Experimental report

05/02/2020

Proposal: **9-11-1903** **Council:** 10/2018

Title: Equilibration and reversibility inpolymer/fullerene nanocomposites

Research area: Soft condensed matter

This proposal is a new proposal

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Samples: Polystyrene
Bis(1-[3-(methoxycarbonyl)propyl]-1-phenyl)-[6,6]C62 "Bis-PCBM"

Instrument	Requested days	Allocated days	From	To
D17	3	2	28/08/2019	30/08/2019

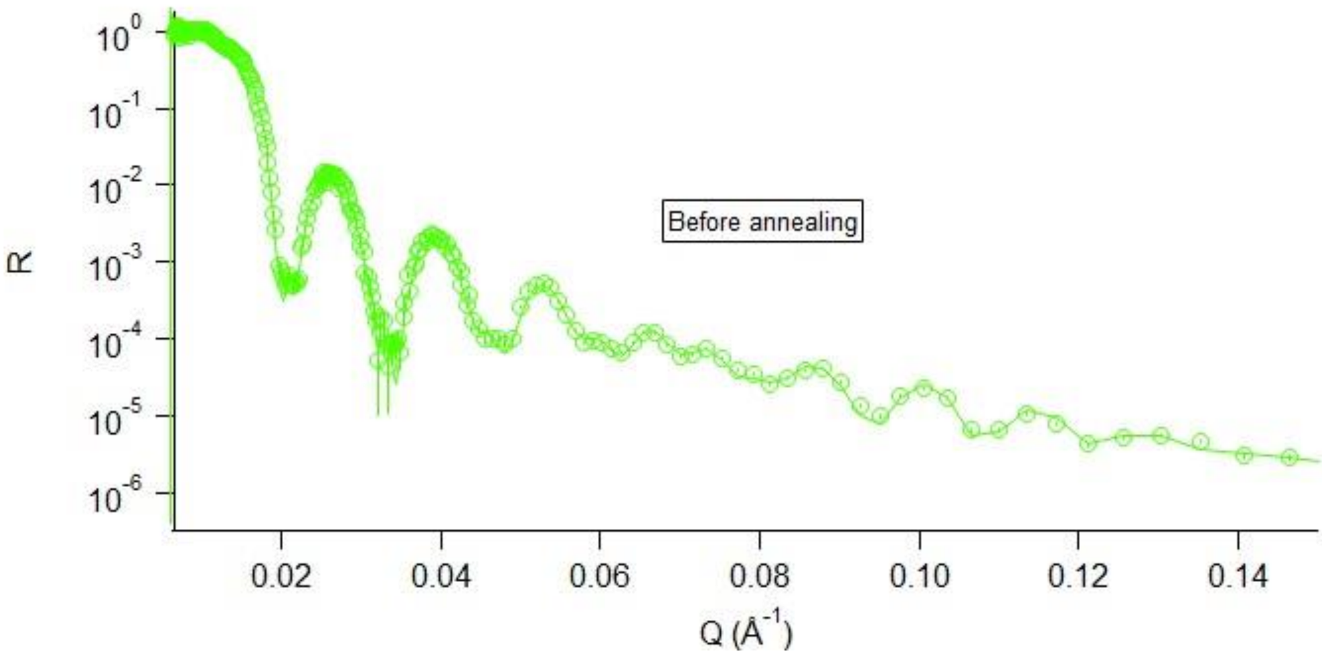
Abstract:

