

Supporting Information

MoS₂ nanoplatelet fillers for enhancement of the properties of waterborne pressure sensitive adhesives

Vesna Daniloska^a, Radmila Tomovska^{a,b}, José M. Asua^a, Joseph L. Keddie^{c,}*

^a POLYMAT and Departamento de Química Aplicada, Facultad de Ciencias Químicas, University of the Basque Country UPV/EHU, Joxe Mari Korta zentroa, Tolosa Hiribidea 72, Donostia-San Sebastián 20018, Spain

^b IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Spain

^cDepartment of Physics and Surrey Materials Institute, University of Surrey, Guildford, Surrey GU2 7XH, United Kingdom

The Flory–Huggins interaction parameter was calculated as [1]:

$$\chi_{PVP-P2EHA} = \frac{V_m}{RT} (\delta_{PVP} - \delta_{P2EHA})^2 \quad (1)$$

where, $\chi_{PVP-P2EHA}$ is the polymer–polymer interaction parameter, V_m is the geometric mean of the polymer segment molar volumes, R is the gas constant, T is the absolute temperature, and δ_{PVP} and δ_{P2EHA} are the solubility parameters for PVP and P2EHA, respectively. For the PVP solubility parameter, the literature value of 16.7 MPa^{0.5} was used [2]. The P2EHA solubility parameter was calculated by Group Contribution Method of van Krevelen [3] to be 17.03 MPa^{0.5}, assuming that the properties of the soft polymer are similar to that of poly(2-EHA). The polymer-polymer interaction parameter, estimated by Equation 1 was $\chi_{PVP-P2EHA}=0.0065$. The critical interaction parameter, ($\chi_{cr}=0.017$), was calculated on the base of the degree of polymerization for PVP and P2EHA according Equation 2.

$$\chi_{cr} = 0.5 \left[\frac{1}{\sqrt{r_{PVP}}} + \frac{1}{\sqrt{r_{P2EHA}}} \right]^2 \quad (2)$$

where, r_{PVP} and r_{P2EHA} are the corresponding degree of polymerization of PVP and P2EHA, respectively.

As $\chi_{PVP-P2EHA} < \chi_{cr}$, the polymers are miscible and no phase separation should be expected.

References

- [1] Flory PJ. Principles of Polymer Chemistry, Cornell University Press, 1953, New York.
- [2] Adamska K, Voelkel A, Héberger K. J. Chromatography A, 2007;1171:90.
- [3] van Krevelen DW, Properties of polymers, correlations with chemical structures, Elsevier, NY, 1990.