

Surface X-ray Diffraction from an Organic Semiconductor Molecular Crystal

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Introduction

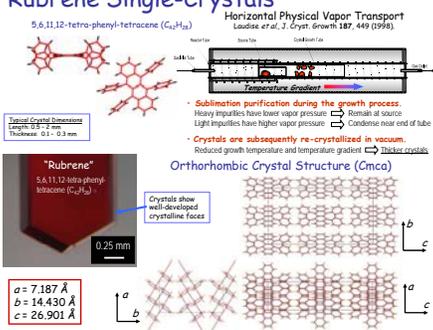
There has been an explosion of interest in organic electronics because of low-cost applications in devices such as field-effect transistors, flexible thin-film transistors and light emitting diodes (see panel on right). Despite significant progress in the field, a fundamental understanding of the mechanism of charge transport in organic semiconductors is still lacking at this time. The recent development of field-effect transistors (FETs) using molecular crystals has provided a means to study the *intrinsic* electronic properties of organic semiconductors. Rubrene (5,6,11,12-tetra-phenyl-tetracene; C₂₆H₂₀), in particular, has shown to be an excellent organic semiconductor with high charge carrier mobility in FET devices. In order to elucidate the role of surface structure in these materials, we have carried out a surface x-ray diffraction study of rubrene using the high-intensity micro-focused beam at 20-ID.

Organic Electronics

OLEDs, OFETs, OTFTs, ... Applications and future fads
[See Forrest, Nature 428, 911 (2004)]

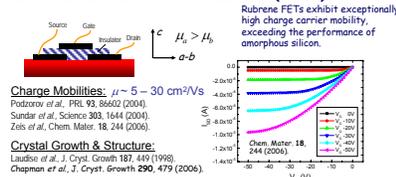


Rubrene Single-Crystals



Motivations

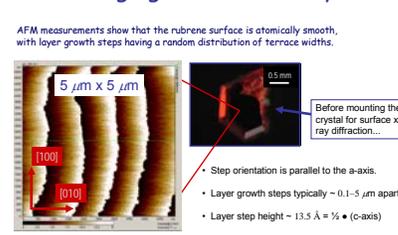
Rubrene Field-Effect Transistors (FETs)



The physics of single-crystal organic FETs is largely determined by the structure at or near the surface of the crystal. In the present study, we addressed the following fundamental questions:

- Is the crystal structure at the surface the same as within the bulk?
- What is the arrangement and conformation of rubrene molecules at and near the surface?
- Is there intercalation of oxygen at the surface?

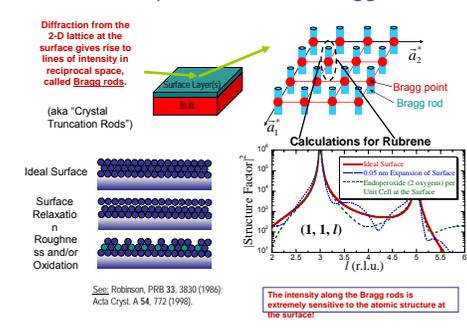
AFM Imaging of Rubrene Crystals



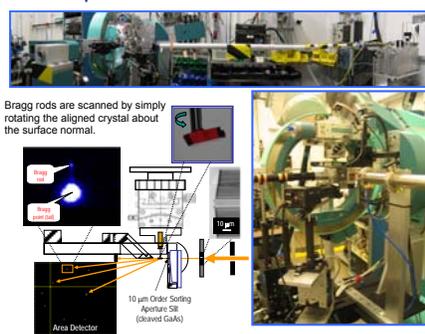
Consistent with other published AFM measurements:
Single-Crystals, Menard et al., Adv. Mater. 16, 23 (2004).
Thin-Films, Haemori et al., Jpn. J. Appl. Phys. 44, 3740 (2005).

X-rays are more sensitive to the atomic structure at and near the crystal surface, and can probe below the surface.

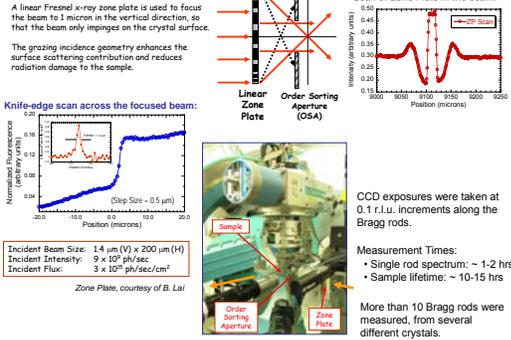
Surface X-ray Diffraction: Bragg Rods



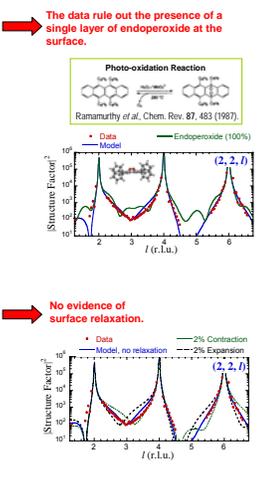
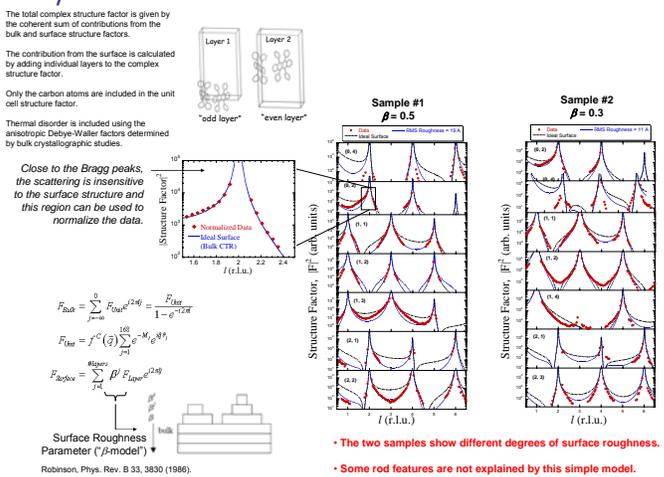
The Experiment, 20-ID



Linear Zone Plate



Analysis and Results



Conclusions

- We measured a large set of crystal truncation rods from the free surface of single-crystal rubrene.
- The Bragg rods are well-described by a surface roughness model, consistent with AFM imaging of the surface.
- There is no indication of inter-molecular relaxation of the unit cell at the surface.
- There is no indication of significant levels of endoperoxide residing at the surface.
- COBRA analysis of these data (in progress) may provide more detailed information about the structure at the crystal surface, including thermal disorder.

Acknowledgements

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