Phase Distribution of Carbon Black filler in Polymer Blend

Kiet Pham[a], Kabir Rishi[a], Gregory Beaucage[a]

[a] Department of Materials Science & Engineering, University of Cincinnati, Cincinnati, OH 45221, USA

Introduction

- Properties of processed polymers depend on not only the volume fraction but dispersion of fillers

- In the matrix of immiscible polymer blends, added fillers unevenly distributes to each component of the blend

- The distribution of fillers was previously studied based on the wetting coefficient which is related to interfacial free energy[1]

- In this research, we are studying the distribution of fillers in the polymer blend through pseudo-second order virial coefficient A2.
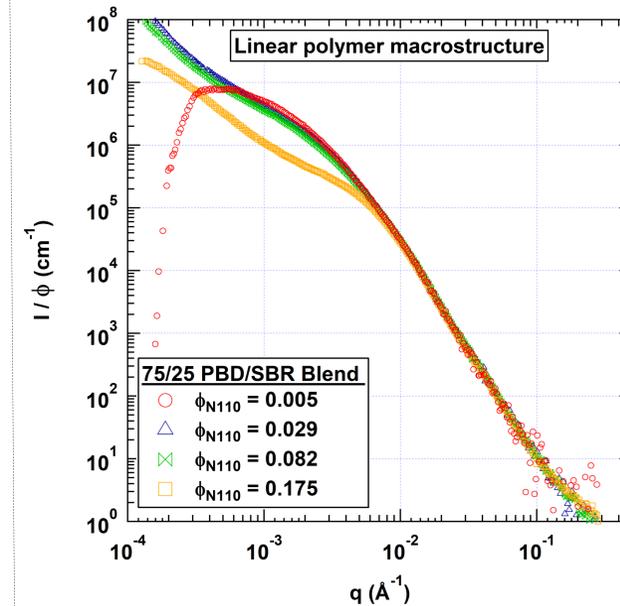
Unified Scattering Model[2]

$$I_0(q)/\phi_0 = \sum_{i=1}^{n}\left[G_i \exp\left(-q^2 R_{g,i}^2/3\right) + B_i(q_i^*)^{-P_i} \exp\left(-q^2 R_{g,i-1}^2/3\right)\right]$$

Random Phase Approximation[3]

$$\phi/I(q) = \phi_0/I_0(q) + \phi\upsilon$$

$$A_2 = \frac{\upsilon\langle\Delta\rho\rangle^2}{2\rho^2} N_A$$

Linear polymer macrostructure

75/25 PBD/SBR Blend
- $\phi_{N110} = 0.005$
- $\phi_{N110} = 0.029$
- $\phi_{N110} = 0.082$
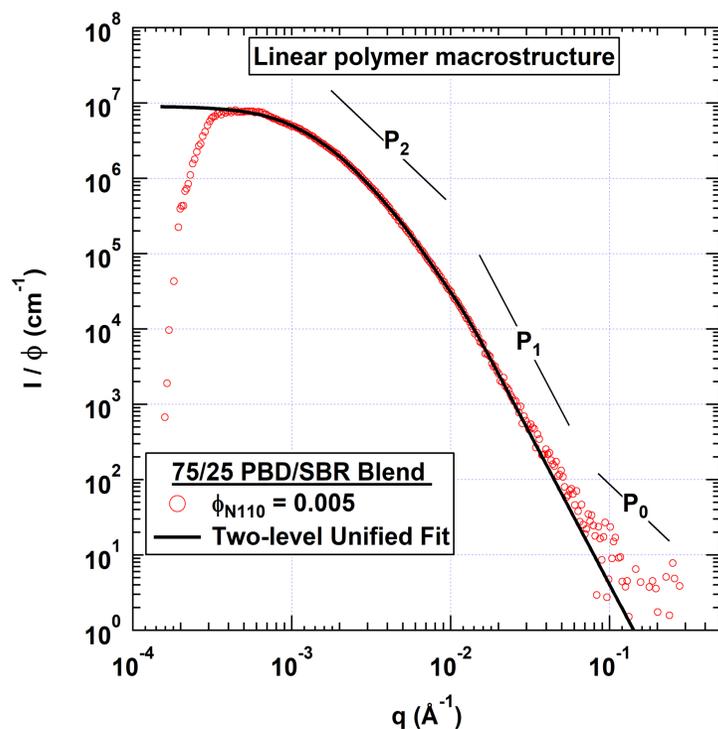- $\phi_{N110} = 0.175$

q (A⁻¹) axis, I / φ (cm⁻¹) axis

Log-log plot of normalized intensity vs. scattering vector for semi-dilute CB filler concentration from USAXS
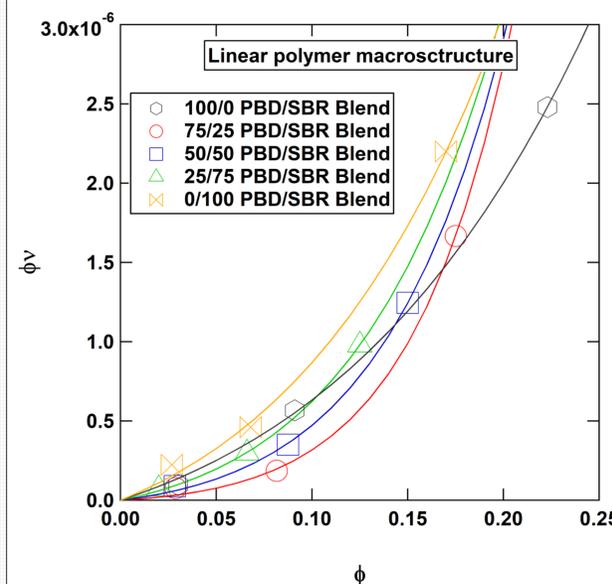
Filler Distribution

