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Experimental core electron density of cubic boron nitride

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The resent progress in powder diffraction provides data of quality beyond multipolar modeling of the valence density. As was recently shown in a benchmark study of diamond by Bindzus et al.[1] The next step is to investigate more complicated chemical bonding motives, to determine the effect of bonding on the core density. Cubic boron nitride lends itself as a perfect candidate because of its many similarities with diamond: bonding pattern in the extended network structure, hardness, and the quality of the crystallites.[2] However, some degree ionic interaction is a part of the bonding in boron nitride, which is not present in diamond. By investigating the core density in boron nitride we may obtain a deeper understanding of the effect of bonding on the total density. We report here a thorough investigation of the charge density of cubic boron nitride with a detailed modelling of the inner atom charge density. By combining high resolution powder X-ray diffraction data and an extended multipolar model an experimental modeling of the core density is possible.[3] The thermal motion is a problem since it is strongly correlated to the changes of the core density, but by combining the average displacement from a Wilson plot and a constrained refinement, a reasonable result has been obtained. The displacement parameters reported here are significantly lower than those previously reported, stressing the importance of an adequate description of the core density. The charge transfer from boron to nitrogen clearly affects the inner electron density, which is evident from theoretical as well as experimental result. The redistribution of electron density will, if not accounted for, result in increased thermal parameters. It is estimated that 1.7-2 electrons is transferred from boron to nitrogen.

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