THEORETICAL AND EXPERIMENTAL STUDY ON THERMODYNAMIC PROPERTIES INTERMETALLIC COMPOUNDS IN THE Zr-Fe BINARY SYSTEM

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Zr-Fe system is the subject of great interest in modern industry of composite and structural steels. Composite materials based on TRIP (transformation-induced plasticity) matrix reinforced by zirconia ceramics are of particular interest due to the wide range of their possible technological, especially, in the nuclear industry and automotive production as structural and functional materials. Development of such composite materials requires the knowledge of thermodynamic properties and phase relations. Thus, the main purpose of this work is the experimental and theoretical study of the thermodynamic properties of the Zr_3Fe and $ZrFe_2$ compounds. Density functional theory (DFT) calculations in combination with the quasi-harmonic approximation have been used to determine the enthalpies of formation, standard entropies as well as isochoric and isobaric heat capacities (CV, CP) for the Zr_3Fe and $ZrFe_2$ compounds form 0 K up to high temperatures. Experimentally, the heat capacities of both compounds was been measured using differential scanning calorimetry (DSC) method. Heat capacity of the Zr_3Fe compound was measured for the first time in the range of temperatures between 100 K and 1023 K. Experimental data on the heat capacity of the $ZrFe_2$ were obtained in the wide temperature range from 100 K to 1473 K and compared with available literature data. By using the combination of theoretical and experimental data, the main thermodynamic properties of the Zr_3Fe and $ZrFe_2$ compounds were described from 0 K up to temperatures close to the upper limits of stability.