Transmissionsoptimierte Einkristallstrukturbestimmung und elektronische Struktur von Bi_3Ni

Transmission-Optimized Single-Crystal Structure Determination and Electronic Structure of Bi_3Ni

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Crystals of Bi_3Ni were synthesized using iodine as mineralizer. X-ray diffraction on a single-crystal including transmission-optimized measurement and optimized absorption correction (μ(Mo-K$_\alpha$) = 1302 cm^{-1}) results in a structure model (*Pnma*; a = 887.96(7), b = 409.97(3), c = 1147.8(1) pm) with significant deviations in interatomic distances compared with previous data from X-ray and neutron investigations. From quantum chemical calculations and from the structural chemistry of the subhalides related to Bi_3Ni the chemical structure of the intermetallic compound can be derived. In the crystal structure the Ni atoms have a capped trigonal prismatic coordination of Bi atoms with strong bonds Ni–Bi and Ni–Ni. The prisms constitute rods $^1_\infty$[$NiBi_{1/1}Bi_{6/3}$] by sharing the non-capped square faces. The bonding between the intermetallic rods is clearly weaker than inside them, leading to a preservation of this structural fragment in the subhalides of Bi_3Ni. In accordance with the low temperature superconductivity of the compound, its electronic band structure shows steep and flat bands at the Fermi level. DFT and ELF calculations reveal a separation of delocalized conduction electrons inside the prism rods and largely localized valence electrons between them.

Key words: Intermetallics, Ultra-High Absorption, Crystal Structure, Bonding, Electronic Localisation