

2D chiral growth of 6,13-pentacenequinone thin films on Si(111)

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Recent progress in the application of organic materials to the microelectronic devices signifies the big advantages of the organic electronics, such as low cost fabrication, biodegradability and flexibility. Among currently investigated organics, the pentacene ($C_{22}H_{14}$, Pn) is studied widely, because of its high field-effect mobility. Pn, however, oxidizes in the presence of oxygen forming 6,13-pentacenequinone ($C_{22}H_{12}O_2$, PnQ) and shows increased saturation current in field-effect transistor (FET) in oxygen atmosphere [1]. The decrease in mobility and on/off ratio in Pn-based FETs induced by a long exposure to air has also been reported [2]. Recently, the n-type electronic transport and intense yellow luminescence in PnQ thin film has been demonstrated [3].

Organic materials are usually highly anisotropic, whether in their molecular or crystal structures, or in the bonding energies. This leads to complicated growth mechanisms, resulting sometimes in the lowering of the crystal symmetry of the film. However, since no direct observation of initial stage of the spontaneous, chiral evolution has been reported yet, there is no well understood mechanism for such evolution, either at mesoscopic level or even at macro level.

In this work the thin film growth of 6,13-pentacenequinone on Si(111) at room temperature (RT) was studied by low energy electron microscopy (LEEM) and *ab initio* density functional theory (DFT) calculations [4]. At the initial stage of film growth, non-crystalline islands or clusters (type-I) nucleate on top of a disordered wetting layer. This is followed by nucleation of crystalline islands (type-II). An anisotropy in the growth of type-II islands has been observed and related to: (1) asymmetric mass incorporation and (2) mass transport from non-crystalline islands via a large diffusion length. The observed left-handed or right-handed chirality is related to the orientation of the *c* axis and associated with the asymmetric mass incorporation. The pronounced, ring-like shapes of the islands originate from the gradual rotation of crystallites associated with asymmetric arrangement of dislocations.

From the observation of the growth and subsequent relaxation of the crystalline PnQ islands, with the support of DFT calculations, we conclude that kinetically stiff direction (here one of the diagonals of the in-plane unit cell) differs from the energetic one. This feature together with the asymmetric mass incorporation associated with molecular tilt and bond anisotropy can determine the chirality (enantiomorphic evolution) of organic growth, and can help to understand the principles of chiral bio-crystallization.

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