

X-Ray Profile Refinement of La_2CuO_4

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Abstract : The Rietveld method of structure refinement from powder diffraction patterns is widely used with neutron data and increasingly so with x-ray data. In this paper the Rietveld method has been explained. As an example the crystal structure of La_2CuO_4 at room temperature has been refined using x-ray powder diffraction data. The crystal structure is orthorombic with $a = 5.3548(4)\text{\AA}$, $b = 5.4006(3)\text{\AA}$, $c = 13.1529(9)\text{\AA}$, and space group C_{mca} . A sample of La_2CuO_4 has been oxidized to $\text{La}_2\text{CuO}_{4+\delta}$ and its magnetic susceptibility as a function of temperature has been studied. The new material is superconductor with $T_c \cong 30\text{K}$. Further investigation is in progress to determine the value of δ and the position of the extra oxygen atoms in the cell.