

XANES and Structure Study of Distorted $\text{BaNi}_x\text{Co}_{1-x}\text{S}_{2-y}$

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The transition temperature of layer compounds $\text{BaCo}_{1-x}\text{Ni}_x\text{S}_{2-y}$ varied in hundred Kelvin range depends on Ni and S concentration. We doped Ca in to $\text{BaCo}_{0.9}\text{Ni}_{0.1}\text{S}_{1.97}$ successful. The bulk samples were prepared specially by vacuum procedure. This new sulfide compounds have Metal-Semiconductor transition at high temperature as shown in Figs. 1 and 2. The result show the transition temperature, magnetization, and resistance can be controlled by Ca concentration.

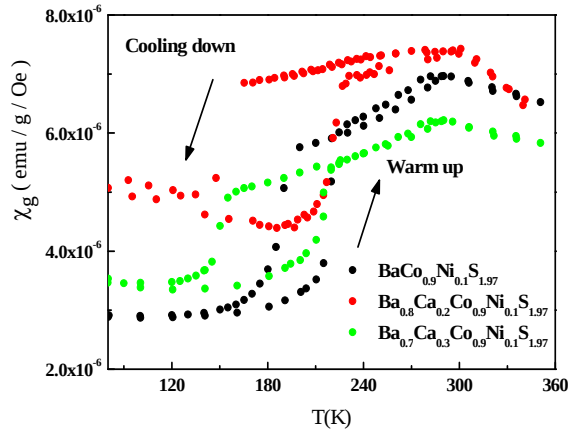


Fig. 1: Magnetization of Ca doped $\text{BaCo}_{0.9}\text{Ni}_{0.1}\text{S}_{1.97}$

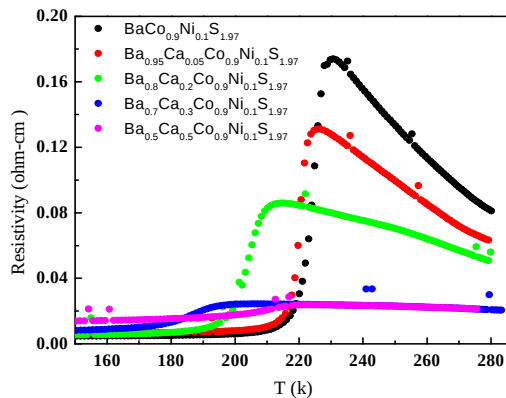


Fig. 2: Resistivity of Ca doped $\text{BaCo}_{0.9}\text{Ni}_{0.1}\text{S}_{1.97}$

The S *k-edge* by fluorescence signal mode measurement were carried out at the 16A beamline of NSRRC in Taiwan. The arrow point out the ligand hole increasing due to the Ca doping.

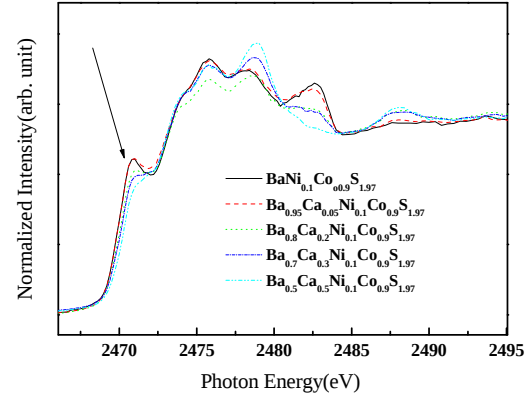


Fig. 3: Normalized S *k-edge* spectrum using intensity between 45 - 300 eV after edge

Co K-edge near edge absorption spectrum (XANES) and extended x-ray absorption fine structure (EXAFS) by fluorescence signal mode were carried out at the 17C beamline of NSRRC in Taiwan. The arrow in figure point out the peak of Co - S 3d-3p orbital hybridization increasing with Ca doping. The EXAFS analysis, not show here, prove the structure distortion by Ca doping also.

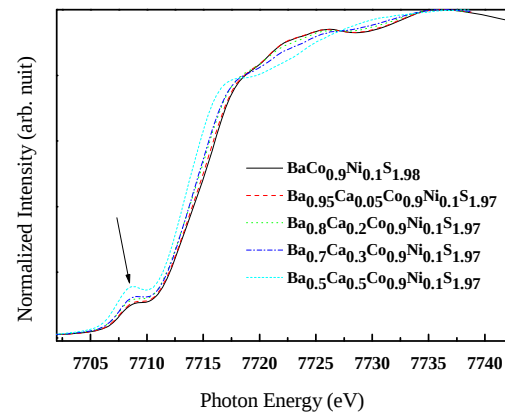


Fig. 4: Normalized Co K-edge spectrum using intensity between 45 - 300 eV after edge

Summary

We make Ca doped $\text{BaCo}_{0.9}\text{Ni}_{0.1}\text{S}_{1.97}$ successful. The transition temperature depends on Ca concentration. From XANES spectrum we measured, we proved the Co 3d- S 3p orbital hybridization increasing with Ca doping.