Accurate Analysis of Molecular Orientation of Organic Semiconductor Material

Clarification of excellent electric properties of transistor devices fabricated by vacuum deposition

Achievements

- Successful fabrication of transistor device with high mobility by **vacuum deposition*** using 2-decyl-7-phenyl [1] benzothieno [3, 2-b] [1] benzothiophene (Ph-BTBT-10), an organic semiconductor with excellent charge transport properties
- Demonstration of excellent charge transport properties (hole mobility, >10 cm^2/Vs) by transistor device evaluation
- Confirmation of thin-film crystal structure (molecular arrangement) that gives Ph-BTBT-10 its high mobility by analysis of deposited thin film by **two-dimensional grazing incidence X-ray diffraction (2D-GIXD)****

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***Spin coating and vacuum deposition:** These are both typical methods for fabricating semiconductor thin films. In spin coating, a semiconductor solution is dropped onto a substrate, which is rotated (spun) at a high speed to coat its surface with the semiconductor. In vacuum deposition, a thin film of a material is formed by vaporizing (evaporating) the material in vacuum, and the vaporized material is deposited on the surface of a substrate.
****2D-GIXD:** When a sample surface is irradiated with an X-ray beam nearly parallel to the surface, faint diffraction signals can be obtained from a thin film layer. This is called grazing incidence X-ray diffraction (GIXD). When the signals are detected two-dimensionally, the preferred orientation of the sample can be evaluated. This is called 2D-GIXD.

Role of SPring-8

Background

Organic semiconductors are lightweight and flexible. Focusing on these advantages, the research and development of organic field-effect transistors (OFETs) have been intensively carried out towards their application in next-generation devices, such as stretchable and bendable electronic circuits and medical sensors that can be attached to the skin.

Ph-BTBT-10 is a liquid crystalline organic semiconductor that is soluble in common organic solvents and has high thermal durability, film formability, and air stability. In a previous study, it was found that an OFET device fabricated using Ph-BTBT-10 by spin coating showed a high hole mobility (>10 cm^2/Vs).[1] In this study, it was also found that a comparable mobility was obtained for a device fabricated by vacuum deposition. To determine the reasons for the excellent electric properties, it was necessary to reveal the thin-film crystal structure (molecular arrangement) in the vacuum-deposited thin film of the organic semiconductor using crystallography techniques.

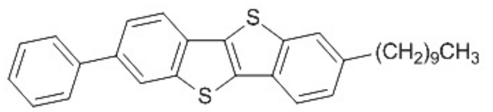
Results

An OFET device using Ph-BTBT-10 was fabricated by vacuum deposition and its transistor characteristics were evaluated. The results revealed that Ph-BTBT-10 was not thermally decomposed and its electrical properties were not deteriorated during the vacuum deposition process. The device fabricated by vacuum deposition showed excellent electric charge transport characteristics (hole mobility, >10 cm^2/Vs) comparable to those of a device fabricated by spin coating.

The molecular arrangement of the deposited thin film was analyzed by 2D-GIXD at SPring-8. The X-ray obtained from SPring-8 beamlines has an intensity much higher than that of general X-ray diffraction systems and enables the fast and accurate analysis of the molecular arrangement of organic thin films. The analysis results suggest that the crystal structure (molecular arrangement) of the vacuum deposited thin film was the same as that of the spin-coated thin film, verifying the high mobility of the device fabricated by vacuum deposition.

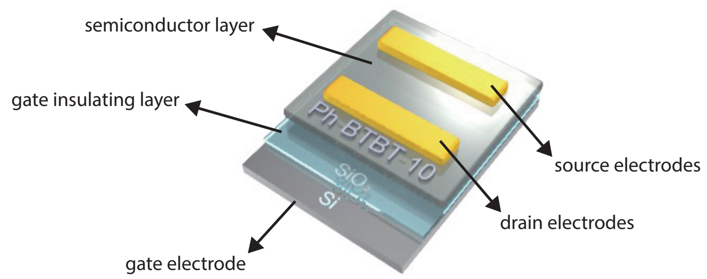
Ph-BTBT-10

Ph-BTBT-10 (upper) is a commercially available (lower) p-type organic semiconductor material with excellent transistor properties.



