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

Holger Kohlmann\textsuperscript{a} and Clemens Ritter\textsuperscript{b}

\textsuperscript{a} FR. 8.1 Anorganische und Analytische Chemie und Radiochemie, Universität des Saarlandes, Postfach 15 11 50, 66041 Saarbrücken, Germany
\textsuperscript{b} Institut Laue-Langevin, 6, Rue Jules Horowitz, BP 156, 38042 Grenoble Cedex 9, France

Reprint requests to Dr. H. Kohlmann. Tel.: +49 681 302 3378. Fax: +49 681 302 4233. E-mail: h.kohlmann@mx.uni-saarland.de


Dedicated to Dr. Bernard Chevalier on the occasion of his 60\textsuperscript{th} birthday

The ternary indium palladium intermetallics \(\text{In}_3\text{Pd}_5\), \(\text{InPd}_2\), and \(\text{InPd}_3\) 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 \(\text{In}_3\text{Pd}_5\) (\(Pbam\), No. 55, \(a = 1104.20(2)\), \(b = 561.346(8)\), \(c = 424.263(6)\) pm, \(\text{Rh}_5\text{Ge}_3\)-type) and \(\text{InPd}_2\) (\(Pnma\), No. 62, \(a = 561.676(6)\), \(b = 421.710(4)\), \(c = 822.78(8)\) pm, \(\text{Co}_2\text{Si}\)-type). X-Ray powder diffraction apparently confirms the \(\text{TiAl}_3\) structure type proposed in the literature for \(\text{InPd}_3\). However, Rietveld refinement on neutron powder diffraction data reveals an \(\text{In}/\text{Pd}\) distributional disorder. Therefore, we describe the crystal structure of \(\text{InPd}_3\) in a \(\text{AuCu}\)-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 \(\text{In}_3\text{Pd}_5\) and \(\text{InPd}_2\), which can be considered to be line compounds, \(\text{InPd}_3\) shows a non-negligible homogeneity range with unit cell volumes ranging from 0.126132(5) nm\(^3\) for the indium-rich to 0.125474(8) nm\(^3\) for the palladium-rich \(\text{In}_{1+x}\text{Pd}_{3-x}\) phases. Mean In–Pd distances in these indium palladium intermetallics range from 272.3 pm (In1 in \(\text{In}_3\text{Pd}_5\)) with coordination number 8 for indium to 281.2 pm for 12-coordinated In in \(\text{InPd}_3\).

\textit{Key words:} Intermetallic Compounds, Palladium, Neutron Diffraction, Powder Diffraction, Disorder