



ESRF

	Experiment title: Carbon K-edge x-ray Raman study of polyfluorene	Experiment number: HE-2021
Beamline: ID16	Date of experiment: from: 16-Nov-05 08:00 to: 21-Nov-05 24:00	Date of report: 16-Feb-06
Shifts: 17	Local contact(s): Dr. Simo Huotari	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): S. Galambosi*, J. A. Soininen, K. Hämäläinen* Division of X-ray Physics, Department of Physical Sciences, University of Helsinki, 00014 University of Helsinki, Finland M. Knaapila* Department of Physics, University of Durham, South Road, Durham DH1 3LE, United Kingdom		

Report:

There is a significant interest in understanding the electronic and optical properties of π -conjugated polymers. The development of efficient optoelectronic devices requires a deep knowledge on the fundamental electronic properties of polymer systems of wide varieties. Polyfluorenes represent the modern era of conjugated polymers showing high efficiency, full color range in emission and excellent stability [1].

We have performed momentum transfer dependent x-ray Raman scattering (XRS) experiment at the carbon K-edge of poly[9,9-bis(ethylhexyl)-fluorene-2,7-diyl] (PF2/6). We have extended the use of XRS from hard condensed matter into the field of organic π -conjugated polymers. We also showed that using the momentum transfer dependence of XRS together with a recently proposed computational scheme [2] the unoccupied density of electron states can be decomposed into various symmetry components.

The experiments were carried out at ID16 using the eV-resolution spectrometer. The total energy resolution of 1.3 eV was achieved by using the Si (555) analyzer crystal in near backscattering geometry. In order to reduce the power density at the sample unfocused incident beam was used. The XRS spectra of the partly orientated polyfluorene samples were measured in a vacuum environment and the samples were held at a temperature of 20 K throughout the experiment.

As the unoccupied electronic states associated with the aromatic rings in the backbone of polyfluorenes are highly anisotropic, the directional dependence of the XRS spectra gives information on the macroscopic orientation of the polymer. In figure 1 the prepeak in the energy loss spectrum at 285 eV can be uniquely assigned to states perpendicular to the plane of the aromatic rings. Our calculations based on a full multiple scattering approach reproduce the essential features of the directional dependence near the edge region quite well.

By exploiting the subtle momentum transfer dependence of the XRS spectra, we have successfully performed the decomposition of the unoccupied density of states into two major symmetry components. Specifically, it is evident from figure 2, that the peak at 285 eV has a pure p -type symmetry, whereas the increased intensity of the XRS spectrum at larger energy transfer values is due to s states.

We have additionally gained valuable experience on the behavior of organic compounds under a heavy irradiation of x rays. By performing additional *ex-situ* diffraction and optical spectroscopy studies we were able to show, that while oxidation of the samples remain negligible, some cross linking of the polymers occurs.

We find that our results carry scientific importance and demonstrate the feasibility of XRS in the field of soft condensed matter. The manuscript is submitted for publication.

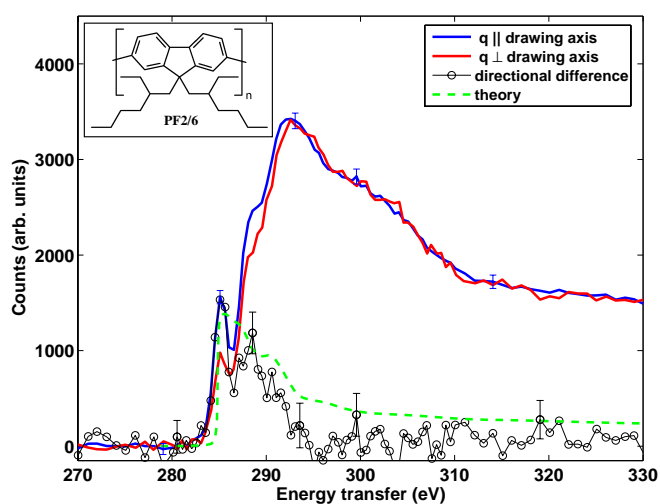


Figure 1

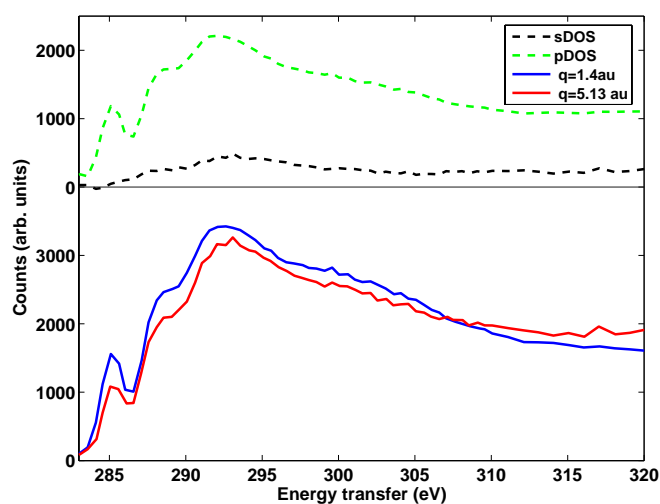


Figure 2

References

- [1] U. Scherf and E. J. W. List, *Adv. Mater.* **14**, 477 (2002).
- [2] J. A. Soininen, A. L. Ankudinov, and J. J. Rehr, *Phys. Rev. B* **72**, 045136 (2005).