Compact Titanium Oxycarbide: A New Substrate for Quantitative Analysis of Molecular Films by Means of Infrared Reflection Absorption Spectroscopy

SUPPORTING INFORMATION

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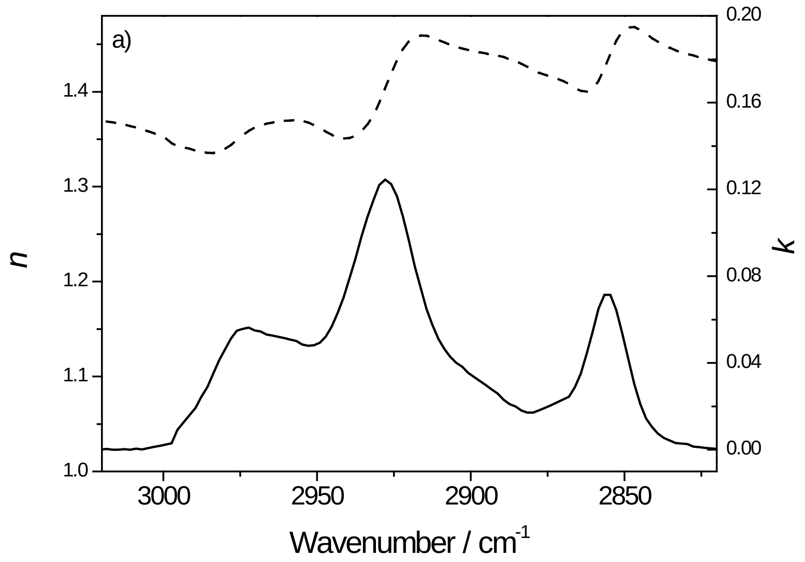
SI. 1 The optical constants of arachidic acid in IR spectral region.

The optical constants of the arachidic acid ($C_{19}H_{39}COOH$) dissolved in CCl_4 were determined from IR transmission measurements. The refractive index (*n*) and extinction coefficient (*k*) are shown in figure SI1.



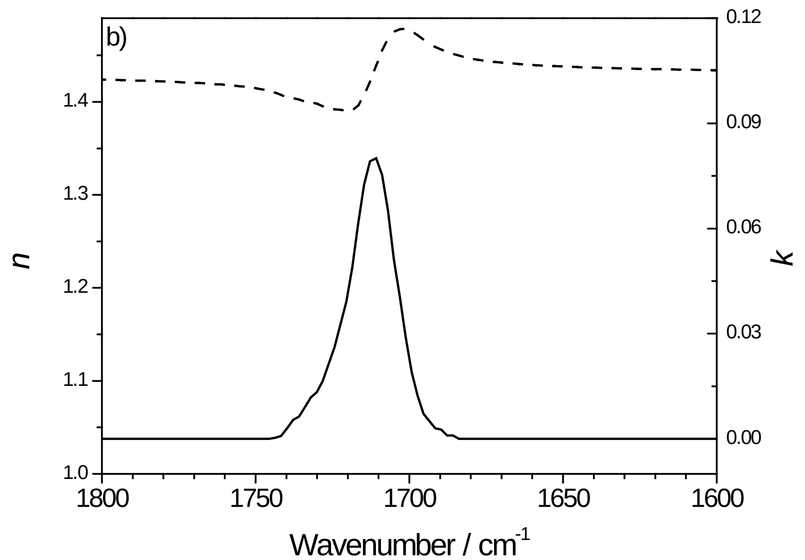


Figure SI 1. The refractive index (*n*; dahed line) and extinction coefficient (*k*; solid line) of arachidic acid in a) CH stretching and b) C=O stretching mode region.

SI. 2 PM IRRA spectra of Langmuir Blodgett (LB) monolayers of $C_{19}H_{39}COOH$ on Au

Figure SI 2 shows the PM IRRA spectra of LB monolayers of $C_{19}H_{39}COOH$ on Au and the PM IRRA spectrum calculated from optical constants for randomly distributed $C_{19}H_{39}COOH$ in a monolayer thick film. In the calculation of the PM IRRA spectrum, the optical constants shown in figure SI1 were used. The stratified system was composed of air|2.7 nm thick $C_{19}H_{39}COOH$ film|Au, the angle of incidence was set to 68 °.

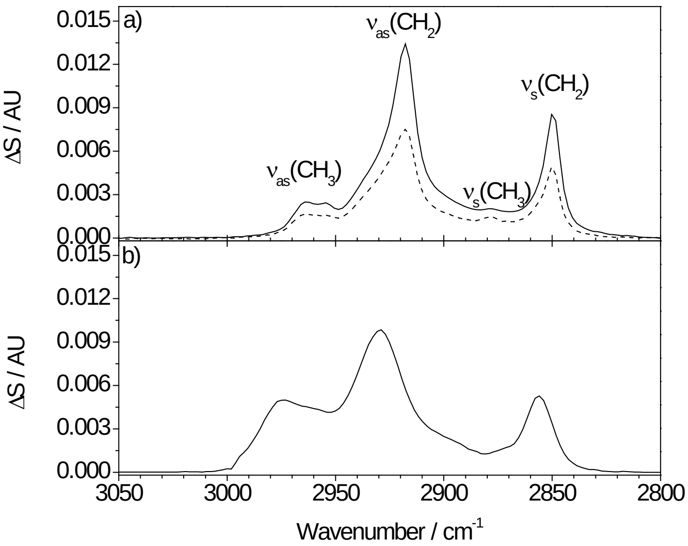


Figure SI 2. PM IRRA spectra of arachidic acid monolayers on Au; a) LB monolayers transferred at a surface pressure equal to 15 (dashed line) and 40 (solid line) mN m^{-1}, and b) calculated PM IRRA spectrum for randomly distributed molecules in a monolayer thick film.

