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Crystal structure solution from thin films: software requirements

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The presence of a surface during the crystallization process of a molecular material can induce new polymorphs, as is frequently observed for organic electronic molecules and, recently, also in pharmaceuticals.[1] Such so-called surface-induced phases (or surface-mediated phases) are only present within thin films, so determining a crystal structure from these phases is challenging, as currently there is no established procedure to solve crystal structures from thin films. Conventional single crystal diffraction techniques cannot be applied, since the typical extension of the crystals are in the thickness range of several tens of nm and they are attached to a substrate. Even powder X-ray diffraction methods cannot be used, since strong preferred orientations of the crystallites are present within thin films. One experimental possibility is the use of grazing incidence surface X-ray diffraction (GIXD) using synchrotron radiation. Within the talk, the progress in the field of crystal structure solution from thin films will be introduced, but also the difficulties, open problems and limitations of the method will be discussed. A special focus will be drawn to the software requirements for crystal structure solution from thin films. The indexation of diffraction patterns collected by GIXD is a first step of structure solution; however, until now no reliable software routines have been developed to perform this step. For the second step, where the molecular packing is determined based on the crystallographic unit cell, currently available software packages can be used. One possibility is rigid-body refinement of molecular structures against experimentally observed structure factors.[2] A second possibility is a purely theoretical approach based on energy minimisation by using molecular dynamics (MD) simulations and density functional theory (DFT). Examples based on rod-like aromatic molecules, conjugated molecules with flexible side chains and hydrogen-bonded molecules will be introduced.[3,4] Finally, the differences in the molecular packing between surface-induced crystal structures and bulk structures will be discussed to understand the basic mechanisms for the formation of surface-induced phases.

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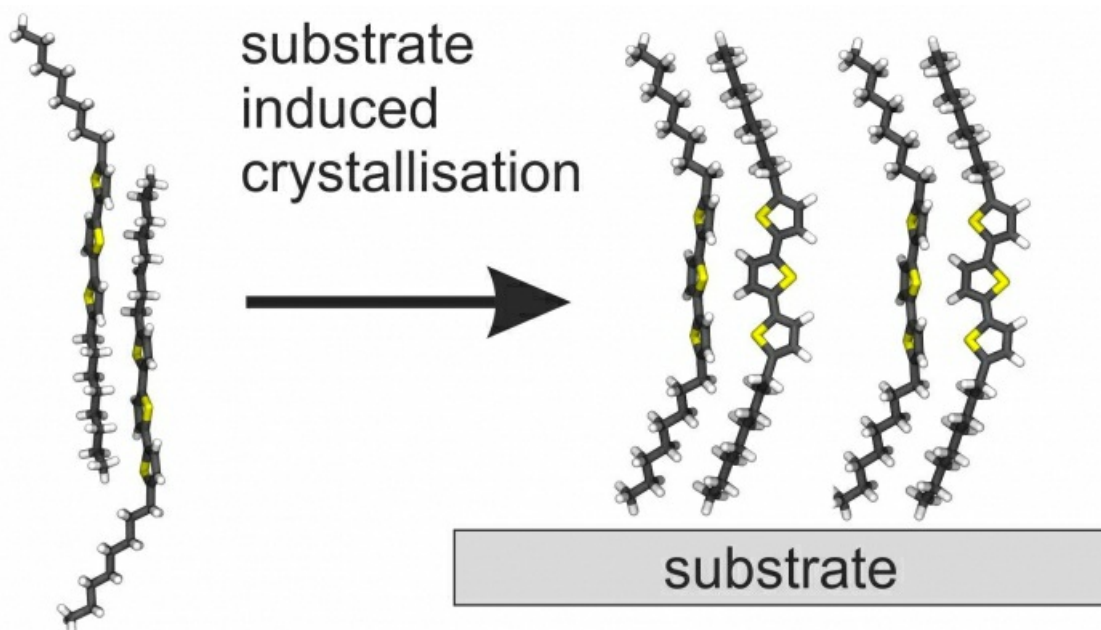
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