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Exploration of New Superconducting Phases in a Scandium Borocarbide System

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Superconducting materials containing light elements are advantageous to emerge the relatively high critical temperature (T_c), because high-frequency vibration of phonons due to the light mass enhances its T_c within the BCS theory. Indeed, there are various superconductors in alkali, alkali-earth, and d transition-metal borides and carbides [1-3].

In this study, we searched for a new superconductor in the ternary Sc-B-C system using an arc-melting method. Although a moderately high- T_c superconductor is expected in combination with the comparatively small ionic radius of Sc and potentially high Debye frequencies originating from B and C, this system remains unexplored.

We attempted to synthesize the Sc-B-C compounds under various conditions of the starting composition, and found that a superconducting transition was observed at around 7.7 K only when the B-poor sample (e.g. nominal composition of Sc:B:C=37:2:61) was prepared [4]. Note that neither B-free nor B-excess samples exhibited the superconductivity down to 2 K. The structural refinements through the Rietveld analysis demonstrated that the compound belongs to the tetragonal space group of $P4/ncc$. By using the density functional theory calculations, the precise atomic positions of a small amount of B were examined. As a result, a chemical formula of the present superconducting phase was found to be expressed as $\text{Sc}_{20}\text{C}_{8-x}\text{B}_x\text{C}_{20}$ ($x=1$ or 2).

The sample exhibited the typical type-II superconductivity below $T_c=7.7$ K. Our specific-heat measurements revealed that $\text{Sc}_{20}\text{C}_{8-x}\text{B}_x\text{C}_{20}$ was classified as an intermediately coupled superconductor. The electronic structure studies by first principles calculations proposed that the contribution of Sc- $3d$ orbitals was mainly responsible for the superconductivity.

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