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Atomically resolved data for oxide surface analyzed using a local crystallography analysis method ZHENG GAI, WENZHI LIN, K. FUCHIGAMI, T. WARD, P. SNIJDERS, J. SHEN, STEPHEN JESSE, SERGEI KALININ, ARTHUR BADDORF, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — The emergent physical phenomena of oxides have attracted increasing scientific attention. Here, we report an approach for studying local surface chemistry and order parameter fields based on a local crystallographic analysis of scanning probe microscopy data of oxide surfaces. We obtained initial estimated atom locations by finding the centroid of the remaining isolated regions of pixels, after applying thresholds to the topographic images. Then we determined the refined positions by automatically fitting each atom individually using a shape function. With the refined locations, we can further derive and quantify properties that are not readily clear in the topographic images. This approach was applied to analyze scanning tunneling microscopy data for the surface of La5/8Ca3/8MnO3 (001) and demonstrated distortion domains with different distortion orientations. These studies provide a new pathway to extract and quantify local properties for scanning probe microscopy images. Research was supported (W.L., S.V.K.) by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division. This research was conducted at and supported by (Z.G., S.J., A.P.B.) the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

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