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THERMOCHEMISTRY OF FORMATION OF IRON AND ANTIMONY ALLOYS: EXPERIMENT AND MODELING

The thermochemical properties of binary liquid Fe-Sb alloys were determined by high temperature isoperibolic calorimetry. The determination of the partial enthalpies of mixing was carried out at 1723-1820 K in purified helium medium. It is shown that the process of alloying formation is accompanied by slight heat effects. The minimum value of the integral enthalpy of mixing ($\Delta_m H_{min}$) in the Fe–Sb system is evaluated to be (-2.3±0.2) kJ·mol⁻¹ at mole fraction of antimony equal to 0.5. The values of partial enthalpies for components at infinite dilution are equal to (-8.2±0.9) kJ·mol⁻¹ for iron and (-7.2±1.0) kJ·mol⁻¹ for antimony. These facts indicate a weak chemical interaction between the components of investigated alloys of iron with antimony due to the great size difference of the components. It is found that estimations of thermodynamic properties of liquid alloys based on the data for solid phases are not sufficiently reliable. Preference should be given to data obtained directly from the experiment. The simulation of mixing enthalpies of Fe-Sb melts is also performed using the model of "surrounded atom" and the associated ideal solution model. The complete applicability of these models to description of concentration dependences of the enthalpies of mixing for this system is shown. This fact allows wide use of these models for predictions of thermochemical properties of multicomponent systems which are difficult for direct experimental investigation.

Keywords: iron; antimony, high temperature calorimetry, enthalpy of mixing, model of "surrounded atom", ideal associated solution model.