Tuesday Evening Poster Sessions

Novel Trends in Synchrotron and FEL-Based Analysis
Focus Topic
Room: Hall D - Session SA-TuP

Synchrotron Analysis Poster Session

SA-TuP1 Soft X-ray Spectroscopy Reveals Chemical Information beneath the Surface of Organic Photovoltaic Devices, *Claudia Fleischmann*, IMEC, Belgium, *P. Hönicke, M. Müller, B. Beckhoff,* Physikalisch-Technische Bundesanstalt (PTB), Germany, *E. Voroshazi, J. Tait, T. Conard,* IMEC, Belgium, *W. Vandervorst*, IMEC, KU Leuven Belgium

While inorganic photovoltaic devices (PV) remain the main choice for large-scale energy production, *organic photovoltaic devices* (OPV) show great potential for future, environmentally friendly energy sources. Their semi-transparency, light-weight and unique opto-electrical properties combined with the possibility to shape OPV devices at will enable new applications where PV has never been used before. Similar to their inorganic counterparts, the underlying physical mechanisms and hence the performance and efficiency of organic devices is directly linked to their physicochemical properties. Revealing these properties is often very challenging due to the limited sensitivity and specificity of standard analytical techniques used for inorganic semiconductor characterization. In addition, it is highly desirable to probe the device structure as close as possible to a real one, which typically comprises organic-inorganic interfaces, intermixed phases being based on the same constituent atoms, or multilayer structures of a few tens to hundreds of nanometer thickness.

In this contribution we will examine the capabilities of *Near-Edge X-ray Absorption Fine Structure Spectroscopy* (NEXAFS) for the chemical characterization of (complete) bulk-heterojunction OPV device structures based on conjugated polymers and fullerene derivatives including P3HT, PCDTBT, DPP and PCBM. We will show that the high chemical sensitivity of the carbon K-edge (~290eV) NEXAFS permits to distinguish between the common organic semiconductors in these devices, providing a tool for compositional analysis and miscibility studies. By using fluorescence yield detection the information depth is extended far beyond the surface, in contrast to electron yield detection, allowing to probe non-destructively the bulk properties of (buried) layers in the OPV structure. In this context, we will also illustrate the remaining metrology challenges and investigate the sensitivity of the sulfur and nitrogen K-edge NEXAFS to be used for degradation studies. Finally, we will discuss the stability of these organic materials under x-ray irradiation, which is particularly critical for synchrotron radiation-based methods.

SA-TuP2 Exact, Efficient Calculation of Synchrotron Radiation--Proximity and Angle Effects, *Eric Shirley*, NIST

We evaluate synchrotron radiation for a circular orbit using Graf's addition theorem for Bessel functions. Using Debye's and Olver's asymptotic expansions, the exact radiation fields can be calculated without recourse to assuming large distance from the tangent point and without using truncations as in Schwinger's work. Thus, the present results should be both numerically robust and efficient, requiring no numerical integration. The results are applied to assessing the accuracy of the Schwinger formula for radiometric applications. The formulas are particularly well suited for long wavelengths and for measurements at end stations close to the storage ring. Application areas are typically UV and x-ray instrument calibration for such purposes as found on environmental satellites. By carrying out this work, we can gain a quantitative sense on the accuracy of various approximations that can be made, and hence their consequential suitability.

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