MODELLING OF PHASES WITH GENERAL NIAS-TYPE STRUCTURE: WHAT CAN WE LEARN FROM POWDER XRD?

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The general NiAs structure includes the related structure types CdI2, NiAs and Ni2In. It is composed of transition metals T and main group elements B, out of the 13th to 16th group, forming T1+/-xB structures. Due to its ability to include different amounts of transition metal, large homogeneity ranges can be found between T0.5B and T2B. The structure type is widespread among transition metal compounds and therefore present in many different alloy systems. In higher order systems, little is known about occurrence and homogeneity ranges of corresponding solid solution phases. Extrapolations using the Calphad approach are therefore often the method of choice for the prediction of multicomponent systems. For consistent models, however, a detailed knowledge of the underlying crystal chemistry is necessary.

To contribute to this knowledge, some selected ternary model systems were investigated experimentally in a current research project. The NiAs-type solid solutions were characterized by detailed Rietveld refinements of XRD powder patterns. This data helped to clarify open questions regarding the possibility of transition metal ordering and the maximal extension of a continuous phase field. Based on these results, a modified sublattice model for phases with general NiAs structure is proposed. Three endmembers of this model correspond to the boundary structures of the general NiAs type (CdI2, NiAs, Ni2In) so the end member energies can easily be calculated by DFT calculations. This was demonstrated by calculating a small database of energies of formation of (hypothetic) binary Ni-containing NiAs structures with varying main group elements.