

Refinement of the Crystal Structures of Palladium-rich In-Pd Compounds by X-Ray and Neutron Powder Diffraction

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Dedicated to Dr. Bernard Chevalier on the occasion of his 60th birthday

The ternary indium palladium intermetallics In₃Pd₅, InPd₂, and InPd₃ have been synthesized by iodine-catalyzed reactions from the elements. Rietveld refinements on X-ray powder diffraction patterns provide the first accurate crystal structure data for In₃Pd₅ (*Pbam*, No. 55, $a = 1104.20(2)$, $b = 561.346(8)$, $c = 424.263(6)$ pm, Rh₅Ge₃-type) and InPd₂ (*Pnma*, No. 62, $a = 561.676(6)$, $b = 421.710(4)$, $c = 822.78(8)$ pm, Co₂Si-type). X-Ray powder diffraction apparently confirms the TiAl₃ structure type proposed in the literature for InPd₃. However, Rietveld refinement on neutron powder diffraction data reveals an In/Pd distributional disorder. Therefore, we describe the crystal structure of InPd₃ in a AuCu-type model instead (*P4/mmm*, No. 123, $a = 287.224(4)$, $c = 380.079(7)$ pm), with mixed occupancy of one crystallographic site by 50 % In and 50 % Pd. In contrast to In₃Pd₅ and InPd₂, which can be considered to be line compounds, InPd₃ shows a non-negligible homogeneity range with unit cell volumes ranging from 0.126132(5) nm³ for the indium-rich to 0.125474(8) nm³ for the palladium-rich In_{1+x}Pd_{3-x} phases. Mean In–Pd distances in these indium palladium intermetallics range from 272.3 pm (In1 in In₃Pd₅) with coordination number 8 for indium to 281.2 pm for 12-coordinated In in InPd₃.

Key words: Intermetallic Compounds, Palladium, Neutron Diffraction, Powder Diffraction, Disorder