Molecular Ordering and Electrical Characteristics of Pentacene Thin-Film

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1. Introduction
Organic thin-film transistors (TFT’s) are of interest for use of in broad area electronic applications. Organic TFT’s would allow the use of inexpensive, lightweight, flexible and mechanically rugged plastic substrates as an alternative to the glass substrates needed for commonly used a-Si devices.[1-2] The most important factor to determine the performance is the molecular ordering of the organic active-layer, and the molecular ordering is mostly affected by the surface condition on which the organic active-layer is deposited. In this paper we investigated the molecular ordering and electrical characteristics of pentacene thin-film in several deposition conditions and the optimum deposition condition was also extracted.

2. Fabrication and measurement
The powder of pentacene was purchased from Aldrich with the purity of 99.8%. Pentacene thin-films were deposited by OMBD equipped with turbo and ion pump. The chamber was vacuumed to the base pressures of 4×10⁻⁷ Torr and the pentacene powder was evaporated by the thermal heating. TLM structure shown in Fig.1 was fabricated to investigate the electrical characteristics. As the substrate temperature was varied from 30°C to 100°C by 10°C, the deposition rate was maintained on 5Å/sec and 0.3Å/sec at each temperature. The molecular ordering of thin-films were measured and analyzed with X-ray diffraction and atomic force microscopy (AFM).

Fig.2. shows the X-ray diffraction pattern of pentacene thin-film with average thickness of 100nm deposited on SiO₂ at 30°C and 70°C. As the substrate temperature increases, the intensity of peaks becomes large, which represents the enhancement of molecular ordering. The expected crystal structure of pentacene is triclinic[3] with a=7.90Å , b=6.06Å , c=16.01Å , α=101.9°, β=112.6°, γ=85.5°. This leads to the plane spacing of 14.9Å on (001) plane. In Fig.2 the peak of 14.6Å decreases with temperature while the peak of 15.7Å becomes dominant. Therefore, the pentacene film in this work produced (001) crystal orientation with the plane spacing of 15.7 Å.

Fig.3 AFM images of these films are presented various substrate temperatures and deposition rates.
We estimate that the pentacene film would be re-evaporated from the substrate at the higher temperature. When annealed for 1 hr at 100°C, the conductivity was increased up to 30%. In conclusion the molecular ordering was enhanced at the high substrate temperature and at low deposition rate. The optimum vacuum deposition conditions in this work were found that the substrate temperature was 80°C and the deposition rate 0.3Å/sec.

Fig.3. Atomic force microscopy (AFM) images for a several substrate temperatures and deposition rates. (substrate temperature ; deposition rate)

At the same deposition rate the grain size becomes large as the substrate temperature increases. However, even the lower temperature the grain size becomes large when the deposition rate is small. Therefore the lower deposition rate and the large substrate temperature was effective on the enhancement of molecular ordering since those conditions provide the sufficient time and active energy for the molecules of pentacene to find the stable and the low energy states.

I-V characteristics were measured by HP4155A and conductivity was extracted from the relation of distance and resistance, and depicted in Fig.4. The conductivity was also produced the similar trend. It increases with the substrate temperature and the slope of increment becomes large when the deposition rate is small. The maximum conductivity of 6×10⁻⁶ S/cm was reached at 80°C and it saturated beyond 80°C. The results presented above show a strong correlation between molecular ordering and deposition conditions. The molecular ordering and the conductivity were enhanced at the high substrate temperature and at the low deposition rate. The optimum vacuum deposition condition in this work was found that the substrate temperature was 80°C and the deposition rate 0.3Å/sec.

Fig.4. Conductivity on various substrate temperatures and deposition rates

3. Conclusions

The results presented above show a strong correlation between molecular ordering and deposition conditions. The molecular ordering and the conductivity were enhanced at the high substrate temperature and at the low deposition rate. The optimum vacuum deposition condition in this work was found that the substrate temperature was 80°C and the deposition rate 0.3Å/sec.

Acknowledgments

This work was supported by the National Program for Tera-level Nanodevices of the Ministry of Science and Technology as one of the 21 century Frontier Programs.

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