

## Structure analysis of thin-films with new high performance organic semiconductor small molecules for self-assembled monolayer field-effect transistors (SAMFETs), organic thin-film transistors (OTFTs) and memory devices

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We performed grazing incidence X-ray diffraction (GID) and X-ray reflectivity (XRR) in ambient conditions using a photon energy of 22 keV on self-assembled monolayers (SAMs) used by the OMD group, i.a. BTBT-C<sub>12</sub>-PA (Fig. 1) and BTBT-C<sub>11</sub>-PA consisting of an insulating and semiconducting part for the use in monolayer field-effect transistors. As a solvent for all samples 2-propanol was used for the preparation of solutions with a concentration of 0.2 mM and 0.02 mM respectively. SAMs were deposited from solution in the OMD laboratory in Erlangen on aluminum oxide films (10 nm), grown by atomic layer deposition (ALD) as well as on sapphire with a crystal structure of (1-102) or (0001). The presence of SAMs was examined prior to the experiment by static contact angle measurements to verify a proper film formation.

XRR measurements were performed on smooth aluminium oxide films, grown by atomic layer deposition (ALD), to obtain information about the vertical alignment of the SAM. The reflectivity profile and corresponding fit for BTBT-C<sub>12</sub>-PA is shown in figure 1 a). The scattering length density (SLD) profile is illustrated in Fig. 1b) depicting a confined peak of 0.76 nm of highly ordered BTBT moieties that are responsible for the charge transport in electronic devices. The length of hydrocarbon spacer chain (1.50 nm) is also well-resolved by the fit and corresponds well to the theoretical length.

GID measurements were successfully performed for these systems. For each sample several GID patterns were recorded at 3 different positions of PILATUS detector with varying counting times between 3 and 20 s and moving sample position.

Due to the excellent high flux of ID10 and the short counting times severe radiation damage could be averted (compared to previous beamtime at BM28). Three Bragg rods were found for BTBT-C<sub>12</sub> (Fig. 1c) and BTBT-C<sub>11</sub> and could be attributed to the (11), (02) and (21) reflexes. A resulting unit cell with a herringbone structure and the lattice parameter could be deduced (Fig. 1d). Similar rods could be observed for several other samples, e.g. SAMs of C<sub>10</sub>-PA/C<sub>14</sub>-PA/C<sub>16</sub>-PA/C<sub>18</sub>-PA/F<sub>15</sub>C<sub>18</sub>-PA/F<sub>21</sub>C<sub>12</sub>-PA mixed with semiconducting C<sub>60</sub>-C<sub>18</sub>-PA and thermally evaporated sexithiophene semiconductor (Et-6T-Et) on top of a mixed SAM making these results extremely valuable for the OMD group.

All our materials were previously tested in electrical devices; the combination of electrical results with information about the structure of used materials is of great value for the community of organic electronics.

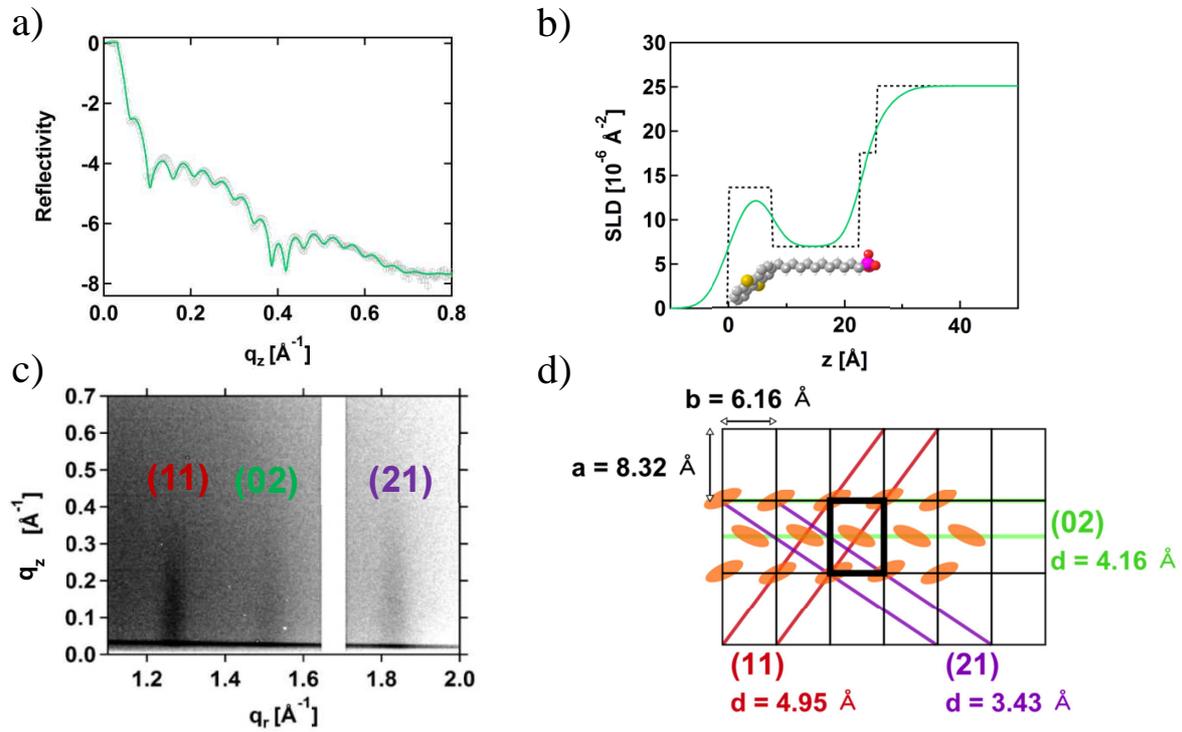


Fig. 1: a) Reflectivity profile of a BTBT-C<sub>12</sub>-PA SAM on ALD AlO<sub>x</sub> (10 nm) with corresponding fit. b) 3 layer SLD profile of the BTBT-C<sub>12</sub>-PA SAM resolving the PA anchor-group, insulating hydrocarbon chain (C<sub>12</sub>) and the benzothienothiophene (BTBT) head-group (0.76 nm). c) Grazing incidence X-ray diffraction shows the presence of three Bragg rods and can be attributed to the (11), (02) and (21) reflex. d) The resulting unit cell with a herringbone structure and the determined lattice parameter.