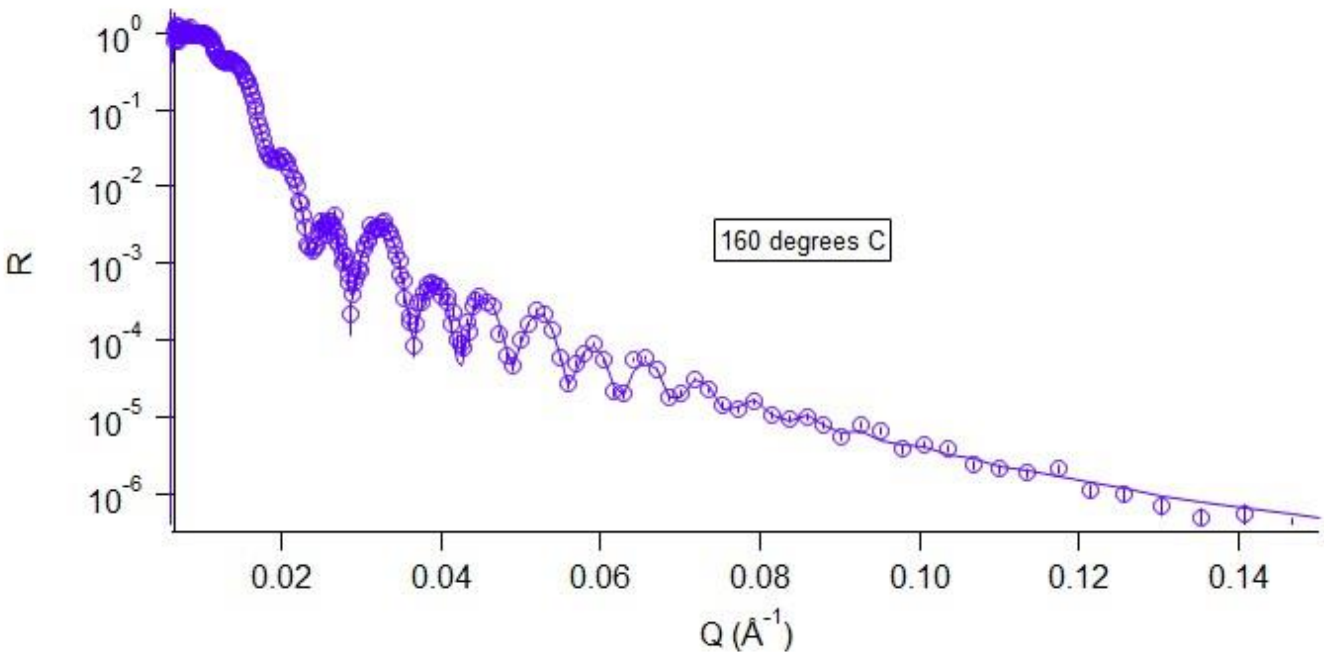
Organic photovoltaics (OPVs) are candidates for the large-scale capture of solar radiation, due to the potential to process these materials in large areas at low cost. However, considerable challenges exist in terms of lifetime and robustness of performance. Polymer/fullerene blends are bench-mark OPVs. However, there is considerable variation in the efficiency of these complex devices as a result of the sensitivity to a host of material and processing parameters. This proposal forms part of a wider effort in which our motivation is to reduce complexity and complement device optimisation strategies with an in-depth study of structure and kinetics in polymer/fullerene systems aimed at increasing the fundamental understanding of the materials science within polymer nanocomposite thin-films. This proposal focusses on a model polymer/fullerene system, in a bilayer geometry, in which neither component crystallises. We propose to characterise bis-PCBM/polystyrene at elevated temperatures, and robustly probe the behaviour of what we hypothesise is a liquid-liquid equilibrium system, as a function of annealing temperature, MW and starting point (composition profile before annealing).

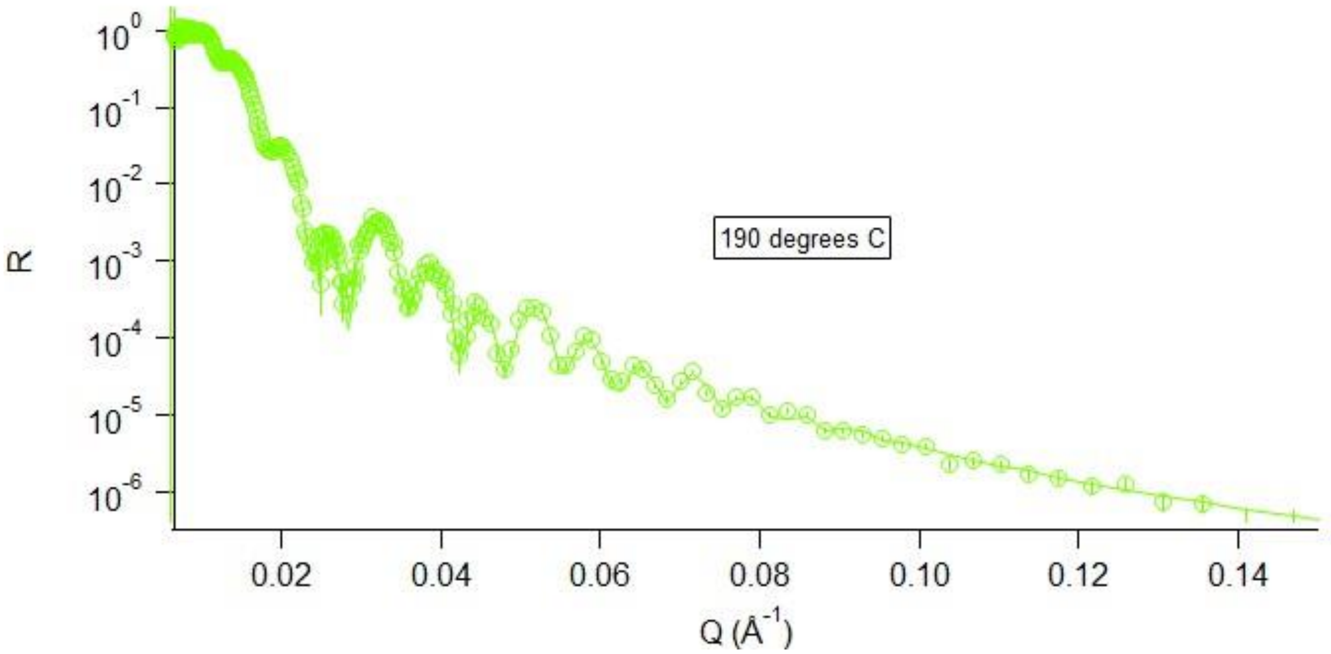
Experimental Report for D17 experiment 9-11-1903: August 2019