1. Filler predominantly distributes to PBD or SBR phase

2. Filler segregates at interface

3. Filler uniformly distributed between SBR and PBD phases

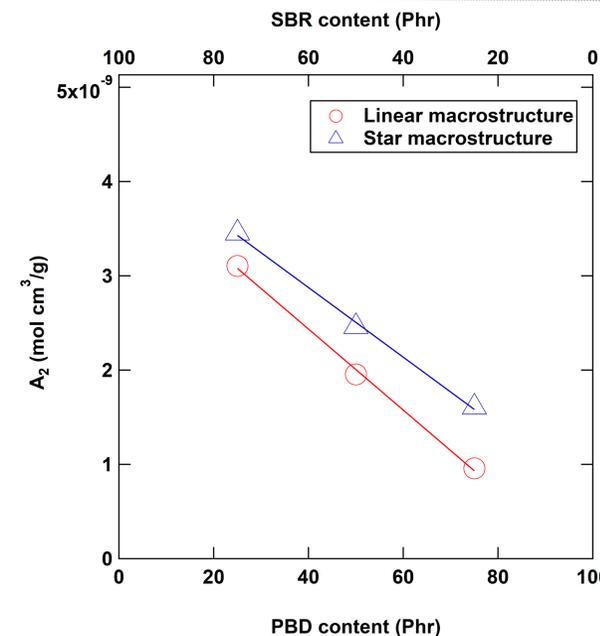4. Filler partially segregates between SBR and PBD phases

Methods

- Polymer blend used is PBD/SBR
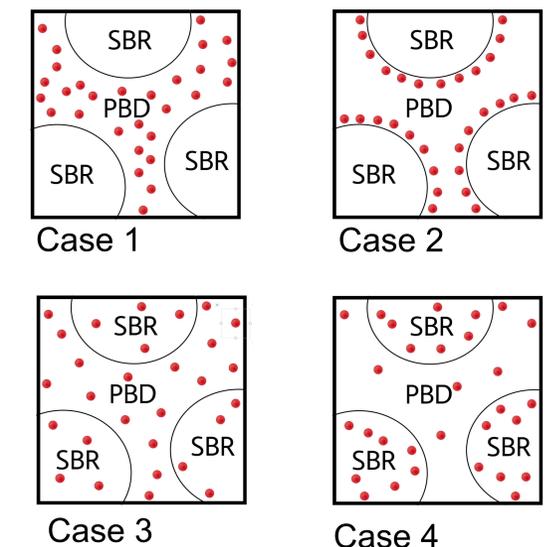- Filler used is Carbon Black N110 (CB)

Linear polymer macrostructure

P₂, P₁, P₀

75/25 PBD/SBR Blend
- $\phi_{N110} = 0.005$
- Two-level Unified Fit

I / φ (cm⁻¹) vs q (A⁻¹)

Log-log plot of normalized intensity vs. scattering vector for dilute CB filler concentration from USAXS

Linear polymer macrostructure
- 100/0 PBD/SBR Blend
- 75/25 PBD/SBR Blend
- 50/50 PBD/SBR Blend
- 25/75 PBD/SBR Blend
- 0/100 PBD/SBR Blend

$\phi\upsilon$ vs ϕ

Plot of filler concentration ϕ versus $\phi\upsilon$ in PBD/SBR Blend

SBR content (Phr)
- Linear macrostructure
- Star macrostructure

A_2 (mol cm³/g) vs PBD content (Phr)

Plot of A2 coefficient versus PBD content

Case 1: SBR, PBD, SBR, SBR
Case 2: SBR, PBD, SBR, SBR
Case 3: SBR, PBD, SBR, SBR
Case 4: SBR, PBD, SBR, SBR

Filler distribution in SBR/PBD Blend, $\phi_{SBR} < 0.5$

References

1. S. Asai , K. Sakata , M. Sumita and K. Miyasaka , *Polym. J.*, 1992, **24** , 415 —420
2. Beaucage, G. Approximations Leading to a Unified Exponential/Power-Law Approach to Small-Angle Scattering. *J. Appl. Crystallogr.* 1995, *28* (6), 717–728. https://doi.org/10.1107/S0021889895005292
3. Beaucage, G. Determination of Branch Fraction and Minimum Dimension of Mass-Fractal Aggregates. *Phys. Rev. E* 2004, *70* (3), 031401. https://doi.org/10.1103/PhysRevE.70.031401

For further information, please contact:
Gregory Beaucage beaucag@ucmail.uc.edu