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Elastic Modulus of the Crystalline Regions for High Performance Polymer Single Fibers

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The elastic modulus, E_l, of the crystalline regions of polymers in the direction parallel to the chain axis provides important information on the molecular conformation and its relations to the mechanical properties. We have been engaged in measuring the E_l value for a variety of polymers using X-ray diffraction, where polymer fibers are constantly stressed on the goniometer and the lattice strains were detected *in situ*. Synthetic polymer is well known to bring weaker diffraction spots, thus, for the X-ray diffraction experiments using the laboratory equipment, a bundle of the polymer fibers has been used in order to get enough diffraction intensity. However, stress imhomogenity among the fibers in the bundle may seriously influence on the results. On the contrary, high beam intensity of synchrotron source will be expected to give enough diffraction even from a single organic fiber. So the single fiber experiments were planned in this project. First, the stretching device was especially designed for this purpose, and set on the Huber goniometer in BL46XU. The stretching device was connected with a stepping motor (for the elongation of the single fiber) and a load cell (for the stress detection on the single fiber). The single fiber of poly(*p*-phenylene terephthalamide) (PPTA), kindly supplied from Toray-Du Pont as Kevlar 49, was experienced. The diameter of the fiber is ca.12 μ m, which corresponds to the cross-sectional area of 1.1 X10^{-6}cm^2.

The fiber was adjusted on the center of the goniometer, then, the diffraction profile was measured as shown in Figure. The diffraction peak located around 2 θ =25.6° (wave length = 0.9490Å) could be asigned as the 006 meridional reflection. It took about 17 min / 2 θ degree. The results reveals that the single fiber experiments could be successfully performed using a newly developed stretching device. However, unfortunately, the machine time was quite restricted, because the beam was shut down during 5 shifts among the 6 shifts (from June 20 to June 22). So the experimental results were limited to confirm the validity of the apparatus and the setting technique. Even though, these are believed to be very useful for further investigations on the E_l measurements for high performance polymer single fibers.

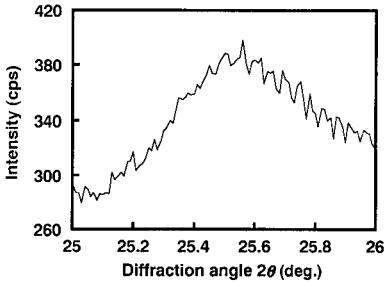

Fig. X-ray diffraction profile of poly(*p*-phenylene terephthalamide) single fiber.

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Extensive observation of superlattice peaks associated with a CDW order in $La_{1.875}Ba_{0.075}Sr_{0.05}CuO_4$

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A lattice distortion associated with an incommensurate charge-density-wave (CDW) order have been systematically studied on co-doped $La_{1.875-x}Ba_{0.125-x}Sr_xCuO_4$ (LBSCO) by neutron scattering [1]. Furthermore, hard X-ray diffraction measurements performed at BL02B1 as well as at BL46XU have also detected the CDW order. However, observed signals in neutron as well as X-ray diffraction have been limited in narrow Q-region because of the very weak intensity ($\sim 10^8$ times weaker than that of fundamental Bragg intensity in X-ray measurements). Therefore no quantitative information about atomic displacements due to the CDW order have been obtained so far. In the present work, we succeeded in observing the signals of the CDW order in a wide Q-region for LBSCO of $x = 0.05$.

X-ray diffraction experiments were performed at Research & Development beamline BL46XU, where the undulator is inserted. X-ray energy was tuned at 20 keV by using a Si111 double monochromator.

The incommensurate satellite peaks for the CDW order located around (4 0 L), (6 0 L), (4 4 L), and (5 3 L) points with $0 \leq L \leq 17$ were observed. The total number of collected reflections are more than 100. The typical profile of the CDW peak at (6+2ε 0 11/2) is shown in Figure 1 (a). Quite interestingly, as displayed in Figure 1 (b), the intensity of the CDW peak has a strong L-dependence. Furthermore, the CDW peaks at low-q positions (closed circles) show a completely different L-dependence from those at high-q positions (opened squares). These results indicate that the direction of an atomic displacement due to the CDW order occurs not only parallel to CuO_2 planes but also perpendicular to the planes. We performed a model calculation based on the so called *stripe* model. However, the possible models are not in an agreement with the obtained results, which strongly suggests that the origin of a CDW order might *not* be based on the simple stripe model.

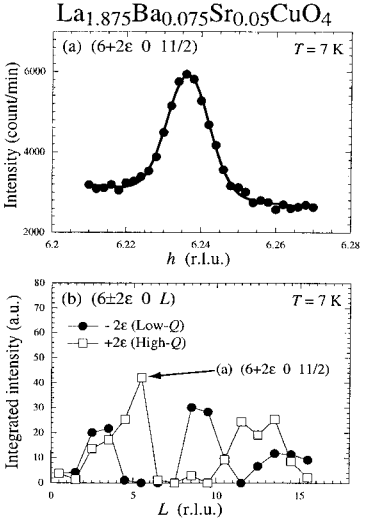

Figure 1: (a); h-scan profile through the (6+2ε 0 11/2) point taken at 7 K and (b); Integrated intensities of CDW peaks at (6±2ε 0 L) as a function of L. Closed circles and open squares denote the data taken at h=6-2ε and at h=6+2ε, respectively.

[1] M. Fujita *et al.*, PRL**88**, 167008, (2002).