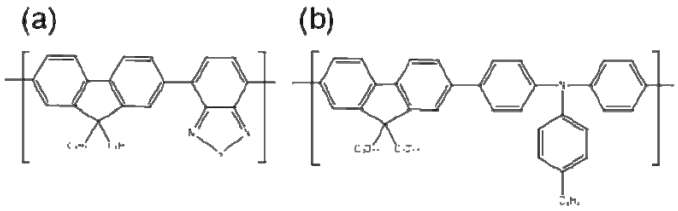
MLF Experimental Report	提出日 Date of Report
課題番号 Project No.2010A0025 実験課題名 Title of experiment 中性子反射率法による高分子薄膜／高分子薄膜界面の構造解析 実験責任者名 Name of principal investigator 簗嶋 裕之 所属 Affiliation 住友化学株式会社	装置責任者 Name of responsible person 瀬戸秀紀 装置名 Name of Instrument/(BL No.) Arisa II (BL-16) 実施日 Date of Experiment 2010/11/27-29

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)
Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.

In order to study the interface between poly(9,9-dioctylfluorene- co-benzothiadiazole) (F8BT, Fig. 1a) and deuterated poly(9,9-dioctyl fluorene-co-N-(4- butylephenyl) diphenylamine) (dF8-TFB, Fig.. 1b) , a dF8-TFB layer was deposited on a Si wafer by spin coating and thermally annealed at 200°C for 1hr in N2 to prevent the dF8-TFB being removed when a next F8BT layer was spin coated on top.



2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。)
Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.

The neutron reflectivity (NR) experiment was carried out on the time-of-flight neutron reflectometer, Arisa II (BL-16, J-PARC) to examine the interfacial mixing between dF8-TFB and F8BT. We used three incident angles, 0.3, 0.8 and 2.1degree to cover the q range from 0.07 to 2 nm^{-1} using neutron wavelength from 0.25 to 0.88 nm. Resolution dq/q was set ~5% by changing the slit width. Reflected intensities were normalized by the direct beam.

Figure 1 shows neutron reflectivity curves of a single layer of polymers (dF8-TFB or F8BT) on Si. The data were analyzed using Motofit software [1]. Good fits were obtained by fitting parameters of the polymer layer on native Si oxide / Si layer and the scattering length density and the film thickness of the polymers were determined.

In order to study the degree of mixing induced by thermal annealing at the interface between F8BT and dF8-TFB, the bi-layer sample was mounted on the hot stage and NR curves in Fig. 2 were gathered at various temperatures in vacuum. We waited for 10 min to start each run to stabilize the temperature.

2. 実験方法及び結果（つづき） Experimental method and results (continued)

The data is representative of the quality of the data using Arisa II, with a low background and going out to a high Q value of 2 nm^{-1} in the reasonable duration time (ca 3 hours for each). By annealing at 110°C, fringes were shifted toward lower q direction due to the thermal expansion of the polymer thickness. The reflectivity decreased more rapidly compared to the data at RT, which were observed more distinctly by annealing at higher temperature, especially at 170°C. These changes indicate that the mixing of the polymer interface was enhanced by annealing at higher temperature.

These structural changes of the polymer interface, observed by NR, might directly relate to charge injection at the polymer interface. Further data analysis and experiments are required to extract the width of interface between F8BT and dF8-TFB to compare to the device characteristics.

References

[1] Nelson, A. (2006). "Co-refinement of multiple contrast neutron / X-ray reflectivity data using MOTOFIT." Journal of Applied Crystallography 39: 273-276.

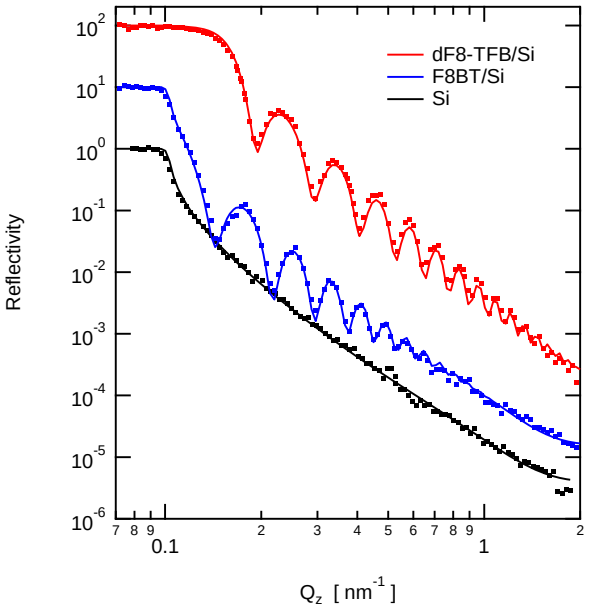


Fig. 1 Neutron reflectivity curves of reference samples: dF8-TFB, F8BT and Si. The data are offset for clarity.

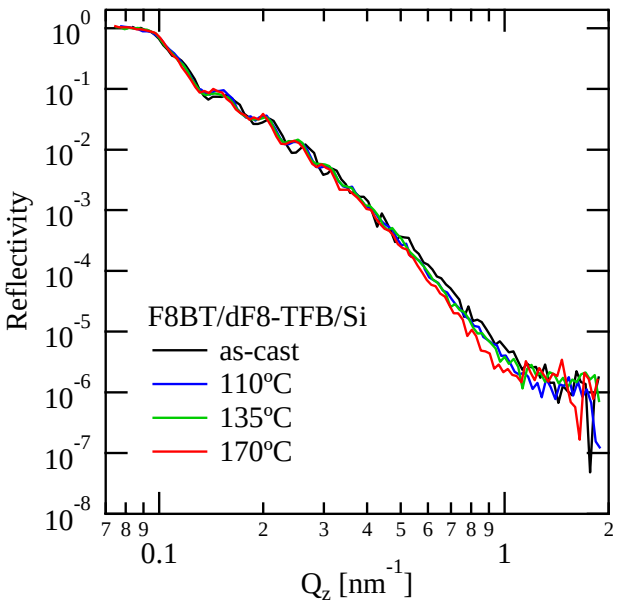


Fig. 2 Neutron reflectivity curves of bi-layer samples measured at various temperatures.