The Mo_2FeB_2- and Mn_2AlB_2-Type Modifications of RE_2Ni_2Cd (RE = La, Pr, Nd, Sm, Tb, Dy)

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The rare earth metal (RE)–nickel–cadmium intermetallics RE_2Ni_2Cd (RE = La, Pr, Nd, Sm, Tb, Dy) were prepared from the elements in sealed niobium or tantalum tubes in a water-cooled sample chamber of a high-frequency furnace. They crystallize with a tetragonal Mo_2FeB_2 type low-temperature modification, space group $P4/mbm$, and an orthorhombic Mn_2AlB_2 type high-temperature modification, space group $Cmmm$. The cadmium compounds were characterized through their X-ray powder patterns. Five structures of the low-temperature modifications were refined from X-ray single crystal diffractometer data: $a = 763.76(9)$, $c = 387.26(8)$ pm, $wR2 = 0.046$, 205 F^2 for $La_2Ni_{1.67(1)}Cd$; $a = 752.93(7)$, $c = 380.95(6)$ pm, $wR2 = 0.061$, 260 F^2 for Pr_2Ni_2Cd; $a = 750.88(9)$, $c = 378.33(7)$ pm, $wR2 = 0.051$, 195 F^2 for Nd_2Ni_2Cd; $a = 743.6(1)$, $c = 374.0(1)$ pm, $wR2 = 0.036$, 386 F^2 for $Sm_2Ni_{1.93(1)}Cd$; $a = 734.9(1)$, $c = 366.1(2)$ pm, $wR2 = 0.030$, 252 F^2 for $Dy_2Ni_{1.94(1)}Cd$, with 13(12) variables per refinement. The 4g nickel site is only fully occupied in the neodymium and the praseodymium compound. Both modifications can be considered as intergrowths of distorted AlB_2 and CsCl related slabs. In both modification the nickel and cadmium atoms build up two-dimensional $[Ni_2Cd]$ networks. In the low-temperature modifications the nickel atoms form pairs, while nickel zig-zag chains occur in the high-temperature modifications. These nickel fragments are condensed *via* the cadmium atoms. The crystal chemistry and the chemical bonding in these intermetallics is discussed.

Key words: Rare Earth Compounds, Cadmium, Phase Transition, Crystal Chemistry