Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Information

Packing and emergence of ordering of rods in a spherical monolayer

Dharanish Rajendra, Jaydeep Mandal, Yashodhan Hatwalne, Prabal K. Maiti

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This supplementary material contains results to show that 1. there is no positional ordering in the low-density phase, 2. The finite size effect for the system 3. shape anisotropy has a similar effect on the radial order parameter as compared to the nematic order parameter, and 4. there can be short ranged positional ordering below the critical anisotropy A_c.

1. No positional ordering in the low density LC phase

As is mentioned in the main text, the system shows different phases depending on the density. These phases show different positional and orientational ordering. We have showed that in the 2D LC phase, there is orientational ordering but no positional ordering. Through the nematic and radial order parameters, and orientational correlation we have then shown that there is a weak orientational ordering in the low density LC phase. While the radial distribution function in the main text indicates that there is no positional ordering in the low densities, we confirm this fact by the calculation of structure factor at $\eta \sim 0.30$ (Fig. S1). The structure factor does not show any other peak apart from the one at $q = 0$. This confirms our observation of lack of positional ordering in the low densities.

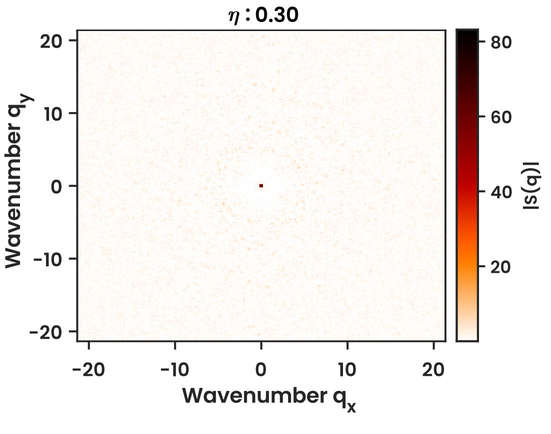

Figure S1: Structure factor for a packing fraction of $\eta = 0.3$ for a system of $N = 2500,\ T^* = 5,\ A = 5$. The absence of any peak apart from the $q = 0$ peak confirms the lack of positional ordering at this and lower densities.

2. Effect of finite size for the system

We show the effect of increasing system sizes for the system of spherical monolayer. We note that for this case as well, the nematic as well as the radial order parameter increase monotonically with density. Even at very low densities the nematic order parameter takes values $S > 0$ (Fig S2) implying the absence of isotropic phase for such systems.

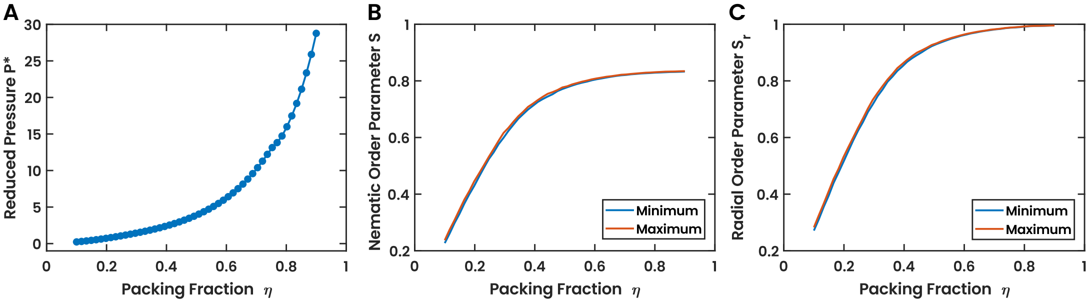

Figure S2: (A) Equation of state of the system i.e. reduced pressure P^* vs packing fraction η of a system of 25000 particles with $A = 5$, $T^* = 5$. (B) Nematic order parameter S and (C) radial order parameter S_r as a function of the packing fraction η for the same system.

3. Radial order parameter shows similar nature as nematic order parameter for different shape anisotropy

For shape anisotropy $A = 3$, the maximum and minimum values of radial order parameter is same over the surface of the sphere, indicating homogeneous ordering of the spherocylinders in the full range of densities (Fig. S3A). Whereas, for $A = 4$, orientational defects arise at high densities and there is a large difference between the maximum and minimum values of radial order parameter S_r over the surface of the sphere (Fig. S3B). This shows that there exists a critical shape anisotropy A_c below which orientational defects can no longer arise.

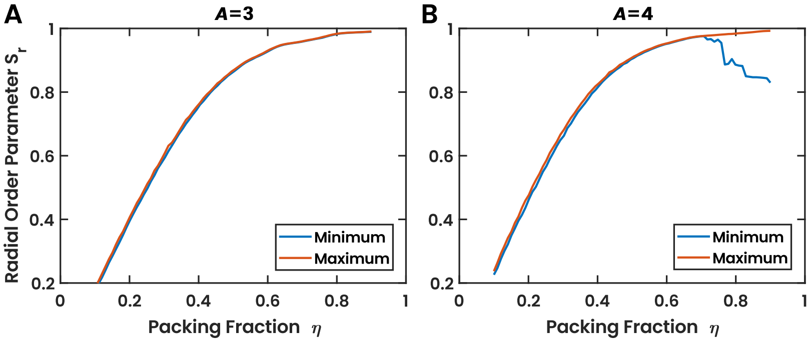

Figure S3: Radial order parameter S_r as a function of packing fraction η for shape anisotropies of (A) $A = 3$, and (B) $A = 4$. Both are calculated for systems with $T^* = 5$, $N = 2500$.

