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Crystal structure of niobium chromium nickel, $Nb(Cr_{1-x}Ni_x)_2$ (x = 0.49)

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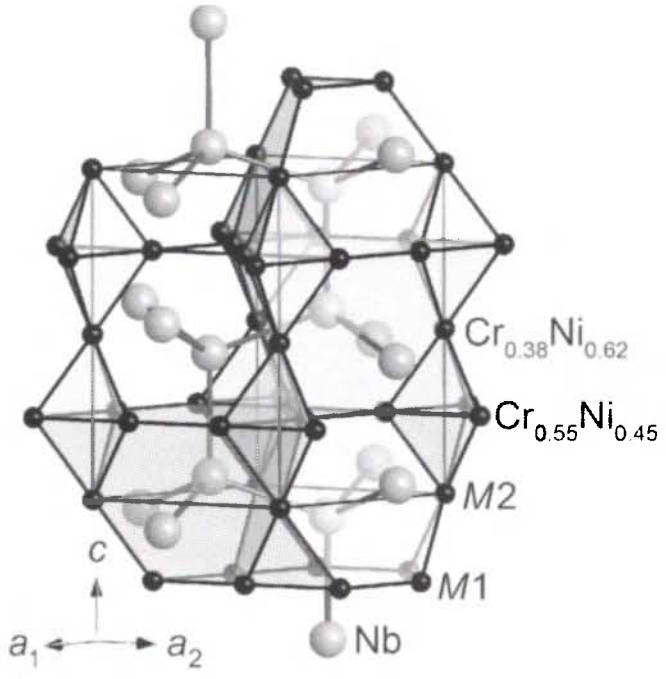

Abstract

$Cr_{1.02}NbNi_{0.98}$, hexagonal, $P6_3/mmc$ (no. 194), a = 4.8692(5) Å, c = 7.9628(8) Å, V = 163.5 Å^3, Z = 4, $R_{gt}(F)$ = 0.052, $wR_{ref}(F^2)$ = 0.111, T = 293 K.

Source of material

A single crystal of irregular shape and metallic luster was obtained from a sample of nominal composition NbCrNi. The sample was prepared by arc-melting a mixture of the elements (Nb, 99.9 %, Starck; Cr, 99.99 %, Ni, 99.99 %, Chempur) on a water cooled copper hearth in Ar atmosphere. For the following heat treatment at 1373 K for 30 days the sample was weld-sealed in a niobium ampule, which was in turn held within an evacuated and sealed fused silica jacket. Finally, the sample was quenched in cold water.

Experimental details

The unit cell parameters were determined from least-squares refinements of the 2θ values of 28 reflections (Cu $K_{\alpha 1}$ radiation, λ = 1.54056 Å) in the range 20° < 2θ < 100° using Si powder SRM640c (a = 5.431195 Å) as an internal standard. Metallographic examination confirms the phase purity (C14) of the sample. Elemental analysis – (nominal NbCrNi) found by ICP-OES: Nb, 33.5(4) at %; Cr, 33.2(4) at %; Ni, 33.3(3) at %.

Discussion

The title compound is a Laves phase of C14 structure type [1]. Cr and Ni atoms (M) occupy randomly the vertices of a six-connected net composed of distorted M_4 tetrahedra. These units are joined alternately point-to-point and base-to-base, thereby forming infinite chains along c of apically-fused trigonal bipyramids. These chains are linked together in the a_1,a_2 plane, thus forming large polyhedra with the geometrical shape of truncated M_{12} tetrahedra. The Nb atoms (Nb1) occupy the center of these polyhedra and form a four-connected net of wurzite type, which in turn interpenetrates the net of the M atoms. The Nb and the M atoms are coordinated by Friauf polyhedra (CN = 16) and by icosahedra (CN = 12), respectively. The crystal structure comprises triangular and Kagome layers with stacking sequence aBβBaCγC along c. The symbols β, γ denote Kagomé layers composed of Cr/Ni atoms at M1 whereas a and B,C denote triangular layers of Cr/Ni atoms at M2 and Nb atoms, respectively. The crystal structure is significantly distorted compared with an idealized crystal structure based on a hard sphere model. The distortion is manifested by the deviation of c/a = 1.6353 from the ideal ratio (1.6329) and by that of x(M1) and z(Nb1) from the idealized parameters ⅙ and ⅝, respectively. The nature of the distortion is described as an expansion of those $(M1)_3$ triangles (d(M1—M1) = 2.483(1) Å) of the Kagomé layers, which are capped by the M2 atoms at 2.453(1) Å, and a contraction of the uncapped triangles (d(M1—M1) = 2.387(1) Å). The Nb net is slightly distorted with d(Nb—Nb) = 3 × 2.980(1) A and 1 × 2.993(2) A). The interatomic distances d(Nb—M) range from 2.841(1) Å to 2.858(1) Å. No Laves phase is reported for the Nb-Ni system, but a C15 and above 1850 K a C14 polytype is known in the Nb-Cr system. Thus, alloying Ni to $NbCr_2$ stabilizes the C14 structure type at lower temperatures forming the solid solution phase $Nb(Cr_{1-x}Ni_x)_2$. It was found that x ranges at 1275 K from 0.07 to 0.58 [2]. For the title compound (x = 0.49, T = 1373 K) the Cr atoms occupy preferentially the Kagomé layer positions (55 %) and Ni atoms the triangular layer positions (62 %).

Table 1. Data collection and handling.

Crystal:	metallic light silvery, irregular, size 0.015 × 0.025 × 0.065 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	241.23 cm^{-1}
Diffractometer, scan mode:	Rigaku R-AXIS RAPID, φ/ω
$2\theta_{max}$:	143.64°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	5023, 560
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 522
$N(param)_{refined}$:	12
Programs:	SHELXL-97 [3], DIAMOND [4]

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

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
$M(1)$*	6*h*	0.16995(7)	2x	¼	0.0062(1)	0.0043(2)	0.0062(3)	0.00216(8)	0	0
Nb(1)	4*f*	⅓	⅔	0.56206(8)	0.0066(1)	U_{11}	0.0066(3)	½U_{11}	0	0
$M(2)$**	2*a*	0	0	0	0.0066(2)	U_{11}	0.0055(5)	½U_{11}	0	0

* $M(1) = Cr_{0.55(3)}Ni_{0.45}$

** $M(2) = Cr_{0.38(4)}Ni_{0.62}$

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