Synthesis and Characterization of Bulk BC8 Si

HAIDONG ZHANG, TIMOTHY STROBEL, Geophysical Laboratory, Carnegie Institution of Washington — Silicon, an essential element for modern industry, has several allotropes existing at ambient conditions. Among them, one of the most important phases is the metastable Si-III (BC8) structure. Although it has been known since 1960s, experimental characterization of its properties is still rare primarily due to lack of large bulk samples. Common methods produce BC8 Si samples with the size of micrometers in dimension, preventing definitive experimental measurements. In this work we report synthesis of phase pure bulk BC8 Si with the size of a few millimeters through the multi-anvil press method. The structure was confirmed by powder X-ray diffraction and further supported by the Raman spectrum. Its electrical resistance exhibits clear temperature dependence, increasing from 300 K to 2K. A crossover region occurs around 80 K to 100 K, showing a stronger dependence below 80 K. We also report its optical properties, thermal stability and phonon density of states.

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