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Crystal structure of praseodymium dimolybdenum disilicide carbide, $PrMo_2Si_2C$

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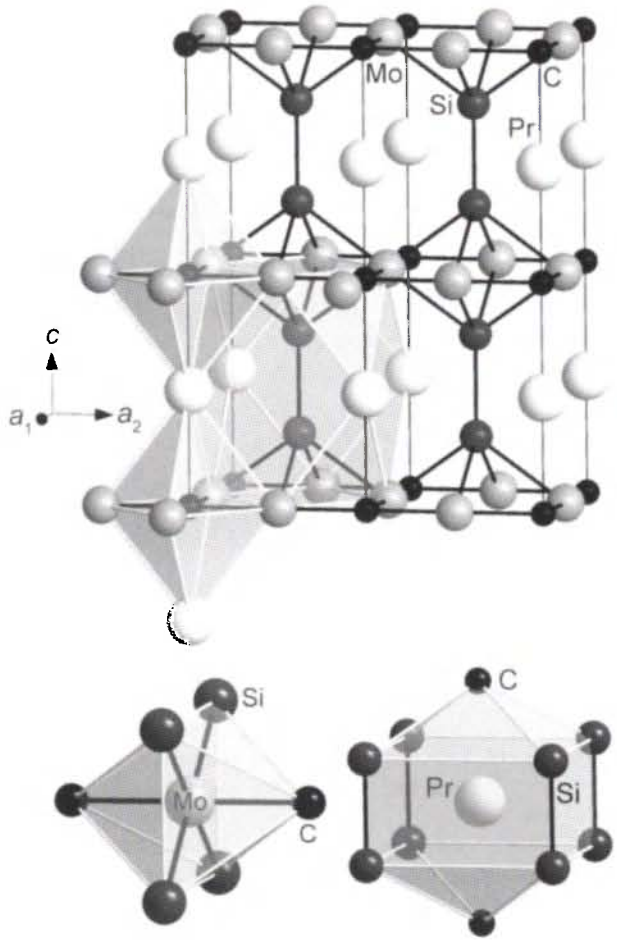

Abstract

CMo_2PrSi_2, tetragonal, *P4/mmm* (no. 123), $a = 4.2139(3)$ Å, $c = 5.4093(4)$ Å, $V = 96.1$ Å^3, $Z = 1$, $R_{gt}(F) = 0.020$, $wR_{ref}(F^2) = 0.042$, $T = 295$ K.

Source of material

Single crystals with platy habit and with a metallic dark gray luster have been obtained by a two-step high-temperature synthesis. A cold-pressed pellet containing a mixture of the elements Pr (99.9 %, Alpha Aesar), Mo (99.9 %, Chempur), Si (99.99 %, Chempur) and graphite (99.9 %, Chempur) in molar ratio 1:2:2:1 was arc-melted under argon atmosphere. Due to the sensitivity of the bulk material against air and moisture all handling was done in a glove box. The sample was then annealed at 900 °C for 10 days in an evacuated and sealed silica tube and finally quenched in water. The sample contains traces (<2 %) of the second phase Mo_2C.

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Experimental details

The single crystal has been mounted in an argon-filled and sealed Lindemann capillary. The lattice parameters were determined from the least-squares refinements of the 2θ values of 14 reflections ($CuK_{\alpha 1}$ radiation, $\lambda = 1.54056$ Å) in the range $10° < 2\theta < 85°$ using LaB_6 powder SRM660a ($a = 4.15692$ Å) as an internal standard.

Discussion

The title compound crystallizes in the $CeCr_2Si_2C$ structure type [1,2]. The Pr and Mo atoms form an 8-connected network with a space-filling packing of distorted octahedra and cuboctahedra ($c/a = 1.284$) with packing ratio of 1:1. The arrangement of polyhedra is similar to that in a tetragonal perovskite where the oxygen atoms are located at the vertices. However, in this case the polyhedra are much more stretched. In the metal substructure square layers of Pr atoms (d(Pr—Pr) = 4.2139(3) Å) alternate along [001] with square layers of Mo atoms (d(Mo—Mo) = 2.9797(2) Å). The Mo layers are shifted relatively by $\frac{1}{2}a_1$ compared to the Pr layers. The Mo atoms have 4 Mo at 2.9797(1) Å and 4 Pr atoms as nearest metal neighbors while all Pr atoms are adjacent to 8 Mo atoms with d(Mo—Pr) = 3.4285(2) Å. Monoatomic carbon species occupy the octahedral sites, Mo_4Pr_2, of the polyhedra packing. The stretched cuboctahedra, $Mo_4Pr_4Mo_4$, are occupied by Si_2 dimers, which are aligned parallel to the fourfold axis. The interatomic distance d(Si—Si) in the dimer is 2.393(4) Å, somewhat greater than the single bond distance of 2.352 Å in elemental silicon. The Mo atoms are surrounded octahedrally by 2 C atoms at 2.1070(1) Å) and by 4 Si atoms at 2.591(1) Å. The eight faces of this octahedron are capped by four Pr and four Mo. The Pr atoms are surrounded linearly by 2 C at 2.7046(2) Å and in a tetragonal prismatic arrangement by 8 Si atoms at 3.2110(7) Å.

Magnetic susceptibility measurements in the temperature range 100 K – 400 K show Curie-Weiss type paramagnetism with an effective moment of 3.6 μ_B per Pr atom consistent with a $4f^2$ configuration, i.e., Pr^{3+} ion ($\mu_{free} = 3.578\ \mu_B$).

Table 1. Data collection and handling.

Crystal:	metallic dark gray plate, size 0.01 × 0.02 × 0.04 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	192.93 cm^{-1}
Diffractometer, scan mode:	Rigaku AFC-7 & Mercury 70 CCD
$2\theta_{max}$:	65.52°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	813, 131
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 130
$N(param)_{refined}$:	12
Programs:	SHELXL-97 [3], DIAMOND [4]

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}
Si	2*h*	½	½	0.2788(3)	0.0052(4)	U_{11}	0.0064(7)	0	0	0
Mo	2*f*	0	½	0	0.0038(3)	0.0049(3)	0.0064(3)	0	0	0
Pr	1*b*	0	0	½	0.0059(2)	U_{11}	0.0064(3)	0	0	0
C	1*a*	0	0	0	0.007(2)	U_{11}	0.007(4)	0	0	0

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