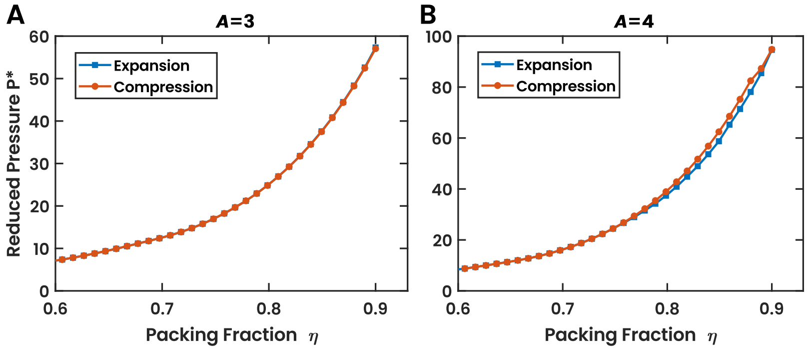

Figure S4: Equation of state for expansion and compression of a system of SRS particles on a sphere with $N = 2500$, $T^* = 5$ for (A) A=3 and (B) A=4. For $A = 4$, the expansion and compression curves show a disagreement indicating a first-order transition between LC and solid. For $A = 3$, the expansion and compression curves closely match throughout, indicating a continuous transition

4. LC–solid transition is continuous below A_c

In addition to orientational defects not being possible when the shape anisotropy is below the critical shape anisotropy A_c, the LC–solid transition becomes continuous. This can be seen from Fig. S4. For $A = 4$, above A_c, the equation of state shows a disagreement or hysteresis during compression and expansion of the system. This is a sign of a first order transition between LC and solid phases. However, for $A = 3$, below A_c, the equation of state during compression and expansion show good agreement throughout and do not show any kind of hysteresis. Therefore, we can say that below the critical shape anisotropy A_c, the LC–solid transition becomes continuous.

5. Positional ordering below A_c

When the shape anisotropy is below the critical shape anisotropy A_c, we have seen that orientational defects are no longer possible in the range of packing fractions. Even within this range of packing fractions, there is a gradual emergence of short ranged hexagonal positional ordering. This can be seen in the case of $A = 3$ (Fig. S5), which shows one or two rings in the structure factor plot at high packing fractions.

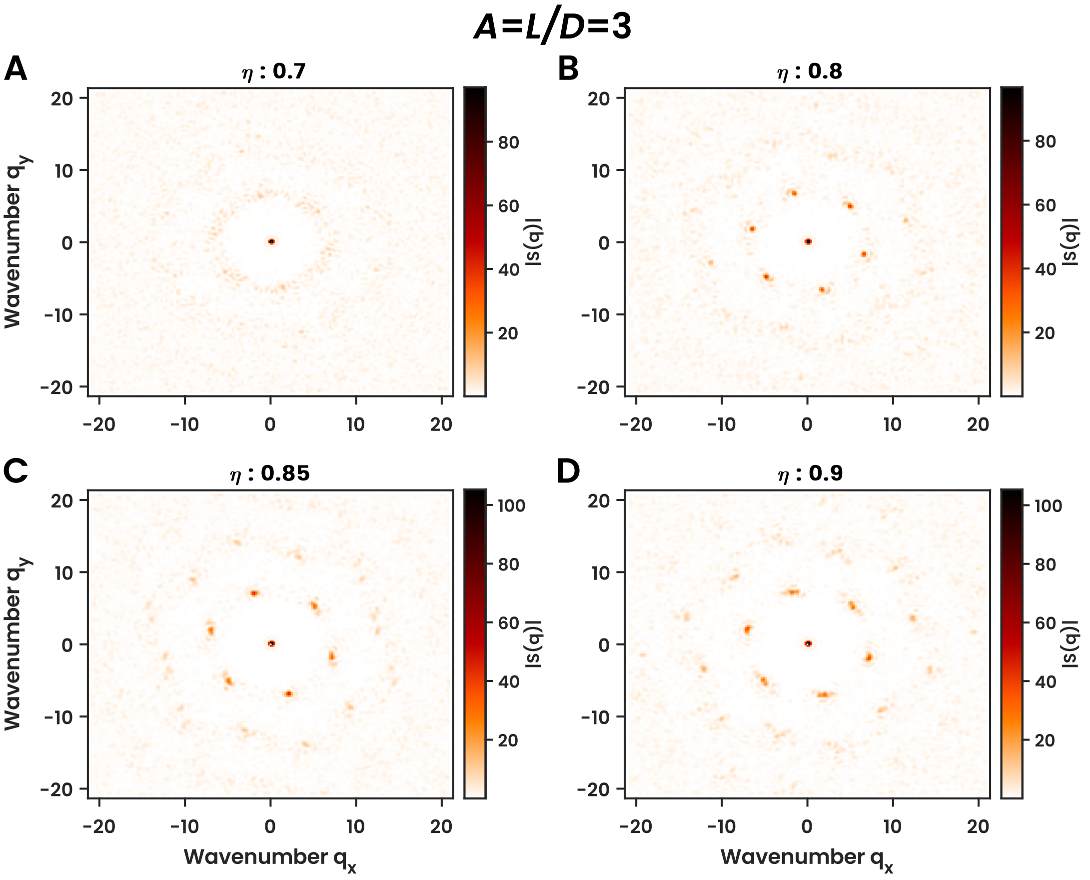

Figure S5: Structure factor for different packing fractions η for a system of SRS particles with shape anisotropy $A = 3$ i.e. below the critical shape anisotropy A_c. It shows a gradual emergence of short-ranged positional ordering, only one or two rings in the structure factor plot.