Pearson's Handbook of Crystallographic Data for Intermetallic Phases

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by

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About the Cover

The motivation for producing this reference book, in addition to publishing a very complete, critical, and up-to-date compilation of crystal structure data, was to encourage scientists to use these data as a basis for predictions about those alloy systems for which only limited or no information is available. Recently, many investigators have correlated experimental data with semiempirical models to predict the features and properties of uninvestigated systems (Ref 1-10). The application of models is particularly important for ternary and quaternary systems, for which the large quantity of data necessitates the use of guidelines.

For example, quantitative relations have been established between atomic- and/or physical-property expressions of elements and the crystal structures of binary intermetallic compounds, as well as compound formation versus noncompound formation in binary systems. In four isostoichiometric, three-dimensional structural-stability diagrams, excellent separation into domains was achieved using the difference $\Delta (r_s + r_p)^Z_{AB} = | (r_s + r_p)^Z_A - (r_s + r_p)^Z_B |$ of the Zunger's pseudopotential-radii sums, the difference $\Delta X^{MB}_{AB} = | X^{MB}_A - X^{MB}_B |$ of the Martynov-Batsanov electronegativity, and the sum ΣVE_{AB} of the number of valence electrons as axes. Further, assuming an overlap of two different structure types in a binary system (three in a ternary) in regions containing phases that have two (or three) polymorphic structural modifications, over 3,000 binary A_1B_1, A_1B_2, A_1B_3, and A_3B_5 intermetallic compounds can be classified into distinct structure-type domains with only 2.2% violations (Ref 11-13).

Using a semiempirical approach in another investigation, three atomic-property expressions were discovered that allow separation of binary compound-forming and noncompound-forming systems by means of two three-dimensional diagrams with a 96% degree of accuracy. One diagram comprises 1,107 combinations of the isostructural elements, whereas the second diagram contains the 2,379 combinations of elements with different crystal structures. The three expressions yielding the best separation are: (1) the difference of Zunger's pseudopotential-radii sums, (2) the ratio of the melting temperatures $T_A | T_B$ ($T_A > T_B$), and (3) the difference $| \Delta VE_{AB} |$ of the number of valence electrons. In addition, the noncompound-forming systems can be separated into four types: solubility, insolubility, eutectic, and peritectic systems with a 90% degree of accuracy (Ref 14).

The cover of this book illustrates two examples of sections through one of these three-dimensional diagrams (Ref 11).

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