

MS21-P1 Structural impact of Pt on a γ -brass related composite structure in the Zn-Pd system: a guided view by (3+1)-dimensional space description Partha Pratim Jana,^a Sven Lidin,^b *a,b CAS Chemical Centre, University of Lund, Sweden*
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The γ -brass Hume-Rothery [1] phases which adopt at *vec* values near about 21/13 presently attract most 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 [2], Ni-Zn [3] and Pd-Zn [4] 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 Pd-Zn phase diagram is investigated using single crystal X-ray diffraction. In the course of a preliminary investigation of the Pd-Zn system, a γ -brass related composite structure ($a = 1292.9(3)$ pm, $b = 911.2(4)$ pm, $c = 33.32(1)$ pm, $Cmce$, $oC276$), $Pd_{24.3}Zn_{75.7}$ has been refined from single crystal X-ray diffraction data in the conventional 3D space group using supercells [5]. It can be refined with the (3+1) dimensional space description as well by considering as commensurate modulated structure [6].

In order to gain an insight into expressions, cause and mechanism and structure-property relationship for such phases, we studied the impact of substitution of zero-valent palladium and bi-valent zinc by zero-valent platinum on the evolution of the structure of ternary derivatives of $Pd_{24.3}Zn_{75.7}$ by the use of (3+1) formalism.

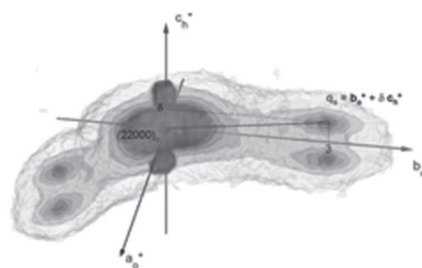
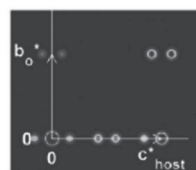
This presentation will discuss about the understanding of the complexity of the atomic arrangement through the various modulation which correlates with the variation of composition of the ternary phases.

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Keywords: intermetallic compounds crystal chemistry; X-ray diffraction; aperiodic materials.

MS21-P2 Multidimensional crystallography applied to critical phenomena. Céline Mariette,^a Laurent Guérin,^a Philippe Rabiller,^a Bertrand Toudic,^a *^a Institut de Physique de Rennes, UMR 6251 au CNRS, Université de Rennes 1, 35042, France*
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Much work has been in the past dedicated to the study of phase transitions in aperiodic crystals. The simplest cases concerned the structural instability leading to modulated incommensurate phase. There, the high symmetry phase is periodic, the phase transitions are usually continuous and a Landau-type approach was successfully applied to described both the symmetry lowering and the associated critical phenomena [1]. Here, we will consider materials which are aperiodic by construction, which means that even their high symmetry phase requires a superspace crystallographic description. A prototype example is given by aperiodic host-guest composite. We focus here on n-nonadecane/urea which present the particularity to show a group/subgroup phase transition from a four dimensional superspace group towards a five dimensional one. X-ray and neutron diffraction were used to characterise this particular symmetry breaking. The static aspect of the pretransitional fluctuations of the order parameter is studied around the transition temperature, using high resolution X-ray diffraction technique. Quite specific observations are reported, related to the persistence in the high symmetry phase of very long correlation lengths along the internal direction of the crystallographic superspace.



Up: 4D to 5D group/subgroup phase transition in n-nonadecane/urea [2,3]. Down: Pretransitional diffuse scattering associated to the transition.

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Keywords: aperiodic composites; phase transitions; X-ray diffuse scattering