Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Information: Temperature dependence of micelle shape transitions in copolymer solutions: the role of inter-block incompatibility

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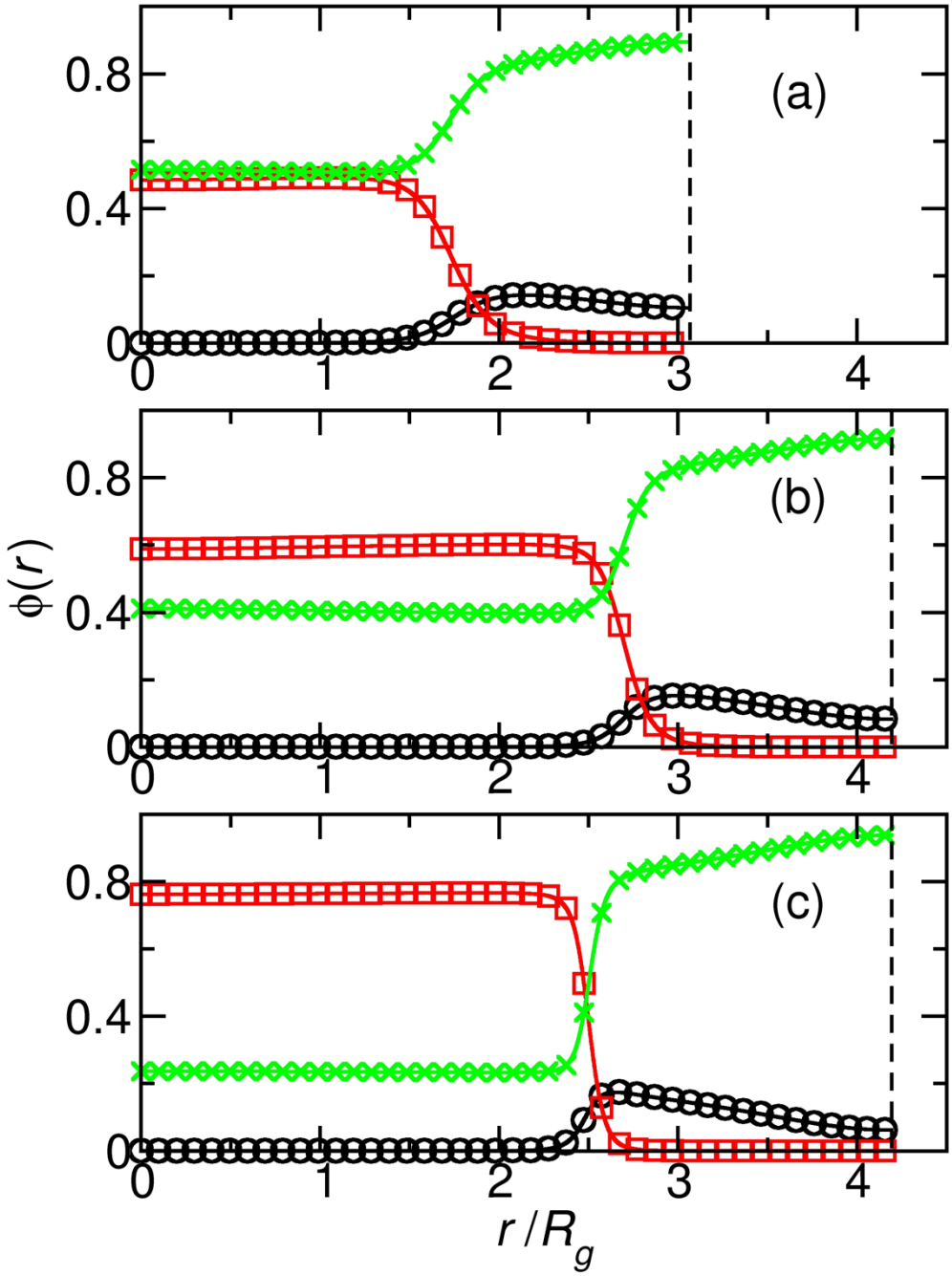

