

TcSUH Bi-Weekly Seminar

Texas Center for Superconductivity at the University of Houston

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Raman Spectroscopy of Ferroelectric $\text{Co}_3\text{B}_7\text{O}_{13}\text{X}$ (X=Cl,Br,I) Boracites (Phonons, X-Sublattice Instability, Raman Imaging of Twin Transformations)

Friday, January 23, 2009

Room 102, University of Houston Science Center
12:00noon– 1:00 p.m.

Abstract

The boracites with general formula $\text{M}_3\text{B}_7\text{O}_{13}\text{X}$ (M=divalent metal, X=Cl,Br,I), shortly denoted as M-X, are the first known multiferroic materials. They exhibit a sequence of transitions from the high temperature paraelectric cubic phase to ferroelectric orthorhombic, monoclinic, trigonal phases, and finally to a monoclinic phase at low temperatures, where both ferroelectric and magnetic orders coexist. The lattice dynamics of boracites has been scarcely studied, the main problem with non-cubic phases being the coexistence of twin variants with different crystallographic and polarization orientation. We will present results of our detail temperature-dependent Raman study of Co-X and Ni-Br boracites. The spectra in the paraelectric cubic phase are analyzed in close comparison with results of ab initio (DFT) calculations of lattice dynamics. The analysis provides clear evidence for structural instability of the halogen sublattice, which triggers the ferroelectric cubic-to-orthorhombic transition. The spectra of the non-cubic ferroelectric phases of Co-Cl and Co-Br were obtained after Raman visualization of the twin variants. Using Raman microscopy imaging we were able to follow the twin-domain transformations through the crystallographic transitions, obtain Raman spectra from untwined domains in exact scattering configurations, determine the Raman mode symmetries, and assign Raman lines to definite atomic motions. The effect of elemental substitution at the X and M sites is also discussed.

Bio

Milko Iliev received his Ph.D. degree in Physics in 1973 at the University of Sofia, Bulgaria, and worked there as assistant, associate, and full professor and Dean of the Faculty of Physics until 1996. During 1976-77 he worked as a postdoctoral researcher and later (1992, 1995) as a visiting scientist in the group of Prof. M. Cardona at the Max-Planck-Institute for Solid State Research, Stuttgart, Germany. Since 1996, Dr. M. Iliev has been a Research Professor and Project Leader in TcSUH. His research interests are in the field of Raman and infrared spectroscopy of HTS and related materials. He has over 130 publications in peer-reviewed journals.

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