In-situ thermal annealing and neutron reflectometry measurements were performed on polymer/fullerene (polystyrene/bis-adduct phenyl-C60-butyric acid methyl ester (bis-PCBM)) bilayers. Experiments were done using i) pure components in each layer before annealing and ii) using layer compositions before annealing that were (polymer/fullerene) blends, rather than single components.

Pure component layers before annealing. Figure 1 shows reflectivity, R, versus momentum transfer, Q, with bilayer fits (two uniform layers with Gaussian interfacial roughness) for a 300k-polystyrene/fullerene bilayer, at four time points (in chronological order, room temperature, 160 ^oC, 190 ^oC 120 ^oC) before and during annealing. Very good fits were obtained using bilayer composition profile models. Significant changes in R(Q) occur on annealing, indicative of fullerene diffusion into the top (initially pure polystyrene) layer to give an equilibrated volume fraction of fullerene of ~0.15 to 0.2. The bottom layer remains pure fullerene. This can be seen in the SLD profiles (see Figure 2), in which the top layer gets thicker, the bottom layer gets thinner and the SLD of the top layer increases, on annealing. The interface also broadens on annealing.







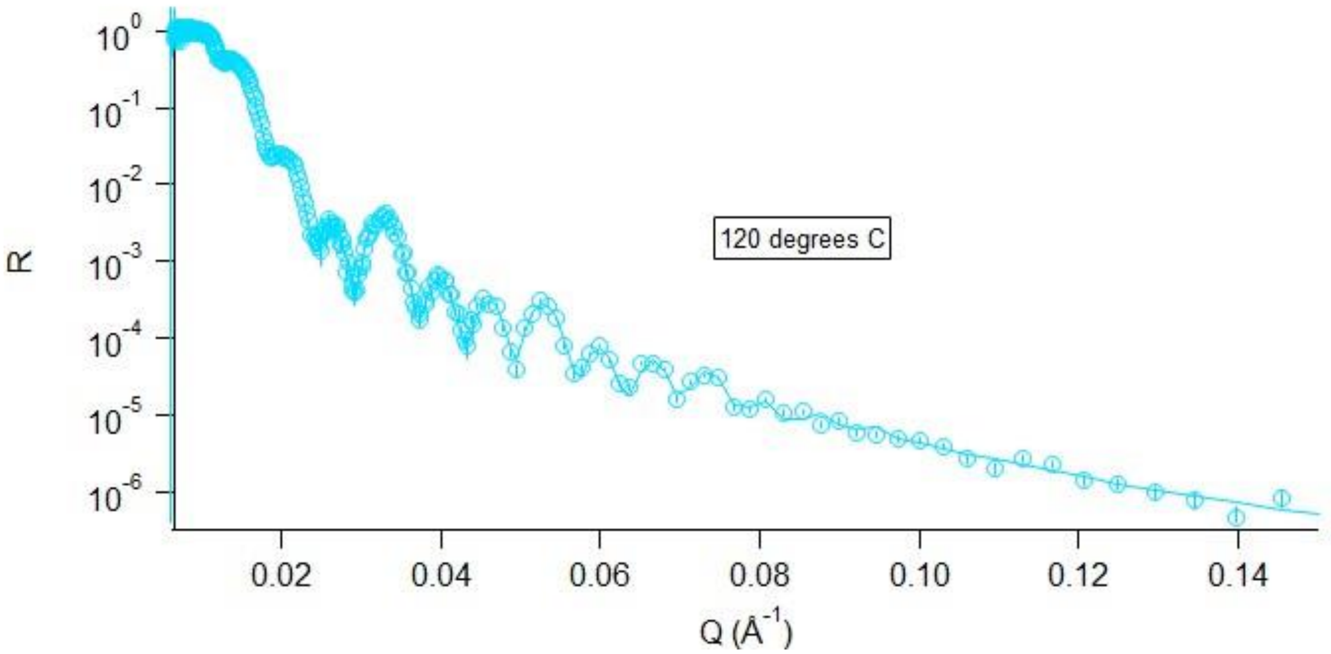


Figure 1; Reflectivity curves and bilayer fits for an in-situ annealed 300k-polystyrene/bisPCBM sample, at four different temperatures.

