Oral Contributions

[MS34 - 02] Surface induced crystal structures for organic electronic applications: thin film growth and structure solution

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The structural order in thin films of organic semiconductors strongly impacts the performance of organic electronic devices. A large number of organic semiconductors exhibits polymorphism and well-known phenomena are specific crystallographic phases which are present exclusively in thin films. Such crystallographic phases are often denoted as surface induced phases (other used terms are surface mediated phases or thin film phases), since the presence of a surface during the crystallisation is of primary importance for their formation. In general, such thin-film polymorphs do not exist as macroscopic free standing single crystals. A number of surface induced crystal structures of conjugated molecules have been solved during the last few years. In particular, examples include application relevant molecules like pentacene [1-4].

In the first part of the talk the method of crystal structure solution from thin films is introduced. Different methods are developed to solve the crystal structures of surface induced phases, which combine both experimental and theoretical approaches (grazing incidence x-ray diffraction and theoretically based molecular packing considerations). In the second part of the talk the crystallisation behaviour of different thiophene based conjugated molecules will be described in detail: sexithiophene, dioctyl-terthiophene and dihexyl-terthiophene. It is found that surface induced phases are formed by various techniques of thin film preparation. Solution based methods as well as physical vapour deposition can yield surface induced phases [5]. Important parameters for preparation are the type of surface, the evaporation rate (or deposition rate) of the solvent during the thin film preparation and the temperature of the substrate during the crystallisation process [5-7]. Similarities and differences in the molecular packing between known crystal structures and surface induced phases will be discussed in detail [1,2,4,8]. One typical crystallographic feature of surface induced phases is the low mosaicity of the crystals. Of particular importance for the formation of surface induced crystal structures is the formation of the first molecular monolayer on a surface [5,9,10,11]. Despite the variety of experimental observations, some general features of surface induced crystal structures are introduced and discussed.

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