ABSTRACT

This PhD thesis is dedicated to the preparation and characterisation of new zirconium-based compounds. The analysed literature and experimental data on the phase equilibria in the studied systems and the crystal structures of the resulting compounds greatly expand the understanding of the interactions of the components in zirconium-based systems and are important for both inorganic chemistry and materials science in general and can be used to search for new useful materials. The results obtained enable the prediction of component interactions in other related systems, which simplifies the task of systematic research. The data on the crystal structures of the studied compounds can be used to identify new phases in the development of new materials and as supporting material for specialists in crystal chemistry and metallurgy.

The dissertation consists of 5 chapters. The first chapter provides literature data on the phase diagrams and crystal structures of known compounds in the binary system associated with the studied Zr-Cu-Bi and Zr-Fe-Bi ternary systems. Tri-component systems similar in electronic structure to the studied systems were characterised. The main methods for metal hydride-based hydrogen storage and hydride cells were analysed. A literature review on zirconium hydrides and their alloys was conducted. Chapter two contains the thesis and objectives of the work. The third chapter describes the basics of the research methods. The fourth chapter contains the research results and their discussion, and presents the results of scanning electron microscopy (SEM), X-ray energy dispersive spectroscopy (EDS), X-ray phase analysis (XRD), calorimetric analysis (DSC), theoretical calculations, electrochemical studies and gas-phase hydrogen sorption/desorption studies. Conclusions are presented in chapter five.

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