Structural symmetry of Cd$_2$Re$_2$O$_7$ from nonlinear optics

JESSE C. PETERSEN, MICHAEL D. CASWELL, J. STEVEN DODGE, Department of Physics, Simon Fraser University, Burnaby, British Columbia, Canada, JIAN HE$^1$, DAVID MANDRUS, Department of Physics and Astronomy, The University of Tennessee, Knoxville and Solid State Division, Oak Ridge National Laboratory — Cd$_2$Re$_2$O$_7$, a superconducting metallic pyrochlore, undergoes a second-order structural phase transition at 200 K from a cubic to tetragonal lattice. Landau theory predicts that any second-order cubic-to-tetragonal phase transition must also possess an order parameter associated with broken inversion symmetry. By observing optical second-harmonic generation, we provide a direct demonstration that the 200 K transition in Cd$_2$Re$_2$O$_7$ involves broken inversion symmetry. Moreover, we have used the polarization dependence of SHG to refine the crystal structure. We find that the low-temperature crystal symmetry is that of the $F42m$ space group.

$^1$Now with Department of Physics and Astronomy, Clemson University, Clemson, SC

Jesse C. Petersen
Simon Fraser University

Date submitted: 19 Dec 2005