Crystal structure of iron nickel phosphide, $Fe_{1.65}Ni_{1.35}P$, *a Rhabdite extracted from Morasko meteorite*

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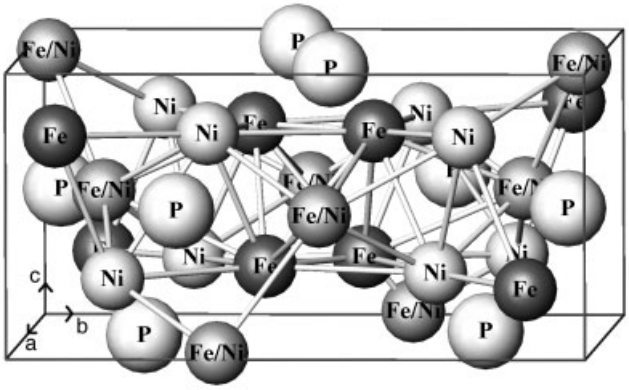

Abstract

$Fe_{1.65}Ni_{1.35}P_8$, tetragonal, $I\bar{4}$ (No. 82), a = 9.059(2) Å, c = 4.479(1) Å, V = 367.6 Å^3, Z = 8, $R_{gt}(F)$ = 0.022, $wR_{ref}(F^2)$ = 0.049, T = 293 K.

Source of material

Single crystals of the phosphides from "Morasko" were obtained by using a solution with HNO_3 (3%) and methanol. After dissolving the meteorite samples only sulphides, carbides, oxides, phosphides and other crystals remained. The solution with the crystals was filtered and the phosphides were picked up from the filter material. They were prepared and fixed on glas fibres for X-ray experiments. The chemical composition was determined by electron microprobe analysis (Cameca SX 100). The crystals are homogenous and don't show zonations, twinnings or intergrowth sections.

Discussion

The $(Fe,Ni)_3P$ single crystals (ideomorph variant named Rhabdite) from the "Morasko" meteorite with a Fe:Ni-ratio of 1.2:1 ($Fe_{1.65}Ni_{1.35}P$) show a body centered tetragonal crystal structure with the well known space group $I\bar{4}$ typical for meteoritic phosphides. The distribution of Fe and Ni on the three symmetry independent metal positions was determined earlier on Rhabdites from "North Chile" meteorite using a Co-tube with a wavelength near by the Fe absorption edge. This result showed that Ni prefers the M2 and M3 sites avoiding M1 [1] (cf. also [2]). Additional measurements with synchrotron radiation (HASYLAB at DESY, Hamburg) near the Fe absorption edge in order to separate Fe and Ni using the anomalous dispersion and the delta synthesis [3,4] showed the same ordering: Fe prefers the M1 and M2 sites whereas Ni prefers the M2 and M3 sites. Considering this fact, the site occupancy factors of the Fe and Ni atoms were fixed during refinement [5]. The best R-value is evoked by a distribution with Fe on M1, Fe/Ni on M2 and Ni on M3.

Table 1. Data collection and handling.

Crystal:	bronze tetragonal prism, size 0.030 × 0.265 × 0.500 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	268.49 cm^{-1}
Diffractometer, scan mode:	Stoe IPDS, ϕ
$2\theta_{max}$:	47.72°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2135, 292
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 273
$N(param)_{refined}$:	39
Program:	SHELXL-97 [5]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	8g		0.0782(1)	0.1081(1)	0.2301(3)	0.0090(6)	0.0103(6)	0.0124(8)	0.0003(5)	–0.0005(6)	0.0009(7)
Fe(2)	8g	0.65	0.3619(1)	0.0336(1)	0.9793(3)	0.0084(6)	0.0090(6)	0.0098(6)	0.0006(4)	0.0002(6)	–0.0006(6)
Ni(2)	8g	0.35	0.3619	0.0336	0.9793	0.0084	0.0090	0.0098	0.0006	0.0002	–0.0006
Ni(3)	8g		0.1682(1)	0.2189(1)	0.7485(3)	0.0123(6)	0.0118(6)	0.0135(7)	0.0021(4)	–0.0001(5)	–0.0006(6)
P	8g		0.2923(2)	0.0501(2)	0.4834(6)	0.009(1)	0.010(1)	0.011(1)	0.0005(8)	–0.001(1)	0.002(1)

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