phase AlNi3 slants to the nickel-rich side at lower temperatures. Both problems likely result from describing all of these phases with the single function. It should be also noted that the region of single-phase Al3Ni2 is overestimated at higher temperatures and underestimated at lower temperatures. This may be caused by the substitutional sublattice model description used in this assessment. It has been experimentally observed that on the nickel-rich side of the nominal stoichiometry, nickel atoms fill structural vacancies; on the aluminum-rich side, nickel atoms are substituted by aluminum. This has been considered in the most recent assessment by Ansara et al. This assessment also includes a description of the Al3Ni5 phase as a stoichiometric compound, though its homogeneity range has been ignored. The phase diagram obtained from this assessment is in very good agreement with the observed diagram. It should be noted that the calculated phase diagram not only reproduces the experimentally observed phase diagram, but also provides the thermodynamic functions for extrapolation into higher order systems or use in the modeling of, for example, casting solidification. A disadvantage of this iterative process with improved descriptions is that the descriptions used in previous assessments may be incompatible with newer assessments that are based on recently developed model descriptions. Despite this, significant progress has been made in recent years, and an increasing number of databases have become available for use with multicomponent systems. Most of the model descriptions used for alloy and ceramic systems are common to all these programs; however, not every package has other specific model descriptions e. Another important feature of these software packages is the availability of a module for the optimization of the Gibbs energy functions. For these applications, the user needs only to supply a bulk composition and temperature limits for the calculation, and the programs generate the remaining conditions that are needed for the calculation. For the incorporation of phase-equilibria calculations into micromodeling e. Several thermodynamic databases have been constructed from the assessments of binary, ternary, and quaternary systems. For the description of commercial alloys, it is quite likely that at least a dozen elements need to be considered. The number of constituent subsystems of an n-component system is determined by the binomial coefficient , where k is the number of components in the subsystem. A 12 component system consists accordingly of 66 binary, ternary, and quaternary subsystems. These numbers suggest that is impossible to obtain descriptions of all the subsystems in reasonable time. However, as mentioned previously, only rarely are quaternary excess parameters needed. If the database is for base element X, it is sufficient to consider only the X-based ternary systems, hence, considerably reducing the number of needed assessments. Also, if more than one element occurs only in fairly small quantities in the alloy family of interest then assessments for binary systems containing only these elements or ternary systems with two or three of these elements are generally not very important for obtaining correct predictions. Based on this information, databases have been developed for various commercial-alloy systems. A review of fully integrated thermochemical database systems that were available in is provided by Bale and Eriksson. As mentioned, extrapolation to higher component systems is one of the staples of CALPHAD, since it provides information where otherwise only educated guesses could be used. When alloys of the Sn-Ag-Bi system were considered as candidate alloys for lead-free solders, no phase-diagram information for the liquid phase could be found. Kattner and Boettinger 65 extrapolated the descriptions of the binary systems to calculate the solidus and liquidus surfaces of the tin-rich corner Figure 3. The silver-rich side of the eutectic troughs should be avoided because the liquidus temperature increases significantly with increasing silver concentration. Figure 3 can be used to identify composition regimes where the freezing range is suitable for solder applications. Two simple models describe the limiting cases of solidification behavior. First, complete diffusion is assumed in the solid as well as in the liquid for solidification obeying the Lever rule at each temperature during cooling. Thus, all phases are assumed to be in thermodynamic equilibrium at all temperatures during solidification. Modeling of real solidification behavior requires a kinetic analysis of microsegregation and back diffusion; however, for most alloys, the predictions of the Scheil model are close to reality. Scheil and Lever rule

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calculations were carried out for six alloy compositions in the solder alloy Ag-Bi-Sn system. The results are shown in Figure 4. The formation of eutectic due to segregation in the Scheil solidification increases the freezing range drastically. A comparison of Figure 4a and Figure 4b shows that as the equilibrium freezing range is increased by adding bismuth , the Scheil solidification curve begins to deviate from that of the Lever rule solidification at smaller values of solid fraction formed. This is an indication that nonequilibrium solidification has a smaller impact on the actual freezing range of an alloy with a small equilibrium freezing range than an alloy with a large equilibrium freezing range. Because it is a practical requirement that solders should have a limited freezing range, this is important information for use in the design of new solder alloys. A phase-fraction diagram vs. Such diagrams are shown in Figure 5 for Lever rule and Scheil calculations of an alloy that is close in composition to the commercial aluminum alloy The composition in weight percent used for this calculation is Al The difference between Lever rule and Scheil solidification becomes most noticeable toward the end of solidification. For both solidification paths, the solidification begins with the precipitation of aluminum and Al6Mn. Finally, after solidification is complete, precipitation of Al2CuMg begins. The microstructures obtained from these paths are quite different, which might result in different mechanical properties. The actual microstructure can be compared to diagrams like those shown in Figure 5 , and casting parameters can be adjusted to obtain the desired microstructure by following a solidification path somewhere between these extremes. Major progress in the application of phase-diagram information has been made in the implementation of such calculations in casting simulation software. Thermodynamic calculation of the phase equilibria of a multicomponent alloy was interfaced with a micromodel for computing the change of fraction solid and temperature, given a specified change in enthalpy during the liquid-solid transformation. This coupling was incorporated into a finite-element package developed for modeling the solidification of castings. The simulation was carried out for a step wedge part and a NiAl-2Ta in weight percent alloy. Further details of the simulation are described by Banerjee et al. One node node 63 cooled approximately twice as fast as the other one node 1. The fraction solid vs. These differences in Scheil behavior and segregation are expected to appear in the final casting and to be reflected in changing microstructure and properties varying throughout the casting. The remaining calculations were carried out with the original Lukas programs Figure 3 or with programs that were using modified code Figures The author thanks H.

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Solubilities of Inorganic and Organic Compounds, Volume 2: Ternary and Multicomponent Systems, Part 2 presents the solubility data of ternary and multicomponent systems. The text arranges the data in a way that the first Tables are systems in which an Element is a component, which are followed by data for systems containing inorganic compounds.

3: Solubilities of inorganic and organic compounds - Caltech Library Catalog

Binary Systems v.2, pt - Ternary Systems (elements, inorganic, metal-organic and organic compounds) v.3, pt - Ternary and Multicomponent Systems (inorganic compounds).

4: Solubilities of inorganic and organic compounds - Caltech Library Catalog

Solubilities of Inorganic and Organic Compounds, Volume 2: Ternary Systems, Part I focuses on a selection from the International Chemical Literature on the Solubilities of Elements, Inorganic Compounds, Metallo-organic Compounds, and Organic Compounds in Ternary and Multicomponent Systems.

5: The Thermodynamic Modeling of Multicomponent Phase Equilibria

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7: Action Record - Solubilities of inorganic and organic compounds.

Volume 1, parts 1 and 2, comprises the solubilities of elements, inorganic compounds, metallo-organic and organic compounds in binary systems. Volume II, parts 1, 2 and 3, comprises the solubilities in ternary and multi-component systems.

8: 1, results in SearchWorks catalog

Solubilities of inorganic and organic compounds. Volume 2, ternary and multicomponent systems, part 2 (Stephen, H.; Stephen, T.).

9: The Thermodynamic Modeling of Multicomponent Phase Equilibria

Solubility-miscibility with water. Experimental methods and data tables. Mutual solubilities and liquid-liquid equilibria of binary, ternary and quaternary systems. Typical solvents and solutes include water, sea water, heavy water, inorganic compounds, and a variety of organic compounds such as.

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