Surface mediated structures: stabilization of metastable polymorphs on the example of paracetamol

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Supporting Information

1.0 wt% solutions of paracetamol (pharmaceutical grade) were prepared by dissolving it in either ethanol (abs, \geq 99.8%, SigmaAldrich) or tetrahydrofuran (\geq 99.8%, SigmaAldrich) completely. The thermally oxidized silicon wafer (150 nm thickness; Siegert Wafer GmbH) were cut into pieces of 2.0 x 2.0 cm² and were extensively rinsed with ethanol (abs.; \geq 99.8%, SigmaAldrich) followed by sonication within a ethanol and dimethylketone (\geq 99.9%, SigmaAldrich) bath in a v/v ratio of 1:1 for 30 min. Afterwards the wafer were rinsed with 2-propanol (\geq 99.9%, Fluka) and dried under a steady nitrogen stream . The spin parameter (17rps in 3sec for 60 sec) were the same for each coating. If not otherwise stated in the manuscript, the as-prepared wafers were dried at room temperature (25°C) in a half covered petri dish for 24 h.

The grazing incidence X-ray diffraction (GIXD) experiments were performed at the European synchrotron radiation facility (ESRF) in Grenoble at the spanish beamline BM25b. The wavelength of the incoming beam was 0.9998 Å and the incidence angle was set to 0.13° for each measurement. The sample to detector distance was 370 mm and a CCD detector with a pixel size of 62.3 x 62.3 µm² was used. The distortion of the detector was determined using the freeware FiT2D²7-30. The further transformation into the q-space as well as the indexation was performed using PyGid³1. The used crystal parameters were obtained from the Cambridge Structural Database; CSD codes are stated within the manuscript. The crystal alignment with respect to the surface was visualized using the freeware version of Mercury 3.3.

Atomic force microscopy (AFM) height imaging was performed using a Nanosurf FlexAFM from Nanosurf GmbH (Switzerland) with a TAP 190 (Budgetsensor, Bulgaria) in non-contact mode. The data evaluation of the AFM images was performed using the freeware Gwyddion.