Poster Presentation

MS10.P04

Y-brass related composite structures : a (3+1)-dimensional space description

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The γ-brass Hume-Rothery [1] phases which adopt at VEC values near about 21/13 presently attract attention due to their structural complexity and challenge for the understanding of the underlying stabilization mechanism. Morton, by electron microscopy studies, revealed that the γ-brass regions of Cu-Zn, Ni-Zn and Pd-Zn do not only accommodate the γ-brass phase but also a bundle of structurally related, complex phases with lower symmetry than that of the γ-phase. A bundle of γ-brass related phases in the Zn-rich region of the Ni-Zn, Pd-Zn, Pt-Zn phase diagram is investigated. Their structures have been refined from single crystal X-ray diffraction data in the conventional 3D space group using supercells [2,3]. In the course of a previous investigation of the Pd-Zn system, the structures of two γ-brass related composite compounds- Pd24.3Zn75.7 and Pd21.2Zn78.8 have been described with the (3+1) dimensional space description (superspace group Xmmm(00γ)0s0 with the following lattice parameters, a = 12.929(3) Å, b = 9.112(4) Å, c = 2.5631(7) Å, q = 8/13 c* and a = 12.909(3) Å, b = 9.115(3) Å, c = 2.6052(6) Å, q = 11/18 c*, respectively) [3]. The aim of this study is to represent the structure of these previously reported phases in a coherent, modulated description to make them more readily comparable. A refinement model with a variety of modulation vectors allows to refine any intergrowth structure in the Zn rich region of the M-Zn (M=Ni,Pd,Pt) system. In order to gain an insight into expressions, cause and mechanism and structure-composition relationship for such phases, we also study the impact of substitution on the evolution of the structure of ternary derivatives of M-Zn composite compounds by the use of (3+1) formalism. For instance, substitution of zero-valent palladium and bi-valent zinc by zero-valent platinum in the structure of Pd24.3Zn75.7. This presentation will discuss about the understanding of the complexity of the atomic arrangement through the various modulation which correlates with the variation of composition of the binary and ternary phases.

[1] *W. Hume-Rothery, J. Inst. Metals 1926, 35, 295.,* ***[2]*** *S. Thimmaiah, Dissertation, University of Marburg, 2005.,* ***[3]*** *O. Gourdon, Z. Izaola , L. Elcoro, et al., Inorg. Chem. 2009, 48, 9715-9722.*

Keywords: Composite structure, Intermetallic compounds, X-ray diffraction