ESRF	**Experiment title:** Study of surface crystalline domains on Poly(3-octylthiophene) thin films by surface x-ray diffraction	**Experiment number**: **25-02- 668**
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Report:

Molecular structure of poly(3-alkyl-thiophenes) investigated by calorimetry and grazing incidence X-ray scattering

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Abstract

A study of the molecular structure of regio-regular bulk poly-3-octyl-thiophene (P3OT) and poly-3- hexyl-thiophene (P3HT) and the phase transitions during heating and cooling scans in a temperature range of –158 to 773 ºC has been performed by means of calorimetry of bulk samples and grazing incidence X-ray diffraction from synchrotron radiation. Additional calorimetric measurements were performed on samples in toluene solution. From the calorimetric temperature diagrams at different scan rates, we obtain the melting and crystallization temperatures, and we identify a low temperature calorimetric glass transition. This transition is expected because of the coexistence of amorphous and crystalline phases, which is further supported by scanning force microscopy images where lamellar structures have been observed. Thin films of both polymers have also been studied by grazing incidence X-ray diffraction, and the evolution of the (100) crystalline peak monitored as a function of sample temperature, showing different behavior in both polymers, d-spacing increases in P3HT and decreases in P3OT for increasing temperatures. The information presented in this article will be useful to design fabrication techniques for organic-based electronic devices, which could include high and low temperature cycles combined with structural quenching procedures.