An *et al.* Reply: Our Letter reported high-resolution transmission electron microscopy on commercial quality boron showing that ~2/3 of the grains exhibit smooth microstructure, leading to an x-ray diffraction pattern of well-known beta boron [1]. The other 1/3 grains exhibit a uniform zigzag pattern that extends across the entire grain and exhibits a very regular twinlike symmetry on every other lattice plane. This second phase gives diffraction patterns that are different from beta.

We then used density functional theory to examine the zigzag crystal structure in boron. We found a second stable phase we termed the tau phase that leads to exactly the same TEM diffraction pattern and x-ray diffraction angles observed experimentally for the grains with the zigzag pattern. The DFT energies for the two phases are very similar, and we claimed that tau was lower. We now know that this resulted from the inconsistent use of pseudopotentials. We have repeated the DFT calculations for three sets of DFT functionals, all of which found beta to be slightly more stable than tau: by 1.7 meV/B for PBE [2], 1.8 meV/B for M06-L [3], and 2.1 meV/B for B3PW91 [4].

The most important point of our Letter is our discovery that commercial high purity boron (>99.2%) is composed of both beta and tau grains, each of which are 100% one or the other. This new tau phase had not been known previously. This raises important issues of how the mechanical and electronic properties of these two phases differ, and how many of the previously measured properties of boron involve such mixtures. This suggests a number of experiments that might be done to characterize these differences, making this PRL a very interesting contribution.

With regard to Werheit's [5] comments about purity, we are aware that six nines boron has been produced in single crystal form and studied using electrical resistivity measurements, but *we do not agree that six nines purity boron is* "*the usual object of reliable investigations*."

For example, in a recent paper on the effect of boron powder purity on superconducting properties of MgB_2, [6] Xu *et al.* state, "*Currently, in order to achieve the highest Jc, high purity amorphous B powers (99%) were used. However, in practical applications, the cost of the materials must be considered. The pure (99%) amorphous boron powder is about 10 times more expensive than the low–grade (96%, 92%) amorphous powders*." This clearly contradicts the claim that six nines purity is the norm.

We also disagree with Werheit that the tau phase probably was caused by mechanical processing. The key point is that *the entire grain is transformed to the tau structure*. Twinning from mechanical processing is nearly always heterogeneously distributed. This occurs because the stresses build up inhomogeneously to trigger localization events like twinning. The idea that twins would be nucleated by mechanical stress and propagate on every other plane across the entire grain is not plausible.

Werheit recommends the use of electrical resistivity as a sensitive way of measuring impurities. However, we cannot make electrical resistivity measurements of individual boron grains.

We reiterate that we studied individual powders (neither boron single crystals nor powder blends). This is why we used energy-dispersive X-ray spectroscopy (EDXS) (Fig. 1) to measure the impurity content of the individual powders that we characterized. Our EELS characterization (Figure S2 of Ref. [1]) also shows pure B for both grains.

Q. A. and M. R. contributed equally to this work.

Qi An,[1] K. Madhav Reddy,[2] Kelvin Y. Xie,[2]
Kevin J. Hemker[2,*] and William A. Goddard III[1,†]
[1]Materials and Process Simulation Center
California Institute of Technology
Pasadena, California 91125, USA
[2]Department of Mechanical Engineering
Johns Hopkins University
Baltimore, Maryland 21210, USA

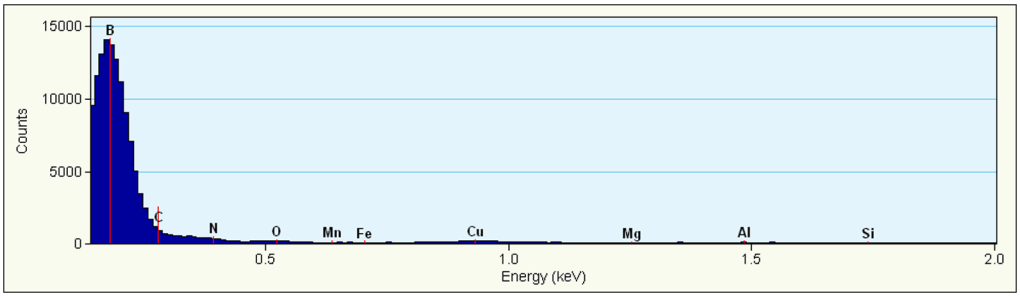

FIG. 1. An x-ray EDXS spectrum obtained at 300 kV from individual $\tau - B$ particles. Peaks are observed for B $K\alpha$ (180 eV) and Cu peaks (Cu $L\alpha \sim 950$ eV Cu $K\alpha \sim 8.0$ keV, and $K_\beta \sim 8.7$ keV) from the TEM grid are visible, but peaks for the proposed impurity elements are not.

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*Corresponding author.
hemker@jhu.edu
†Corresponding author.
wag@wag.caltech.edu

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