Observation of local non-centrosymmetry in weakly ferroelectric YCrO$_3$\(^1\) ANNA LLOBET, KANNADKA RAMESHA, THOMAS PROFFEN, Lujan Neutron Scattering Center, Los Alamos National Laboratory, C.R. SERRAO, C.N.R. RAO, Chemistry & Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research — Using high resolution neutron powder diffraction we have determined the average and local structure of YCRO in order to explain the recently reported ferroelectric character YCRO. Unlike other ferroelectric systems, YCRO has been found to have a centrosymmetric crystal structure which is inconsistent with the development of electric polarization because it requires atomic off-centering. We have characterized the different length scales existent in YCRO and found that, although the average crystallographic structure above and below the ferroelectric transition is orthorhombic and centrosymmetric (\textit{Pnma}), in the ferroelectric state YCRO is locally non-centrosymmetric and Cr is displaced about 0.01Å from its position along \(z\) direction. We conclude that the local character of the Cr off-centering and the small value of the displacement observed could explain the weak ferroelectric behavior. This new concept of “local non-centrosymmetry” might be of great importance for the understanding of unusual properties of other multifunctional materials as well.

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