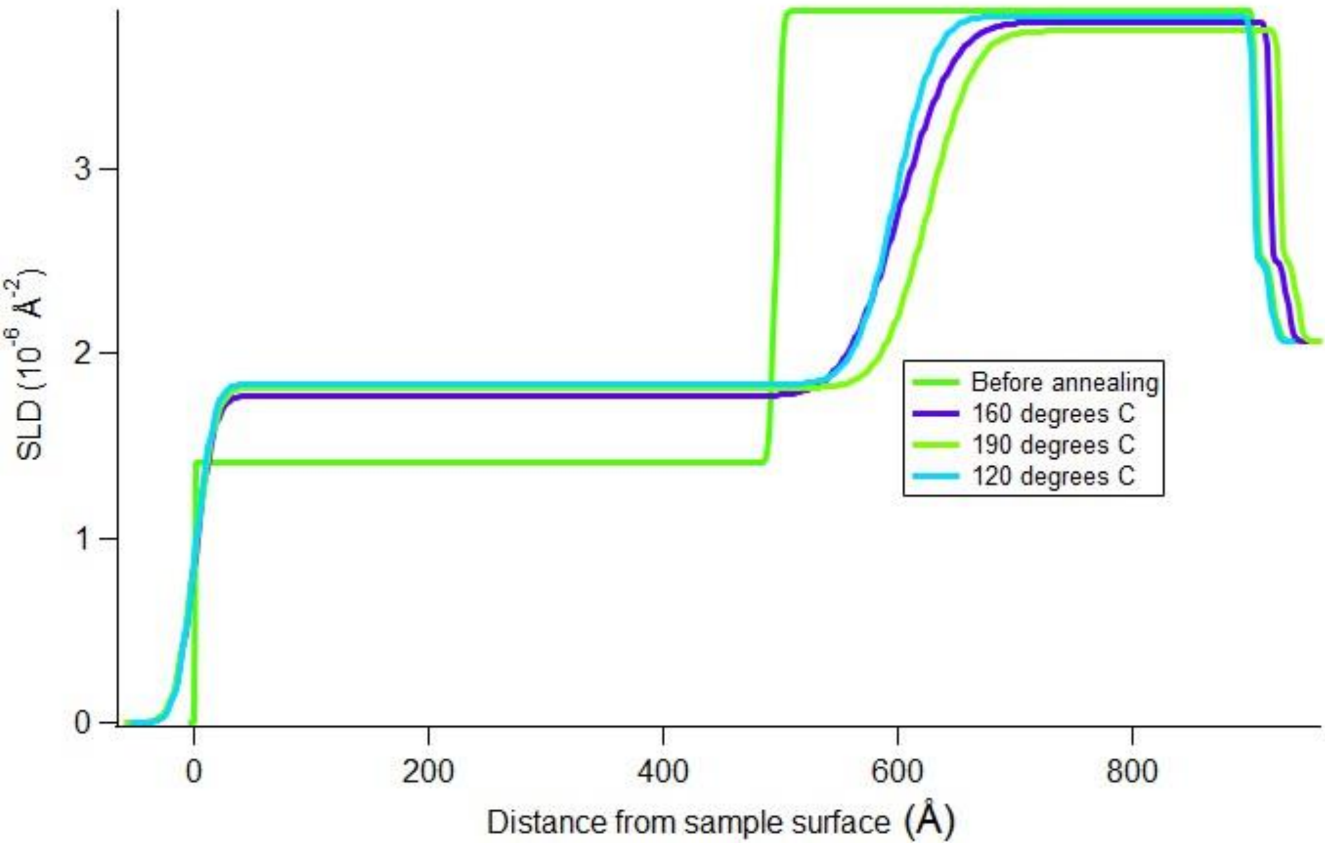


Figure 2; Scattering length density (SLD) profiles corresponding to the four fits shown in Figure 1.

Blended (top) layers before annealing. There were fabricated using several different top layer (polystyrene/fullerene) composition ratios. Good bilayer fits were obtained during annealing, with layer composition profiles evolving towards similar profiles to those obtained from pure component bilayers. However, the kinetics of this evolution process are dependent on the initial composition ratio, resulting in relatively fast diffusion in some cases, and sluggish kinetics in others.