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Structural Determination of Interfaces in Organic Semiconductors using Coherent Bragg Rod Analysis BRANDON CHAPMAN, RONALD PINDAK, Brookhaven National Lab, YIZHAK YACOBY, Hebrew University, JULIE CROSS, Argonne National Lab, EDWARD STERN, University of Washington, CHRISTIAN KLOC, Bell Labs — The low charge carrier mobilities long associated with organic semiconductors have increased by several orders of magnitude in recent years. Charge mobilities in field-effect transistors (FETs) using single-crystals of rubrene (5,6,11,12-tetra-phenyl-tetracene) have been reported with values in the range from 5 to 30 cm²/Vs. However, little information is known about the integrity of interfaces formed by electrical contacts in organic FETs, which can play a significant role in determining device performance. We are using a novel approach called Coherent Bragg Rod Analysis (COBRA) to determine the atomic structure of interfaces in organic FETs. COBRA uses the measured x-ray diffraction intensities along the substrate defined Bragg (crystal truncation) rods to investigate the electron density near the surface, interface and throughout the thin-film. The COBRA method is uniquely suited for probing buried interfaces formed by electrical contact materials on molecular crystals. Here, we present preliminary measurements of Bragg rods from the free surface of rubrene single-crystals and we discuss progress toward measuring a complete set of inequivalent Bragg rods from rubrene that will provide a model-independent determination of the surface structure.

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