三元系 Si クラスレート $K_8Al_7Si_{39}$ の合成と物性

Synthesis and Physical properties of ternary Clathrate $K_8Al_7Si_{39}$

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Earth abundant and non-toxic elements based functional materials have been found commercially viable for applications. Pursuing this, ternary phase clathrate $K_8Al_7Si_{39}$ was synthesized and its physical properties were studied. X-ray diffraction, induction-coupled plasma optical emission spectroscopy (*ICP-OES*), and electron probe micro-analysis have revealed that the synthesized compound is a type-I ternary clathrate $K_8Al_7Si_{39}$ with lattice parameter a = 10.434(1) Å. Chemical composition of as-synthesized sample, determined by *ICP-OES*, was 14.7(2) at.% K, 13.2(1) at.% Al, and 72.1(7) at.% Si, which expresses its chemical formula $K_{7.9(2)}Al_{7.1(1)}Si_{38.9(4)}$. Low temperature (10-320K) transport measurements were performed on the compound. Electrical resistivity measurements suggested that it has metallic nature. Moderate value of Seebeck coefficient with *n*-type conduction was observed. Hall measurement confirmed *n*-type carriers with almost constant concentration (n) of 8.8~14.5*10^{20} cm^{-3} and mobility (μ) of 4.5~10.3 $cm^2V^{-1}s^{-1}$ in the range 10-300K. Slight decrease in thermal conduction was observed with increasing temperature, after a maximum at ~50K, indicating metallic type thermal conduction.