Phase Diagram Activities

Alloy Phase Diagram Symposium of the Materials Research Society Annual Meeting

Among the symposia that have been held by the metallurgical community over the last decade or so, the subjects related to alloy phase formation, phase stability, and phase diagrams in their broadest sense are a recurring theme. These subjects clearly reflect the existing and growing need in both scientific and development areas for a still better understanding of the competition for phase stability, both stable and metastable, that can arise in a particular alloy under a given set of conditions.

The symposium on Alloy Phase Diagrams held recently in Boston (1-4 November, 1982) under the auspices of the Materials Research Society has followed logically from previous such efforts: the Battelle Symposium held in 1966, and the two more recently held AIME Symposia, one in Milwaukee in 1978, on "Calculations of Phase Diagrams and Thermochemistry of Alloy Phases", and the other in New Orleans, in 1979, on "Theory of Alloy Phase Formation".

The Boston symposium has thoroughly covered the background and progress in many of the various topics discussed in previous symposia, but it also has included some additional topics pertaining to rapid solidification, superconductivity aspects, and phase stability under irradiation or shock-pressure loading.

The general theme of the symposium was organized by Drs. Bennett, Massalski and Giessen, but speakers for individual sessions on selected subjects were suggested by co-opted session chairmen as follows: R. E. Watson (Alloy Phase Stability), M. Hillert (Application of Thermodynamics Models in Phase Diagram Data Evaluation), J. Perezpeko and W. J. Boettinger (Phase Diagrams and Rapid Solidification Processing), J. Cahn (Constrained Equilibria), C. Koch (Specialized Phase Diagrams), and K. Russell (Phase Stability Under Extreme External Stimuli).

The session on Alloy Phase Stability covered subjects ranging from "Ab-initio Calculations of Phase Diagrams" to "Solubility Trends in Transition Metal Alloys". The session on the Application of Thermodynamics Models in Phase Diagram Data Evaluation involved presentations by well-known authors in this field, who discussed both simple solution approaches in phase diagram calculations, treatment of sublattice models, thermodynamic properties in multicomponent alloys, and sublattice model calculations.

The two more specialized sessions on phase diagrams involved presentations related to superconductivity, spin glasses, phase transitions, and low temperature phases, as well as a discussion of phase diagram features associated with multicritical points in alloy systems. The session on Phase Stability under Extreme External Stimuli, organized by Prof. Russell, involved talks on "The Effect of Composition Gradients on Phase Diagrams", "Phase Transformation Under Intense Shock-Pressure Loading", and "Atomistic Approaches to Phase Diagrams Under Irradiation".

Altogether there were six symposium sessions over a period of three days. There was also a poster session of an additional twenty-three presentations. As befits the subject, the symposium had an international flavor with several of the invited speakers coming from abroad. A thorough discussion followed some of the papers and it may be expected that the final version of these papers will take into account some of the remarks contributed by the audience. A summary of the papers and posters presented in each session follows.

Alloy Phase Stability

J. Hafner suggested that the combined application of electronic and thermodynamic perturbation theories allows for an ab-initio calculation of the phase diagrams of binary simple-metal alloys.

A. R. Williams and co-authors C. D. Gellatt, Jr., V. L. Moruzzi, and J. W. D. Connolly described the cohesion, compound formation, and phase diagrams derived from first principles.

J. L. Morán-López presented a theory of surface effects of ordering and segregating binary alloys.

A. N. Berker used the renormalization-group approach to obtain global phase diagrams with order-disorder and structural transition.

D. A. Goodman, L. H. Bennett, and R. E. Watson considered both the experimental evidence and theoretical predictions concerning the solubility trends in transition metal alloys, including interpretation by band and valence bond theories.

M. O. Robbins and L. M. Falicov developed an electronic theory for the total energy and short-range order in binary alloys.

E. S. Machlin developed empirical lattice energy functions that allow calculation for prediction of structural properties of alloy phases.

M. Rand indicated the type and precision of information needed by phase diagram calculators for practical calculations.

Application of Thermodynamics Models in Phase Diagram Data Evaluation

L. Kaufman reviewed some of the successful approaches for the predictions of lattice stability values, thermochemical data, and phase diagrams generated by these evaluations.

I. Ansara discussed the representation of thermodynamic properties in multicomponent alloys, derived by adding the properties of the limiting binary systems and by experimental measurements of the interaction parameters specific to the multicomponent systems.