SI. 3 Morphology of the TiO_xC_y substrate

Scanning electron microscopy (SEM) and atomic force microscopy (AFM) were used to analyze the morphology and surface roughness of the compact TiO_xC_y substrate that was produced by carbothermal reduction of an anodic TiO_2 film on polycrystalline Ti at 750 °C in acetylene/argon atmosphere. SEM micrographs were taken with a field emission SEM based on a GEMINI column in a Zeiss CrossBeam NVision 40 system, where the InLens detector was chosen. The acceleration voltage was set to 4 kV at a working distance of 4 mm. Contact mode AFM was performed with a Veeco Multimode 8 instrument using a SNL-10 probe (silicon tip on silicon nitride cantilever). Analysis of the AFM micrographs was conducted with the NanoScope Analysis 1.5 software. The images where pre-processed with plane fit and zero-order flattening procedures. On these images, roughness analysis was performed.

The SEM image in figure SI 3 shows that the TiO_xC_y surface is composed of irregular grains with an average diameter of (16 ± 7) µm.

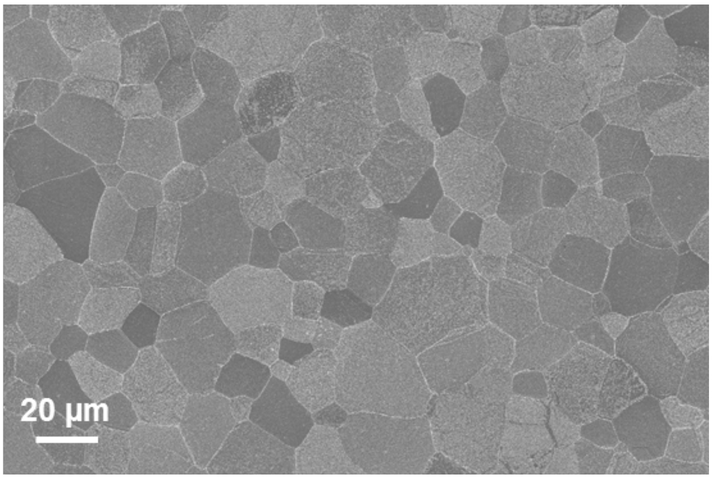


Figure SI 3. SEM image of a TiO_xC_y substrate produced at 750 °C.

Figure SI4 depicts a representative AFM image of the TiO_xC_y surface. One can clearly see protruding borders between various grains and that the surface morphology and roughness differs on different grains. Five zones of each (15 x 15) μm^2 were mapped with AFM and the image root mean square height values (rms) were determined. The mean surface roughness calculated from the rms of these zones is equal to (25.3 ± 5.7) nm.

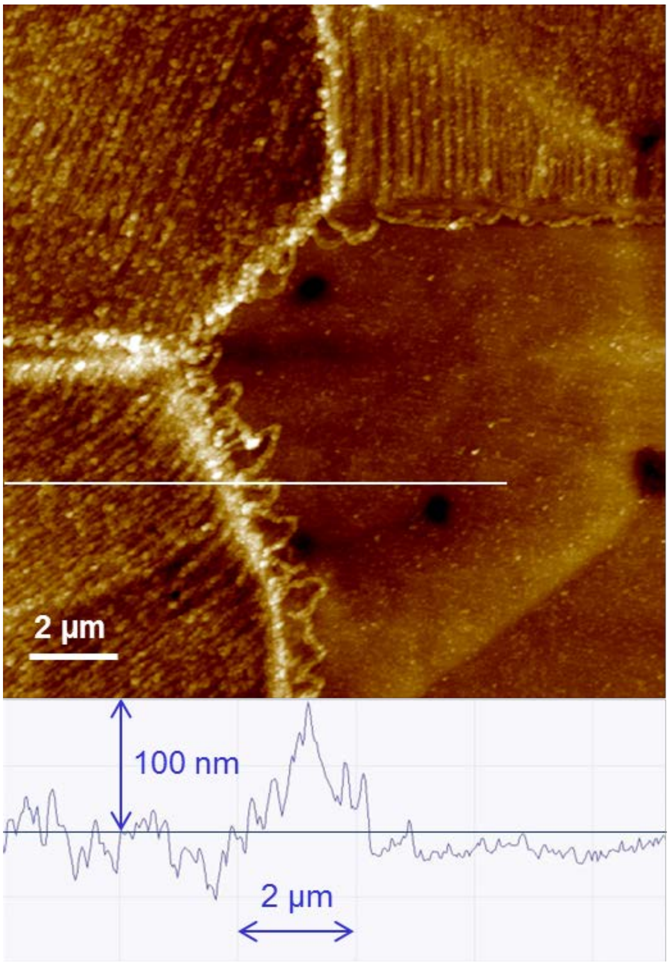


Figure SI4. AFM image of the TiO_xC_y surface with height profile.