Kristallstrukturen und elektronische Eigenschaften von $Ge_{1/3}NbS_2$ und $Ge_{1/4}NbS_2$

Crystal Structures and Electronic Properties of $Ge_{1/3}NbS_2$ and $Ge_{1/4}NbS_2$

Regina Pocha und Dirk Johrendt

Institut für Anorganische Chemie und Strukturchemie, Lehrstuhl II, Heinrich-Heine-Universität Düsseldorf, Universitätsstrasse 1, D-40225 Düsseldorf, Germany

Sonderdruckanforderungen an D. Johrendt. E-mail: johrendt@uni-duesseldorf.de

Herrn Professor Albrecht Mewis zum 60. Geburtstag gewidmet

Z. Naturforsch. **57 b,** 1367–1374 (2002); eingegangen am 2. September 2002

Niobium Sulfide, Intercalation, Germanium, Crystal Structure, Electronic Structure

Single crystals of the intercalation compounds $Ge_{1/3}NbS_2$ and $Ge_{1/4}NbS_2$ have been prepared by heating of the elements at 1073 K and by chemical transport with iodine at 923 to 1073 K. Their crystal structures were determined by single crystal X-ray methods. $Ge_{1/3}NbS_2$ ($P6_3/mcm$, $a = 5.767(1)$, $c = 13.518(3)$ Å, $Z = 6$) crystallizes with a superstructure of 2*H*-NbS_2, characterized by layers of edge-sharing NbS_6 trigonal prisms. The Ge atoms in the octahedral voids of the van der Waals gap are sixfold coordinated by sulfur. The NbS_2-sublattice of $Ge_{1/4}NbS_2$ ($P6_3/mmc$, $a = 3.339(1)$, $c = 37.326(7)$ Å, $Z = 6$) represents a new *6H*-polymorph. Herein, the Ge atoms are located either in the centers of the octahedral voids (c. n. = 6) or shifted from this position along [001] (c. n. = 3 + 3). The unusual electronic state and the bonding situation of germanium in the van der Waal gaps of NbS_2 and the metal-metal bonding are studied in detail by using DFT band structure calculations.