Influence of compatibility on oligomer partitioning in model adhesives.

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Additive surface segregation is a well-known phenomenon in complex polymer formulations. In industrial adhesives, tackifiers – i.e. aliphatic or aromatic oligomers – are added to enhance adhesion by decreasing the polymer's elastic modulus at the interfaces. However, phase separation between the tackifier and polymer could result in loss of adhesion or contamination of adjacent materials.

We combine experiments with theory and computational simulations to develop and validate a model describing oligomers' segregation. A binary model formulation, consisting of an aliphatic oligomer and a rubbery polymer was chosen to mimic the behaviour of tackifiers in hot-melt adhesives.

Compatibility between the two components was rigorously assessed using differential scanning calorimetry (DSC) to quantify deviations from the Fox equation predictions for ideal mixing. Ion beam analysis and neutron reflectometry were further used to visualise and quantify oligomers' partitioning. Subtle changes in interactions between the polymer and oligomer were explored and found to have a significant influence on compatibility. These small compatibility effects resulted in large, quantitative changes in surface and interfacial segregation and, for some model formulations, led to a clear wetting transition.



Figure 1 Expected concentration profiles at low (dashed line) and high (solid line) values of χN showing respectively surface segregation and phase separation.

Figure 2 Neutron reflectometry data and fit (inset) and corresponding composition profiles for 2 to 70 wt% d-squalane in thin polybutadiene films reveal distinct wetting transition with increasing oligomer concentration.

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