Figure S1 The results presented in Figure 2 of C. Y. Liaw, K. J. Henderson, W. R. Burghardt, J. Wang and K. R. Shull, *Macromolecules*, 2015, **48**, 173—183 recalculated using our code. The local volume fractions of the core blocks, shell blocks and solvent are shown with red squares, black circles and green crosses respectively, and the boundary of each calculation box is marked with a dashed line. The overall volume fraction of copolymer is 0.25, the degree of polymerisation N is 534, and the volume fraction of shell-forming blocks in the copolymer is $f_A = 0.348$. The inter-block and shell block/solvent chi parameters are set

to $\chi_{AB} = 0.05$ and $\chi_{AS} = 0.45$ respectively, while the core block/solvent chi parameter is calculated from $\chi_{BS} = 1.45 - 0.0115T$, where T is the temperature in °C (as opposed to the absolute temperature used in the main article). Distances are measured in units of the radius of gyration R_g of the copolymers. (a) The cylinder that forms at 60 °C; (b) the sphere that forms at 50 °C; and (c) a sphere that forms at 25 °C with the system size fixed to that in part (b).

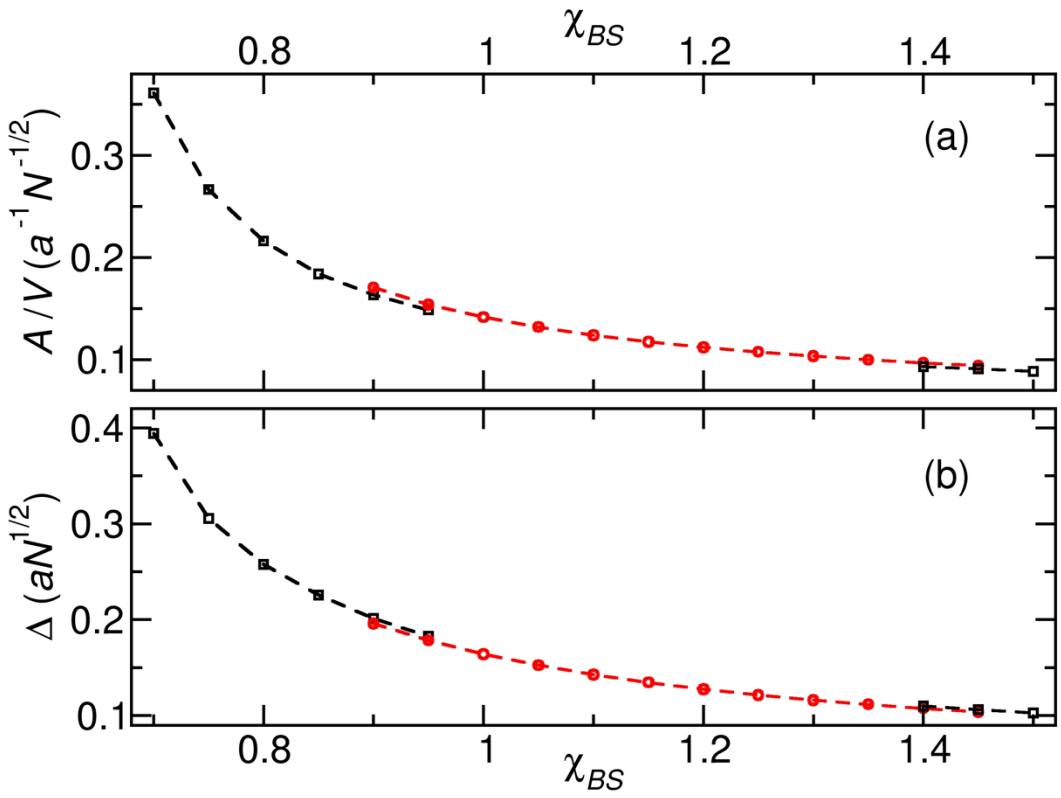

Figure S2 (a) Core surface area of micelles per unit volume (A/V) in the $\chi_{AB} = 0.1$, $N_A = 80$ system in the cylinder and sphere phases, shown by black squares and red circles respectively. The core surface is defined as lying at the value of r where the local volume fractions of the core and shell blocks are equal, so that $\phi_A(r) = \phi_B(r)$. This value of r is used to calculate the core surface area, which is then divided by the volume V of the calculation box. A/V is higher in the sphere phase than in the cylinder phase. (b) Interfacial width Δ in the $\chi_{AB} = 0.1, N_A = 80$ system. Δ is defined as the difference between the value of r at which $\phi_B(r)$ is at 90% of its maximum value and that at which it is at 10% of its maximum value. As A/V becomes larger as the system moves into the sphere phase, the interfacial width is lower in this phase due to the stretching of the interface.