Supporting Information for paper: Pattern formation in two-dimensional hard-core/soft-shell systems with variable soft shell profiles

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I. LATTICE PARAMETERS FOR MECS

For $g \geq 1$, the soft shoulder profile of the HCSS particles is flat enough so that under compression, it is energetically favourable for neighbouring shells to be either fully overlapped or not overlapped. In this section, we show how this interplay between the hard-core and soft-shoulder length scales allows us to calculate the lattice parameters for MECs for $g \geq 1$ and $r_1/r_0 < \sqrt{3}$ using simple geometry.

Low and high density hexagonal phases (HEXL, HEXH)

The unit cell for HEXL is shown in Figure 8(a). The lattice constants $a, b = r_1$ so that the unit cell aspect ratio $\gamma = b/a = 1$, the unit cell angle $\phi = \pi/3$ and the density parameter $\ell = r_1$, where we parameterise the area per particle as $\frac{\sqrt{3}}{2}\ell^2$. On the other hand, the unit cell for HEXH is shown in Figure 8(d). The lattice constants $a, b = r_0$ so that $\gamma = b/a = 1$, $\phi = \pi/3$ and $\ell = r_0$.

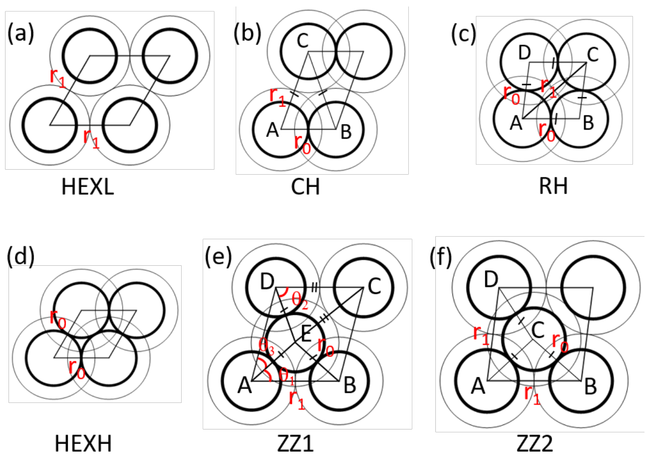

FIG. 1: Unit cells for MECs of HCSS particles with $g \geq 1$ and $r_1/r_0 \leq \sqrt{3}$.

Chain phase (CH)

The unit cell is shown in Figure 8(b). The lattice constants are $a = r_0$, $b = r_1$ so that $\gamma = r_1/r_0$. Since ABC is an isosceles triangle, we have

$$\cos\phi = \frac{r_0}{2r_1} \Rightarrow \phi = \cos^{-1}\left(\frac{r_0}{2r_1}\right). \qquad (1)$$

Using Eq. (1) and the fact that the unit cell area is given by $r_0 r_1 \sin\phi = \frac{\sqrt{3}}{2}\ell^2$, the density parameter is given by

$$\ell = \left(\frac{2r_0 r_1}{\sqrt{3}}\right)^{1/2}\left[1 - \left(\frac{r_0}{2r_1}\right)^2\right]^{1/4}. \qquad (2)$$

Rhomboid phase (RH)

The unit cell is shown in Figure 8(c). The lattice constants are $a, b = r_0$ so that $\gamma = 1$. Since ABC and ADC are identical isosceles triangles, we have

$$\cos\left(\frac{\phi}{2}\right) = \frac{r_1}{2r_0} \Rightarrow \phi = 2\cos^{-1}\left(\frac{r_1}{2r_0}\right). \qquad (3)$$

Finally, using Eq. (3) and the fact that the unit cell area is given by $r_0 r_1 \sin\left(\frac{\phi}{2}\right) = \frac{\sqrt{3}}{2}\ell^2$, we have

$$\ell = \left(\frac{2r_0 r_1}{\sqrt{3}}\right)^{1/2}\left[1 - \left(\frac{r_1}{2r_0}\right)^2\right]^{1/4}. \qquad (4)$$

Zig-zag 1 phase (ZZ1)

The unit cell is shown in Figure 8(e) and the angles θ_1, θ_2 and θ_3 are defined as follows. Since ABE and CDE are isosceles triangles, we have

$$\cos\theta_1 = \frac{r_1}{2r_0} \quad (5)$$

$$\cos\theta_2 = \frac{r_0}{2r_1}. \quad (6)$$

Furthermore, since ADE is an isosceles triangle and AB is parallel to DC, we have

$$\theta_1 + \theta_2 + 2\theta_3 = \pi \Rightarrow \theta_3 = \frac{\pi}{2} - \frac{1}{2}(\theta_1 + \theta_2). \quad (7)$$

The unit cell angle is now given by

$$\phi = \theta_1 + \theta_3. \quad (8)$$

The lattice constants are given by $a = r_1$, $b = 2r_0\cos\theta_3$ so that the unit cell aspect ratio is

$$\gamma = \frac{2r_0}{r_1}\cos\theta_3. \quad (9)$$

Using the fact that the unit cell area is given by $ab\sin(\theta_1 + \theta_3) = 2 \times \frac{\sqrt{3}}{2}\ell^2$ (there are two particles per unit cell for ZZ1), we have

$$\ell = \left[\frac{2r_0r_1}{\sqrt{3}}\cos\theta_3\sin(\theta_1 + \theta_3)\right]^{1/2}. \quad (10)$$

Finally, α, β, the coordinates of particle 2 in terms of the lattice basis set, can be found from $\alpha\mathbf{a} + \beta\mathbf{b} = (r_0\cos\theta_1, r_0\sin\theta_1)$. Solving for α, β, we find

$$\alpha = \frac{1}{r_1}[\cos\theta_1 - \sin\theta_1\cot(\theta_1 + \theta_3)] \quad (11)$$

$$\beta = \frac{\sin\theta_1}{2\cos\theta_3\sin(\theta_1 + \theta_3)}. \quad (12)$$

Zig-zag 2 phase (ZZ2)

The unit cell is shown in Figure 8(f). The lattice constants are $a, b = r_1$ so that $\gamma = 1$. Since ABC and ADC are identical isosceles triangles, we have

$$\cos\frac{\phi}{2} = \frac{r_1}{2r_0} \Rightarrow \phi = 2\cos^{-1}\frac{r_1}{2r_0}. \quad (13)$$

Using Eq. (13) and the fact that the unit cell area is given by $r_1^2\sin\phi = 2 \times (\frac{\sqrt{3}}{2}\ell^2)$ (there are two particles per unit cell for ZZ1), we have

$$\ell = r_1\left(\frac{\sin\phi}{\sqrt{3}}\right)^{1/2}. \quad (14)$$

r_1/r_0	Phase	η
All	HEXH	0.907
1.41	RH ($\approx$ Square)	0.785
1.5	HEXL	0.403
1.5	CH	0.555
1.5	ZZ1	0.653
1.5	ZZ2	0.704
1.618	CH	0.510
1.618	ZZ2	0.631
1.73	ZZ2 ($\approx$ Honeycomb)	0.605

TABLE I: Core area fractions η for different phases and values of $r_/r_0$.

Finally, α, β can be found from $\alpha\mathbf{a} + \beta\mathbf{b} = (r_0\cos\frac{\phi}{2}, r_0\sin\frac{\phi}{2})$. Solving for α, β, we find

$$\alpha = \beta = \left(\frac{r_0}{r_1}\right)^2. \quad (15)$$

The core area fraction $\eta = \pi r_0^2/(2\sqrt{3}\ell^2)$ for the phases above for different values of $r_/r_0$ discussed in the paper are listed in Table 1.