Thermodynamic modelling of formation enthalpies of $Sc_{1-x}TM_xFe_2$ ($0 \leq x \leq 1$, TM - transition metal) alloys

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Based on the semi-empirical Miedema's model and geometric approach, the enthalpies of formation of intermetallics, solid solution, and amorphous phase in $Sc_{1-x}TM_xFe_2$ ($0 \leq x \leq 1$, TM – group 4 and 5 transition metals) alloys are calculated [1], and compared with existing literature data. The desired alloys are intended to be amorphous precursors for further crystallization of Laves phases (crystalline grains embedded in an amorphous matrix). The general aim is to improve the mechanical properties and cycling behavior of composites designed for caloric applications. Enthalpies of formation of intermetallic phases are the most negative, but the formation of glassy structure cannot be neglected for off-stoichiometric compositions and for ternaries with large differences in atomic radii and with significantly negative values of mixing enthalpies (especially those containing Zr and Hf atoms). As an example, ΔH_{am} (enthalpy of formation of amorhpous phase) calculated for $Sc_{0.2}Zr_{0.8}Fe_2$ is equal to -12 kJ/mol and is more negative than the enthalpy of formation of the solid solution. It has been proven that in Zr-Fe binary [2], the amorphous phase can be easily formed (using rapid quenching) close to the eutectic point, and, in this case, calculated thermodynamic parameters are not critical. Nevertheless, due to additional substitutions (growing entropy connected with increasing atomic radii differences) formation of a glassy state can be promoted, and calculated contour maps of enthalpies can serve as a guide for further experimental investigations.

References:

[1] Z. Śniadecki et al., Intermetallics 26 (2012) 72
[2] E. Hellstern, L. Schultz, Appl. Phys. Lett. 49 (1986) 1163

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