Controlling Orientation of phthalocyanine molecules by use of PTCDA ultra-thin template layer

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Introduction
Phthalocyanine (H 2 Pc) and metal phthalocyanine (MPc) have been widely applied to the optoelectronic devices due to their high carrier mobility and high photoabsorbance in visible region. However, single crystalline phthalocyanine shows the anisotropic electric conductivity because the stacking direction of π orbitals mainly contributes to the carrier transport. Therefore, the development of a technique of controlling molecular orientation is of importance for fabricating high performance devices.

It was recently reported that over 75 Å thick perylene tetracarboxylic dianhydride (PTCDA) template layers controlled the stacking direction of H 2 Pc films on quartz [1]. However, definite orientation of H 2 Pc grown on various thick PTCDA layer, particularly in the initial stage of growth, have not been fully understood so far. In the present study, we applied angle resolved ultraviolet photoemission spectroscopy (ARUPS) to determine orientation of H 2 Pc on PTCDA template layers.

Experiment
Highly oriented pyrolitic graphite (HOPG) was cleaved in air and cleaned by annealing at 700 °C in an ultra high vacuum (UHV) chamber. H 2 Pc and PTCDA were purified by temperature-gradient sublimation method. Thin film samples were prepared by vacuum deposition in a UHV chamber. The deposition was performed at a rate of 1-5 Å/min with the substrate held at room temperature. ARUPS was carried out at the station BL-11C of photon factory in the institute of Material Structure Research.

Results and Discussions
Figure 1 shows the ARUPS spectra of H 2 Pc on PTCDA template layer with the incidence angle (α) = 45 ° and hν = 22 eV. The intensity was normalized by the photon flux. With increasing in the detection angle (θ), the π band labeled A in Fig.1 increased up to near 55 °, and then decreased, while peak position was almost independent of θ.

Figure 2 shows the angular distribution of the peak A intensity. The solid curve and the open square indicate the thickness of PTCDA template layer of 7.5Å and 30Å, respectively. The observed angular distribution is very clear and simple giving a maximum intensity of about 55 ° for both samples. In order to analyze the molecular orientation from the ARUPS spectrum, the result of the independent atomic center (IAC) approximation in which molecules are assumed to stay parallel to the substrate surface is shown by solid curve [2]. The observed polar angles of the maximum intensity agree well with the calculated ones. It is thus concluded that H 2 Pc molecules are arranged on PTCDA with their molecular plane parallel to the substrate surface.

References

Fig.1 ARUPS spectra of the 90Å H 2 Pc film grown on the 7.5 Å PTCDA template layer.

Fig.2 Angular distribution of the peak A intensity. The solid circle and open square indicate the thickness of PTCDA template layer of 7.5Å and 30Å, respectively. The thickness of H 2 Pc films is 90Å for both samples. The solid curve shows the result of IAC approximation [2].