
Crystal structure of a non-centrosymmetric system, $\text{CuY}_2\text{Ge}_2\text{O}_8$

Hwanbeom Cho ¹, Hasung Sim ¹, Sanghyun Lee ², Maxim Avdeev ³, Yukio Noda ⁴, and Je-Geun Park ¹

¹ Center for Correlated Electron Systems, Institute for Basic Science (IBS) & Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea, Republic of

² Institute of Materials Structure Science, KEK, Tokai, Ibaraki, 319-1106, Japan

³ Australian Nuclear Science and Technology Organisation, New Illawarra Road, Lucas Heights, New South Wales, 2234, Australia

⁴ Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan

A non-centrosymmetric material doesn't have an inversion symmetry, which could lead to the intrinsic electric polarization. When this system consists of magnetic ions, the electric polarization of the system can be modified by a so-called magnetoelectric coupling under magnetic field. This multiferroic property has been widely studied not only for physical interest but also for industrial application.

We synthesized both single crystal and polycrystalline samples of new multiferroic systems, $\text{Cu}(\text{Y},\text{La})\text{Ge}_2$ and determined the crystal structure at 300 and 450 K using high-resolution powder and single crystal diffraction studies. According to our studies, both samples having magnetic Cu^{2+} ions has a monoclinic unit cell (space group $I1\bar{1}$) without inversion symmetry. We also determined the high temperature structure that has a more symmetric orthorhombic unit cell ($I m m 2$). Using the structural information, we could calculate the theoretical electric polarization at room temperature phase and found that it reaches the electric polarization of $9.88 \mu\text{C}/\text{cm}^2$ along the a -axis.