Multipole refinement and topological analysis of chemical bonding in β-boron

Claudio Eisele[1], Natalia Dubrovinskaia[1], Sitaram Ramakrishnan[1, 2], Jin-Ke Bao[3], Surya Rohith Kotla[1], Carsten Paulmann[4], Leila Noohinejad[5], Martin Tolkiehn[5], Sander van Smaalen[1]

[1]Laboratory of Crystallography, University of Bayreuth, claudio.eisele@uni-bayreuth.de, Germany, [2] Department of Quantum Matter, AdSM, Hiroshima University, 739-8530, Higashi-Hiroshima, Japan, [3]Department of Physics, Shanghai University, China, [4]Mineralogisch-Petrographisches Institut, University of Hamburg, Germany, [5] P24, PETRA III, Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany

Although the crystal structure of β-rhombohedral boron has been established already in 1957 [1], open questions in its details are still remaining [2]. Like other elemental boron-phases, β-boron features a network of interconnected B_{12} icosahedral clusters; in case of β-boron, $(B_{28})_2B$ clusters connecting B_{12} icosahedra and other $(B_{28})_2B$ clusters complete the framework which has in total 15 unique boron sites. Beyond that, interstitial boron (or impurity) atoms can be accommodated in the cavities of this outstanding framework. According to the hitherto most widely adopted model established by Slack *et al.* [4], there are five so-called partially occupied sites (POS) accommodating interstitials in 3.7 to 27.2 % of the unit cells; β-boron crystallizes in the rhombohedral space group $R\bar{3}m$ and contains approximately 320 boron atoms in the hexagonal unit cell of a volume of V ≈ 2465 Å^3.

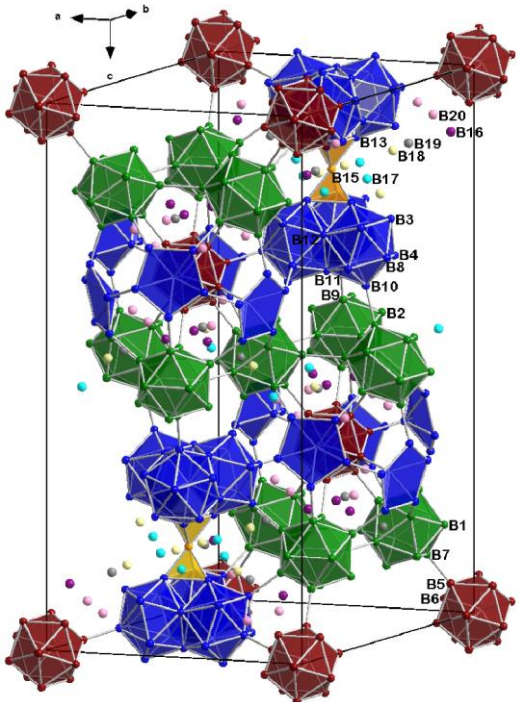

Fig. 1 Hexagonal unit cell of β-boron. B_{12} icosahedra and $(B_{28})_2B$ clusters are depicted as polyhedra, POS are depicted as single atoms. For the sake of clarity, some of the clusters are only partially drawn or completely omitted.

We collected high-resolution X-ray diffraction data using synchrotron radiation and samples of high purity. All main features of Slack's model were confirmed by a routine structure refinement against the experimental XRD data. In order to compute a more sophisticated electron density taking into account deviations from the spherical distribution of atomic electron densities, we performed a multipolar refinement [5].

We will present a characterization of the peculiar chemical bonds in β-boron based on the refined multipole model and the resulting electron density.

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