Structure of a LiKSO₄ single crystal studied by ⁷Li and ³⁹K NMR at low temperature

Ae Ran Lim

Department of Physics, Jeonju University, Jeonju 560-759, Korea

The ⁷Li and ³⁹K nuclear magnetic resonances in an LiKSO₄ single crystal grown by the slow evaporation method have been investigated using a Bruker FT NMR spectrometer. From the experimental data, the quadrapole coupling constant and asymmetry parameter were determined at room temperature and low temperature, respectively. Unlike the case at 300 K, the ⁷Li NMR line consists of three sets at 180 K, while ³⁹K nucleus exhibits six sets for the rotation around the three crystallographic axes. The three resonance lines of ⁷Li and ³⁹K at low temperature can be explained by the existence of three kinds of twin domains, rotated with respect to each other by 120° around the c-axis. The three resonance lines are also related to the crystallographic mirror plane. Structure of ferroelastic LiKSO₄ crystals at 180 K can be directly inferred from the domain pattern obtained by ⁷Li and ³⁹K NMR. The above results show that the equations of the twin boundaries belong to the *mm2F6mm* ferroelastic species. Therefore, the symmetry of phases III and II is given by orthorhombic structure with *Cmc2*₁ (*mm2*) and hexagonal structure with *P6*₃*mc* (*6mm*), respectively.