The Crystal Structure of $Bi_4Au_2O_{14}$: The Use of a Siemens CCD Detector with Short-Wavelength Radiation	X17B1

R. Harlow (DuPont), J. Parise (SUNY at Stony Brook), J. Phillips and C. Campana (Siemens), and J. Hanson (BNL)

The determination of the structure of $Bi_4Au_2O_{14}$ presented two difficulties: absorption (mu for MoKa is approximately 1050 cm-1) and the presence of a superlattice which is 4x the sublattice. Three sets of data have been collected on crystals of this compound: with in-house MoKa radiation using a Siemens CCD and a Rigaku image-plate system, and with 0.185 A synchrotron radiation (where mu is reduced to approximately 30 cm-1) at beamline X17B1, also with a Siemens CCD. At this point, the subcell structure (tetragonal, a = 8.676 and c = 5.832 A, in space group P4212) has been solved and refined using the synchrotron data to an R value of 10.3% using 2094 reflections to a resolution of ca. 0.3 A. All of the atoms were refined with anisotropic thermal parameters, with special attention given to those of the oxygen atoms which are the presumable source of the superlattice. One of the oxygen atoms was found to be disordered over two sites: it is believed that this oxygen will be ordered in the supercell where the c-axis is doubled. This type of disorder was expected because the Bi site in the subcell contains a mixture of Bi^{+3} and Bi^{+5}. Presumably, the latter are also ordered in the supercell. The source for doubling the cell along the a-b diagonal has not yet been determined. Using the in-house data, only the heavy atoms could be refined with anisotropic thermal parameters and some of these ellipsoids were not very realistic. Also, the disorder of the one oxygen atom was not visible from the in-house data. Work continues on modelling the supercell structure, but the benefits of using the (almost) absorption-free data from the synchrotron/CCD combination are already clearly evident.