Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Crystal Structure of Misfit Thermoelectric Compound $[Ca_2CoO_3]_{0.62}CoO_2$ by Electron Diffraction and High Resolution Electron Microscopy P. OLEYNIKOV, V. VOLKOV, Q. JIE, Q. LI, Y. ZHU, Brookhaven National Laboratory, CFN-MSD/BNL TEAM — Layered cobaltates are of great interest from a physics point of view, as shown by their thermoelectric and magnetoresistance properties. In order to understand the origin of physical properties of layered cobaltates and, in particular, of misfit cobalt oxide $[Ca_2CoO_3]_{0.62}CoO_2$ with high thermoelectric power, an accurate determination of the crystal structure is required. Ambiguities of the structure analysis of this compound performed by X-ray methods stimulated us to re-examine its structure by the electron diffraction patterns (DP) and high resolution electron microscopy (HREM) methods. Single crystal $[Ca_2CoO_3]_{0.62}CoO_2$ grown under $SrCl_2$-flux has a misfit lattice structure with rock-salt type $[Ca_2CoO_3]$ slabs and interpenetrating CdI_2-type $[CoO_2]$ layers stacked along c-axis and incommensuration along b-axis. The nearest commensurate structure with ratio of sublattice parameters $b_1/b_2 =$ 5:8 closely matches the 0.62 composition index. Analysis of HREM images and the presence of lines with diffuse scattering and weak spots on the $(h0l)$ DP lead to the tripled a unit cell parameter, which was significantly different from the average structure determined by X-ray and neutrons. Work supported by the U.S. DOE, BES (DE-AC02-98CH10886).

Peter Oleynikov
Brookhaven National Laboratory

Date submitted: 20 Nov 2006 Electronic form version 1.4