polymers

MDPI

Supplementary

The Use of Scattering Data in the Study of the Molecular Organisation of Polymers in the Non-Crystalline state

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Supplementary Information

Characterisation information for the different materials used in this study can be seen in Table 1

Material	M_w	M_n	M_w/M_n	1,2 content (%)	1,4 Content (%)	T_g (^oC)
d-1,4 PBD	75000	79500	1.06	7	93	-103
d-1,2 PBD	72000	77700	1.08	93	7	-13.5
h-1,4 PBD	84000	87360	1.04	7	93	-100
h-1,2 PBD	75300	81300	1.08	93	7	-14

Table S1. Characterisation information for the 1,4 and 1,2-polybutadiene (PBD) systems used in this study. The indices d and h stand for deuterated and protonated systems respectively.

Polybutadiene Blends Sample Preparation and Experimental Procedure

Fully deuterated (>99%) 1,4-polybutadiene and 1,2-polybutadiene was obtained by Polymersource Inc. in Canada. Protonated 1,4-polybutadiene and 1,2-polybutadiene was also obtained by Polymersource Inc. in Canada. Material characterization can be seen in Table 1.

Each sample was dissolved in cyclohexane and casted in a container made of aluminum of 1mm thickness and 36mm diameter. All samples were dried in atmospheric pressure followed by vacuum for 48h and the evaporation of the solvent was checked by weighting. As soon as no changes in weight were observed the samples were assumed that had the majority of the solvent extracted.

Neutron scattering experiments were performed in ISIS Pulsed Neutron Source in the UK using SANDALS Diffractometer. Temperature was controlled by a CCR cryogenic unit with temperature fluctuations of the order of ±2^{o}C. All data were collected for a minimum of 500μA to a maximum of 3,500μA integrated proton current to ensure reasonable signal to noise ratio. Data were collected in all detector banks and normalized to the incident neutron beam and calibrated by a vanadium standard.

Polyethylene Sample Preparation and Experimental Procedure

Fully deuterated (>99%) polyethylene (M_n=109,000, M_w/M_n=1.02) was obtained by Polymersource Inc. in Canada. Sample was dissolved in Toluene and cast into a thin film of 40mm diameter and 1mm thickness. Solvent evaporation was checked by constant weighting at room temperature (~24 hours) and in vacuum (48 hours). After constant weight was reached it was assumed all solvent molecules have been extracted.

Neutron scattering experiments were conducted in ISIS Pulsed Neutron Source in the UK using SANDALS Diffractometer. Data were collected to 1,000μA integrated proton current, in all detector banks and were normalized to the incident neutron beam using a vanadium standard.

Method	l (Å)	φ (deg)	N	θ (deg)	Ref
This work	2.38±0.024	103±3.5		85±5	
RDF Analysis*	2.346±0.013	104±5	1.974±0.205		[1], [2]
MD Simulation	2.35	106		90±40	[3]
MD Simulation	2.3	103	2.1		[4]
MD Simulation	2.37	102.8		92.9	[5]
MD Simulation	2.37	102		100	[6]
MD Simulation	2.38-2.36	104-107±10-19	2-1.88	90	[7] [8]
MD Simulation	2.37	103	1±0.4 2±0.4 3±0.4		[9]
MD Simulation		103	2 (82%-83%) 3 (9-8.5%)	90	[10]
MD Simulation	2.36	106	2 (71%) 3 (18%)	Uniform	[11]
Disordered Chain	2.3-2.4	103-106		102	[12, 13]

Table S2. Comparison between results obtained from this work and previously reported theoretical predictions for the structure of Vitreous Selenium. l corresponds to the bond length, φ to the valence angle, ϑ to the torsion angle and N to the coordination number.

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