Crystal structure of iron nickel phosphide, $\text{Fe}_{1.65}\text{Ni}_{1.35}\text{P}$, a *Rhabdite* extracted from *Morasko* meteorite

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Abstract

$\text{Fe}_{1.65}\text{Ni}_{1.35}\text{P}_8$, tetragonal, $\bar{I}4$ (No. 82), $a = 9.059(2)$ Å, $c = 4.479(1)$ Å, $V = 367.6$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.022$, $wR_{\text{ref}}(F^2) = 0.049$, $T = 293$ 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 glass 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 $(\text{Fe,Ni})_3\text{P}$ single crystals (ideomorph variant named *Rhabdite*) from the “Morasko” meteorite with a Fe:Ni-ratio of 1.2:1 ($\text{Fe}_{1.65}\text{Ni}_{1.35}\text{P}$) show a body centered tetragonal crystal structure with the well known space group $\bar{I}4$ 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 $0.030 \times 0.265 \times 0.500$ mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	268.49 cm^{-1}
Diffraction, scan mode:	Stoe IPDS, ϕ
$2\theta_{\text{max}}$:	47.72°
$N(hkl)_{\text{measured}}, N(hkl)_{\text{unique}}$:	2135, 292
Criterion for $I_{\text{obs}}, N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 273
$N(\text{param})_{\text{refined}}$:	39
Program:	SHELXL-97 [5]

Table 2. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	Occ.	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> 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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References

1. Doenitz, F. D.: Die Kristallstruktur des meteoritischen Rhabdits (Fe,Ni)₃P. *Z. Kristallogr.* **131** (1970) 222-236.
2. Skála, R.; Drábek, M.: Powder Data for synthetic analogue of a mineral nickelposphide. *Powder Diffraction* **17** (2002) 322-325.
3. Wendschuh-Josties, M.: Determination of cation distributions by anomalous dispersion. *Z. Kristallogr.* **209** (1994) 107-112.
4. Moretzki, O.: Experimentelle Studien zur Kationen-Ordnung und Überstrukturbildung in Ba(Ba,Pb,Bi,Sb)O₃-Perowskiten – Röntgenbeugung und Anwendung der Synchrotronstrahlung. Ph. D. Thesis, University of Leipzig, Germany 1999.
5. Sheldrick, G. M.: SHELXL-97, a program for refining crystal structures, University of Göttingen, Germany 1997.