Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Down the primrose path of dalliance: how iterative structural determination routines for thin films may lead to partial or false solutions NAJI HUSSEINI, CODRIN CIONCA, Department of Physics, University of Michigan, Ann Arbor, 48109, YIZHAK YACOBY, Racah Institute of Physics, Hebrew University, Jerusalem, Israel, 91904, ROY CLARKE, Department of Physics, University of Michigan, Ann Arbor, 48109 — Iterative methods are frequently used to solve thin film structures. Convergence, however, may terminate at partial or even incorrect solutions. Coherent Bragg Rod Analysis (COBRA), a direct phase retrieval method with minimal iterations, has had recent success with buried interfaces in perovskite oxides and semiconductors. Here, we investigate the role of iterations in COBRA by means of simulations on a model lattice-matched system of PbTiO3 on SrTiO3 with realistic stochastic noise. Out-of-plane atomic displacements were added in various monolayers of the PbTiO3 film. With increasing iterations, the positions of the heaviest element (Pb) became more accurate at the expense of the lighter elements – particularly the oxygen sublattices. In addition, the error in the central monolayers of the film decreased while the error at both the film-substrate and film-air interface increased. Our results provide new insights on the influence of uncertainties in measuring subtle structural details at interfaces.

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Date submitted: 27 Nov 2007 Electronic form version 1.4