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Yttrium–Nickel YNi with the FeB Structure Type

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Abstract. YNi, orthorhombic, *Pnma*, $a = 7.156$ (3), $b = 4.124$ (1), $c = 5.515$ (2) Å, $Z = 4$, $D_x = 6.02$ Mg m⁻³, $\mu(\text{Ag } K\alpha) = 25.84$ mm⁻¹; final $R = 0.024$ for 235 observed intensities. The structure belongs to the FeB type. No indication of monoclinic symmetry as reported by Smith & Hansen [*Acta Cryst.* (1965), **18**, 60–62] has been found.

Introduction. The equiatomic compounds of the late rare-earth metals (Dy–Lu) and Ni are found to crystallize with the orthorhombic FeB structure type (Abrahams, Bernstein, Sherwood, Wernick & Williams, 1964; Dwight, Conner & Downey, 1965; Palenzona & Cirafici, 1973). For YNi Smith & Hansen (1965) reported, however, a monoclinic structure (space group *P2₁/b*) with a pseudo-orthorhombic unit cell. After an interchange of the axes the proposed YNi structure has similarities to the FeB structure. YNi would be identical to FeB if the y_Y and y_{Ni} values, corresponding to the site set $x\frac{1}{2}z$ in *Pnma*, were exactly $\frac{1}{4}$. The value of $\frac{1}{4}$ is, however, well within the error limits given for the Y and Ni parameters. Thus the question arises as to whether YNi is really monoclinic or crystallizes with the orthorhombic FeB type.

YNi was prepared by conventional arc-melting techniques from metals of high purity (99.99%). The crushed ingot was wrapped in Ta foil and annealed for two weeks at 1073 K. Fragments of the sample (dimensions 135–200 µm) were shaped with an air mill.

A single crystal of ellipsoidal shape (40 × 50 × 60 µm) was selected and mounted on an automatic four-circle diffractometer (Philips PW 1100). Intensities were collected in the θ – 2θ scan mode ($6^\circ < 2\theta < 50^\circ$) with graphite-monochromated Ag $K\alpha$ radiation ($\lambda = 0.5608$ Å). A second data collection was

performed with graphite-monochromated Mo $K\alpha$ radiation ($6^\circ < 2\theta < 54^\circ$). Four sets of equivalent reflections [corresponding to two sets in the monoclinic space group *P2₁/b* proposed by Smith & Hansen (1965)] were measured. The usual background and Lorentz–polarization corrections were applied. Absorption effects were accounted for by a spherical absorption correction ($\mu R = 0.6$ for Ag $K\alpha$). A critical inspection of the systematically absent reflections ($hk0$: $h = 2n + 1$, $0kl$: $k + l = 2n + 1$) indicated space group *Pnma* or *Pn2₁/a*. Special attention was paid to the $0kl$ reflections, since they should be observable with the lower monoclinic symmetry proposed by Smith & Hansen. A weak non-zero intensity was only observed in one setting of the 021 reflection. However, this reflection was absent in the Mo $K\alpha$ data set, which is an indication that it was due to multiple diffraction. Moreover, the equivalent general reflections did not show any systematic intensity differences. Therefore the true symmetry of YNi must be orthorhombic. Averaging the four sets (internal consistency factor 0.025) yielded a unique set of 322 reflections, 235 with $I > 3\sigma(I)$.

The structure was refined by full-matrix least squares with, as starting parameters, calculated atomic positions [equations (8), (13a), (13b), (14a) and (14b) in Klepp & Parthé (1980)]. Isotropic refinement converged to an R of 0.025. Anisotropic refinement resulted in an R of 0.024 [$R_w = 0.037$, $w = 1/\sigma^2(F)$, 257 contributing reflections, including 22 weak reflections calculating greater than the observed]. Scattering factors for neutral atoms were taken from Cromer & Mann (1968), and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974). All calculations were performed with the

XRAY system (1976).^{*} Lattice constants were refined from 22 reflections centred on the diffractometer (Ag $K\alpha$ radiation).

^{*} Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35616 (5 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Fractional atomic coordinates ($\times 10^4$) and interatomic distances (\AA) for YNi up to 4 \AA [space group $Pnma$; all atoms in 4(c)]

The isotropic temperature factor is expressed as $T = \exp(-2\pi^2 U s^2)$ where $s = 1/d_{hkl}$; U values are $\text{\AA}^2 \times 10^4$. The values for the isotropic temperature factors are obtained by recalculation from the anisotropic ones. E.s.d.'s are in parentheses and refer to the last significant figure.

	x	y	z	$U (\text{\AA}^2)^*$
Y	1798 (1)	2500	1325 (2)	92 (2)
Ni	357 (2)	2500	6233 (3)	104 (4)
Y-Ni	2.897 (2)		Ni-Y	2.897 (2)
2Ni	2.898 (1)		2Y	2.898 (1)
2Ni	2.906 (1)		2Y	2.906 (1)
Ni	2.911 (2)		Y	2.911 (2)
Ni	2.991 (2)		Y	2.991 (2)
Y-4Y	3.587 (1)		Ni-2Ni	2.522 (1)
2Y	3.607 (1)		2Ni	3.841 (3)
2Y	3.806 (2)			

* Calculated from $U = \frac{1}{3}(U_{11} + U_{22} + U_{33})$.

Discussion. The final atom coordinates and interatomic distances are listed in Table 1. The coordinates agree with those calculated on the basis of ideal stacking which requires that each Y atom should have six equidistant Y neighbours (Klepp & Parthé, 1980).

There is no doubt that YNi crystallizes with the orthorhombic FeB structure. It seems likely that multiple diffraction was the cause of the two weak $0kl$ reflections observed by Smith & Hansen (1965) which led them to assume that YNi has monoclinic symmetry.

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Structure of Copper-Indium Cu_7In_3

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Abstract. Cu_7In_3 , triclinic, $P\bar{1}$, $a = 10.071(5)$, $b = 9.126(5)$, $c = 6.724(4)$ \AA , $\alpha = 90.22(3)$, $\beta = 82.84(3)$, $\gamma = 106.81(3)^\circ$, $Z = 4$, $V = 586.6$ \AA^3 , $D_c = 8.94$, $D_o = 8.94$ Mg m^{-3} . $R = 0.098$ for 1760 refined reflections. The In atoms are arranged in approximate layers which also contain some of the Cu atoms; the remaining Cu atoms are situated in layers about halfway between these approximate layers.

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Introduction. The cell parameters of the δ phase in the binary system Cu-In have been reported by several authors. Weibke (1939) proposed a cubic cell, Gaun-
eau & Graf (1968) a triclinic one, while according to Fournelle & Clark (1972) the cell is tetragonal with very large parameters. As the structure of this alloy is of interest in understanding alignment in composite materials (Vrolijk & Wolff, 1980) it was desirable to

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