Application of a direct method to solve the structure of $(\sqrt{3}x\sqrt{3})\text{Sb/Au (110)}$ from surface x-ray diffraction measurements\(^1\)

RUSSELL FUNG, VALENTIN SHNEERSON, SOMENDRA PARIHAR, HARRY JOHNSON-STEIGELMAN, PAUL LYMAN, DILANO SALDIN, University of Wisconsin-Milwaukee — Lack of phase information in typical x-ray diffraction measurements makes it very difficult to recover the atomic-scale structure of a crystal by direct inversion of the measured amplitudes. We have developed a direct method for surface x-ray diffraction (SXRD) where the aim is to recover the part of the surface structure that is different from the truncated bulk. The iterative algorithm we have developed employs prior knowledge of the truncated bulk structure and alternately satisfies constraints in real and reciprocal space. Here we report on an application of the method to determine the unknown structure of $(\sqrt{3}x\sqrt{3})\text{Sb/Au (110)}$ from experimental data. In this application, the direct method is adapted to deal with the presence of four symmetry-related domains.

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Russell Fung
University of Wisconsin-Milwaukee

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