Local band structure fluctuation in pentacene thin film investigated by scanning tunneling microscopy/spectroscopy

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In organic semiconductor devices, material inhomogeneity originating from defect, impurity, and grain boundary results in the spatial fluctuation in band structures. Such spatial fluctuation strongly impairs device performance of, for example, carrier mobility. However, no direct observations of such fluctuation have been reported. Here we demonstrate a result of direct observation of spatial distribution in band structure using STM/STS.

A pentacene (Pc) thin film was prepared by vacuum deposition at room temperature on an alkanethiol self-assembled monolayer (SAM) on a Au(111) substrate. Using STM, we confirmed that Pc molecules were orderly packed with atomic steps (Fig. 1). For the STS anlaysis, I-V curves were measured at different areas, from which the dI/dV-V curves were numerically calculated (Fig. 2). To obtain the spatial distribution of the band structure of the sample, the values of dI/dV for different V_s were imaged (Fig. 3).

The dI/dV-V curves show that a new state (gap state) is formed in the band gap of Pc. As shown as the bright areas in Fig. 3, the gap states have a different spatial distribution from the surface topography. To investigate the origin of the gap state, we observed a SAM/Au(111) film and found that the domain boundaries of SAM have a distribution similar to that of the gap state, suggesting that the domain boundary is responsible for the formation of the gap state. Since the SAM packing is not dense at the boundary, the Pc molecules would penetrate to the Au substrate during the growth process and contact with the Au substrate. Thereby, the orbital hybridization is produced and to be the origin of the gap state.

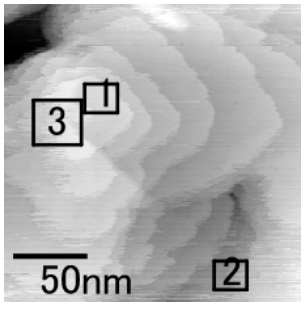

Fig. 1. Topography of pentacene thin film.

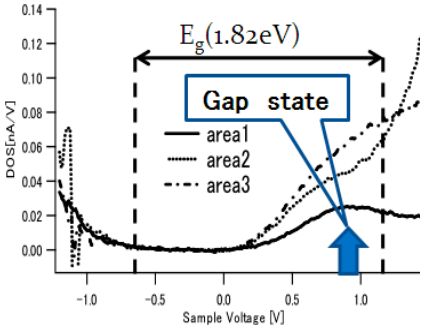

Fig. 2. dI/dV-V curves for each squared area drawn in Fig. 1. Eg denotes bandgap of pentacene.

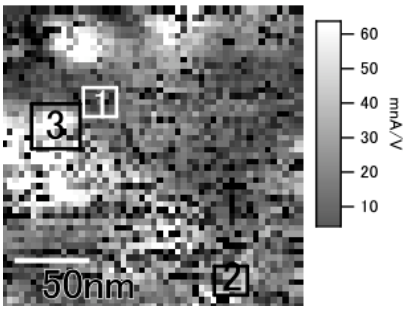

Fig. 3. dI/dV image for sample voltage of 0.8 V.