OFET device fabricated using Ph-BTBT-10

A Ph-BTBT-10 thin film was formed on a silicon wafer (n^+–Si/SiO_2). A gold (Au) layer was deposited on the thin film. Silicon (n^+–Si), silicon dioxide (SiO_2), Ph-BTBT-10, and Au were used as the gate electrode, gate insulating layer, semiconductor layer, and source/drain electrodes, respectively.



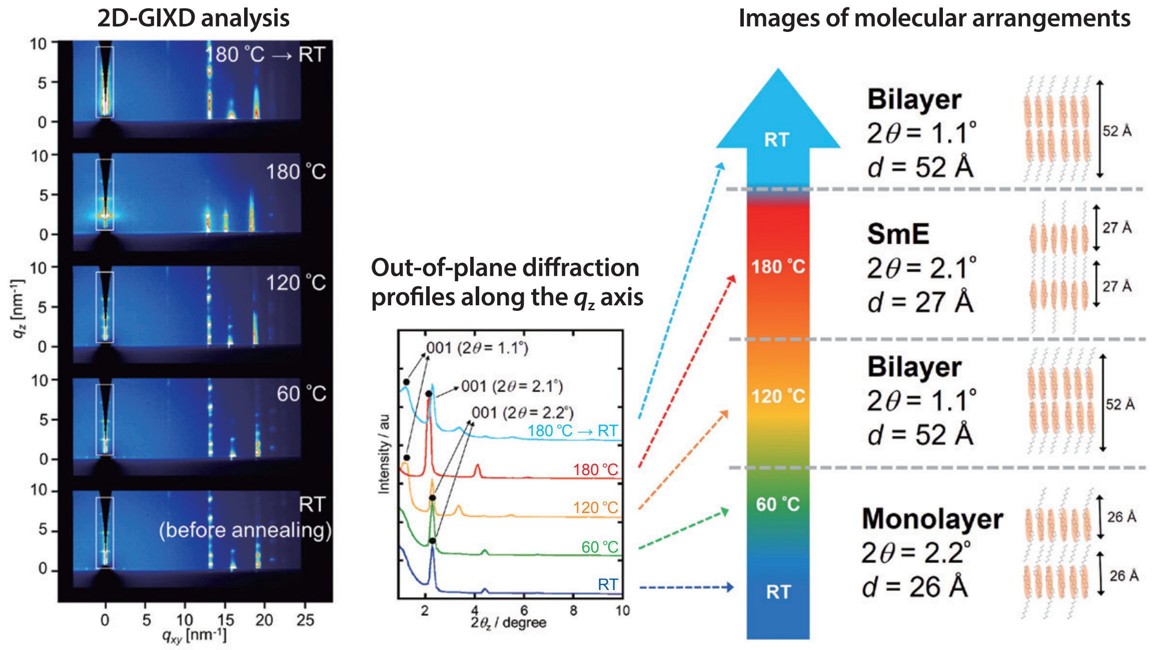
OFET device performance

Stable p-type semiconductor characteristics were observed for the transistor device fabricated by depositing a Ph-BTBT-10 thin film (right table). By annealing the deposited thin film, the transistor performance was greatly improved, that is, a maximum hole mobility of μ_{max} = 14.0 cm^2/Vs was achieved for the octadecyltrichlorosilane (ODTS)-treated substrate.

Fabrication Method	Substrate	Annealing Temp. (°C)	Mobility (cm^2/Vs)	Vth (V)
Vacuum Deposition	Bare (Si/SiO_2)	w/o	0.87 ~ 0.91	-24
		120	4.24 ~ 4.86	-8
	ODTS (Si/SiO_2/ODTS)	w/o	1.40 ~ 1.42	-23
		120	10.3 ~ 14.0	-22

Results of 2D-GIXD analysis

The interlayer distance in the out-of-plane direction was calculated from the diffraction peaks along the q_z-axis (indicated by white boxes). The molecular arrangement of Ph-BTBT-10 in the deposited thin film was predicted at each substrate temperature. The obtained diffraction peaks suggest that the crystal structure (molecular arrangement) of the post-annealed deposited thin film was the same as that of the spin-coated thin film.[1]



Reference H. Iino, T. Usui, J. Hanna, *Nat. Commun.* 2015, **6**, 6828.