Comment on "New Ground-State Crystal Structure of Elemental Boron"

An *et al.* [1] claim to have studied high-purity β-rhombehedral boron. In fact however, the purity level 99.2% of their boron, prepared by H. C. Starck, is far from the high-purity standard 99.9999% (except carbon, 30–60 ppm), established in the 1960s by Wacker-Chemie, Munich, Germany (see [2,3]), and independently, by Research Centre for Crystals (RCC), Warsaw, Poland [4–6]. Both prepared large high-quality single crystals [7,8], whose high purity is proven, for example, by very low electrical conductivity, congruent down to low temperatures [9,10] (see also [11–13] and Refs. therein). At 300 K, the electrical conductivity of high-purity boron is $\sim 2 \times 10^{-7}\ \Omega^{-1}\ \mathrm{cm}^{-1}$.

H. C. Starck, Goslar, Germany, produces boron for industrial applications and does not claim high purity; impurities in Table I.

The sum of impurities (Table I) is compatible with the low grade 99.2% purity referred by the authors. Hence, 75% of the unit cells are statistically affected by impurities. Missing corresponding peaks in their x-ray EDS spectrum do not refute the chemical analysis, but show that the sensitivity of EDS is not sufficient. This holds for their EELS spectrum as well; this is known to be unsuitable to resolve effects of impurities on the structure in boron.

The electrical conductivity of Starck boron at 300 K, $\sim 2 \times 10^{-5}\,\Omega^{-1}\,\mathrm{cm}^{-1}$ [16], exceeds that of high-purity boron by 2 orders of magnitude.

Impurities affect the structure parameters remarkably. Carbon, substituting for boron in polar sites of icosahedra, reduces the unit cell [17,18]; otherwise, this is widened by metal atoms that are interstitially accommodated (see [12,19]).

H. C. Starck produces boron powders like that under discussion from lumps; size typically several cm^3 [8]. At first, the lumps are crushed, and then ground to powder with the grain size requested [14]. Such processing exposes the grains to enormous mechanical stress.

As well-known, the formation energy of twins in rhombohedral structures like boron and boron carbide is low, and mechanical stress induces twins even in small grains. Hence, we can rather safely assume that the twin structures, observed in Starck boron powder, are caused by the method of processing. This seems to be a more plausible explanation of the twin structures than assuming a new ground state structure of boron. Surprisingly, the Letter does not mention any trial to heal these defects, for example, by long-time annealing at high temperatures exceeding the phase transition in β-rhombohedral boron at 550 K [13].

The results presented in the Letter may describe correctly the specific boron samples investigated. However, additional conclusions on the basic structure of boron are daring. The boron samples used are not pure; alternative explanations of the twin structures as well as attempts to heal them are missing.

TABLE I. Impurities in β-rhombohedral boron of H. C. Starck.

Element	Impurities (ppm) Typical [14]	Maximum [15]
C	~1500	3000
N		500
O	~500	1000
Al	~300	1000
Fe	~500	1000
Si	~700	2000
Mg	~100	
Mn		1000
$\sum$	~3600	9500

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