Interaction of Samarium with Nickel and Arsenic: Phase Diagram and Structural Chemistry

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Dedicated to Professor Wolfgang Jeitschko on the occasion of his 70th birthday

Solid-state phase equilibria in the Sm-Ni-As system have been established using X-ray diffraction, scanning electron microscopy and electron probe microanalysis. The samarium-poor region up to 33 at. % Sm was studied at 1170 K, whereas the Sm-rich corner, due to the generally lower melting points, was investigated at 770 K. Six ternary compounds were isolated, among which two have been structurally characterized. The hexagonal structure of SmNiAs (SrPtSb-type) was solved from X-ray single crystal data: space group $P\bar{6}m2$, $a = 4.0904(3)$, $c = 3.8957(4)$ Å, $Z = 1$, $R1 = 0.0221$, $wR2 = 0.0224$ for 134 unique reflections with $I_o > 2\sigma(I_o)$ and 9 variable parameters. The crystal structure of $Sm_6Ni_{15}As_{10}$ ($Tb_6Ni_{15}As_{10}$-type) was determined from X-ray powder diffraction data: full profile refinement, space group $P6_3/m$, $a = 17.0632(4)$, $c = 3.9526(1)$ Å, $Z = 2$, $R_B = 0.079$, $R_p = 0.138$.

Key words: Samarium Nickel Arsenide, Solid-State Phase Equilibria, Crystal Structure