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THE CORRECT CALCULATION OF SOME THERMODYNAMIC PARAMETERS OF NON-IDEAL SOLUTIONS FROM THEIR PHASE EQUILIBRIUM DATA

Abstract

A computational method has been proposed for calculating the correct interaction parameters from experimental phase diagrams, despite reports that this problem was believed to be a "thermodynamically incorrect" one. It has been shown that the presumed difficulties are not of fundamental importance. An original computer program has been applied to two well-known systems Bi-Sb (1) and Bi_2Te_3-Sb_2Te_3 (2), and a good agreement between calculated and observed values has been achieved. The values of interaction parameters Ω^s=7.1±0.4, Ω^l=1.56±0.09 kJ/mole for (1) and Ω^s =5.9±2.5, Ω^l =3.9±2.5 kJ/mole for (2) have been found. The results have been analysed and their statistical reliability has been established. In addition, the possibilities of calculating the liquidus curve from only the solidus experimental data the solidus from the liquidus experimental data have been demonstrated. It has been found that the prediction of liquidus from solidus is much more successful than predicting the solidus from the liquidus.

The results allow one to determine with reliance that the backward problem of modeling regular solutions for finding thermodynamic interaction parameters can be solved correctly. The calculated parameters can be used for both the computational restoration of missing pieces of the experimental phase equilibrium diagrams of binary and multinary systems and for the recognition of the physical nature of regular solutions.