

Effect of Processing Techniques on EMI SE of Immiscible PS/PMMA Blends Containing MWCNT: Enhanced Intertube and Interphase Scattering

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Thermodynamic Prediction of Filler Localization

Wetting coefficient (w) calculation is performed based on Young-Laplace equation equation to predict the thermodynamically favored phase for MWCNT (i.e. predict where MWCNT will locate):

$$w_{1-2} = \frac{\gamma_{\text{polymer2-filler}} - \gamma_{\text{polymer1-filler}}}{\gamma_{\text{polymer1-polymer2}}}$$

$\gamma_{i\text{-filler}}$ represents interfacial tension between the component, i and filler. This calculation assumes thermodynamic equilibrium in polymer blend system^{1,2}. If $w_{1-2} > 1$, the filler is supposed to locate in polymer1; if $w_{1-2} < -1$, then the filler is predicted to locate in polymer2 and interfacial localization of filler is assumed when value of w_{1-2} is in between 1 and -1. Harmonic and geometric mean function^{3,4} base equations are used to calculate interfacial tension (γ_{i-j}) between components, i and j .

$$\text{Harmonic mean: } \gamma_{12} = \gamma_1 + \gamma_2 - 4 \left[\frac{\gamma_1^p \gamma_2^p}{\gamma_1^p + \gamma_2^p} + \frac{\gamma_1^d \gamma_2^d}{\gamma_1^d + \gamma_2^d} \right]$$

$$\text{Geometric mean: } \gamma_{12} = \gamma_1 + \gamma_2 - 2 \left[\sqrt{\gamma_1^p \gamma_2^p} + \sqrt{\gamma_1^d \gamma_2^d} \right]$$

γ_i^p corresponds to the polar contribution and γ_i^d represents non-polar contribution of component, i . Individual surface energy and interfacial tension values for PS, PMMA and MWCNT systems are collected and extrapolated to processing temperature using literature values and correlations⁴⁻⁷. The calculation is shown in Table S1. Calculated values of interfacial tension between the components of the blend, wetting coefficient and predicted filler localization are given in Table S2.

Table S1. Surface tension, and dispersive and polar contribution of the surface tension of PS, PMMA and MWCNT at room temperature (RT) and 230 °C.

	γ (mJm^{-2})	γ^d (mJm^{-2})	γ^p (mJm^{-2})
$\gamma_{PS} (RT)$	40.7	35	6.11
$\gamma_{PMMA} (RT)$	41.1	29.59	11.51
$\gamma_{PS} (230\text{ }^{\circ}C)$	25.6	21.7	4
$\gamma_{PMMA} (230\text{ }^{\circ}C)$	25.14	18.1	7
γ_{MWCNT}^a	27.8	17.6	10.2
γ_{MWCNT}^b	45.3	18.4	26.9

Table S2. Interfacial tension values of polymer-MWCNT and polymer-polymer system at room temperature (RT) and 230 °C.

	<i>Harmonic mean</i>	<i>Geometric mean</i>
$\gamma_{PMMA-PS} (RT)$	2.05	1.04
$\gamma_{PMMA-PS} (230\text{ }^{\circ}C)$	1.28	0.65
$\gamma_{PMMA-MWCNT}^a (RT)$	3.13	1.59
$\gamma_{PMMA-MWCNT}^a (230\text{ }^{\circ}C)$	0.59	0.3
$\gamma_{PS-MWCNT}^a (RT)$	6.56	3.37
$\gamma_{PS-MWCNT}^a (230\text{ }^{\circ}C)$	3.32	1.74
$\gamma_{PMMA-MWCNT}^b (RT)$	8.78	4.54
$\gamma_{PMMA-MWCNT}^b (230\text{ }^{\circ}C)$	11.62	6.42
$\gamma_{PS-MWCNT}^b (RT)$	18.05	9.91
$\gamma_{PS-MWCNT}^b (230\text{ }^{\circ}C)$	17.58	10.56
$w_{PMMA-PS}^a (RT)$	1.67	1.70
$w_{PMMA-PS}^a (230\text{ }^{\circ}C)$	2.14	2.23
$w_{PMMA-PS}^b (RT)$	4.53	5.13
$w_{PMMA-PS}^b (230\text{ }^{\circ}C)$	4.67	6.38

^a According to Barber⁷.

^b According to Nuriel⁶.

Regardless of the methods of wetting coefficient calculation, MWCNT is predicted to locate in PMMA.

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