B. Sundman and J. Ågren introduced a sublattice model suitable to describe phases where the difference in size, charge, or electronegativity causes a deviation from random mixing of the atoms.
L. Brewer discussed mathematical representation of size and electronic factors in determining the relative stabilities of crystal structures and their homogeneous composition ranges.

J. N. Pratt and I. P. Jones examined the use of nearest neighbor pair-wise interaction models for the description of the thermodynamic properties of alloys, including treatment of phases containing several sublattices.

D. de Fontaine defined coherent phase diagrams and the resulting diagrams that can be obtained by means of the cluster variation approximation.

F. Sommer demonstrated the application of an association model for liquid alloys to the calculation of phase equilibria.

G. Inden reviewed the effect of magnetic and chemical ordering on phase stability.

Phase Diagrams and Rapid Solidification Processing

J. H. Perepezko and W. J. Boettinger discussed the use of metastable phase diagrams for the interpretation and prediction of the phases present in rapidly solidified materials.

T. B. Massalski observed the relationships between phase diagrams, the $T_0$ and $T_1$ temperatures, and glass forming ability.

L. E. Tanner discussed a new technology, rapid solidification processing, and its use in phase relation studies.

J. L. Murray examined the influence of thermodynamic factors in the extension of solid solubility in Al-based binary alloys.

B. C. Giessen discussed the crystal chemistry of metastable alloy phases.

Constrained Equilibria

M. Hillert described the history of the para-equilibrium concept.

F. C. Larche presented the effects of lattice constraints on phase equilibria.

M. G. Lagally and T.-M. Lu discussed phase relationships for adsorbed layers on surfaces.

Specialized Phase Diagrams

R. M. White provided a general introduction to order parameters and their relationship to phase transitions.

M. B. Maple discussed the interplay between superconductivity and magnetic order to produce low-temperature phase diagrams.

J. S. Kouvel described transitions between spin-glassiness and ferromagnetism in disordered Ni-Mn alloys.

R. C. Richardson enumerated the low-temperature phases of liquid and solid $^3$He.

S. M. Allen and J. W. Cahn illustrated the phase diagram features associated with multicritical points in alloy systems.

Phase Stability Under Extreme External Stimuli

K. C. Russell discussed atomistic approaches to phase diagrams under irradiation.

K. N. Tu and U. Goesele observed the effect of composition gradients on phase stability.

D. E. Grady described phase transformation of solids under intense shock-pressure loading.

Poster Session

R. Waterstrat compared features of the refractory metal–noble metal phase diagrams, $T_5-T_{10}$.

R. W. Smith, D. Heyding, and F. Unuk described results of a detailed study of the constitution of the Hg-Sn system.

B. Fultz determined the nickel content of precipitated austenite in Fe-9Ni steel.

C. S. Jayanth and P. Nash determined that knowledge of the high-temperature phase equilibria in the Ni-rich region of the Ni-Al-Zr system can be used to select alloys for use in high-temperature, high-strength applications.

W. W. Liang and P. Nash provided data to determine the phase equilibria at 1173 K in the Ni-Co-Al system.

A. A. Prince redetermined the Au-Pb and In-Sn phase diagrams, indicating that Au$_2$Pb is formed at a significantly higher temperature than previously reported, and that the constitution of In-Sn proposed by Heumann and Alpout is generally confirmed.

C. H. Ma and P. Nash explained the procedures used in the selection and development of duplex intermetallic phase alloys for high-temperature applications.

R. W. Smith, N. Blake, and W. B. F. Mackay examined the phase transitions in Hadfield's steel with the idea of improving its mechanical properties and range of industrial applications.

W. Brostow, H. Ertepinar, and M. A. Macip described the methods of prediction of solid + liquid equilibrium diagrams for binary mixtures forming solid solutions with an extremum.

D. A. Goodman developed a procedure for predicting and calculating vapor pressures, activities, and phase stability of binary and ternary sodium alloys.

I. Ansara, J. N. Barbier, and P.-Y. Chevalier presented a thermodynamic approach for the calculation of the C-Cr-Nb-Ni-W phase diagram.

B. C. Giessen and S. Whang described two approaches used to propose metallic glass formation diagrams.

D. Shechtman and L. J. Swartzendruber studied the metastable phase structure in rapidly solidified Al-rich Al-Fe alloys.

J. V. Wood investigated the phase stability in rapidly solidified Fe- and Ni-base alloys.

M. A. Otoomi studied the transition behavior of the amorphous Cu$_{40}$Zr$_{60}$ alloy system during its transition to crystallinity by thermal cycling.