Lattice parameters of the four crystal phases of bowls[†]

We only give the lattice parameters at close packing, because the shape of the unit cells in all cases depends on the packing fraction in a non-analytic way.

1 Inverted crystal (IX)

The inverted crystal of bowls with thickness D and diameter σ (see Figure 1(b) of the letter) has an orthorhombic unit cell with dimensions $a = \sigma$, $b = \sqrt{3\sigma^2 - 4D^2}$, $c = D$. The positions $\mathbf{r}_i$ and direction vectors $\mathbf{u}_i$ of the particles are

$$\mathbf{r}_1 = \mathbf{0}, \qquad \mathbf{u}_1 = \mathbf{c}/c \tag{1}$$

$$\mathbf{r}_2 = \tfrac{1}{2}\mathbf{a} + \tfrac{1}{2}\mathbf{b}, \qquad \mathbf{u}_2 = -\mathbf{c}/c, \tag{2}$$

where $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ are the (perpendicular) lattice vectors of the orthorhombic unit cell.

2 IX' for $D = \sigma/2$

The IX' crystal has a hexagonal unit cell with dimensions $a = \frac{\sigma}{2}\sqrt{3}$ and $c = \sigma$. The positions and direction vectors of the particles in the IX' crystal are

$$\mathbf{r}_1 = \mathbf{0}, \qquad \mathbf{u}_1 = \mathbf{a}_1/a \tag{3}$$

$$\mathbf{r}_2 = \mathbf{a}_1, \qquad \mathbf{u}_2 = \mathbf{a}_1/a \tag{4}$$

$$\mathbf{r}_3 = \mathbf{a}_2, \qquad \mathbf{u}_3 = \mathbf{a}_1/a \tag{5}$$

$$\mathbf{r}_4 = \tfrac{1}{2}\mathbf{c}, \qquad \mathbf{u}_1 = -\mathbf{a}_4/a \tag{6}$$

$$\mathbf{r}_5 = \tfrac{1}{2}\mathbf{c} + \mathbf{a}_1, \qquad \mathbf{u}_5 = -\mathbf{a}_1/a \tag{7}$$

$$\mathbf{r}_6 = \tfrac{1}{2}\mathbf{c} + \mathbf{a}_2, \qquad \mathbf{u}_6 = -\mathbf{a}_1/a, \tag{8}$$

where $\mathbf{a}_1$ and $\mathbf{a}_2$ are two lattice vectors (with length a) in the hexagonal plane. As mentioned above, these lattice parameters are for close packing. At finite pressure, the unit cell is stretched more along the $\mathbf{a}_1$ direction than the perpendicular direction (although the difference is only around 1.5% at coexistence with the fcc[2] phase).

3 Inverted braid-like crystal (IB)

This crystal has a low-symmetry monoclinic unit cell (*i.e.* the lattice vectors obey $\mathbf{a} \cdot \mathbf{c} = 0$, $\mathbf{b} \cdot \mathbf{c} = 0$, $\mathbf{a} \cdot \mathbf{b} \neq 0$ and $|\mathbf{a}| \neq |\mathbf{b}| \neq |\mathbf{c}|$). Furthermore, the positions of the four particles in the unit cell are not described by any of the usual centerings (which are base centered or simple centering for a monoclinic unit cell). We have not been able to derive analytical expressions for the lattice parameters of this complicated crystal. Instead, we give the lattice parameters as obtained from the pressure annealing method for the three values for D where the IB phase is stable ($D/\sigma = 0.3$, 0.4 and 0.45). The lattice parameters we list below are not all independent: $\mathbf{b}/2 = (\mathbf{r}_3 - \mathbf{r}_1)^\perp = (\mathbf{r}_4 - \mathbf{r}_2)^\perp$, $\mathbf{c}/2 = (\mathbf{r}_2 - \mathbf{r}_1)^\parallel = (\mathbf{r}_4 - \mathbf{r}_3)^\parallel$, $(\mathbf{r}_2 - \mathbf{r}_1)^\perp = -(\mathbf{r}_4 - \mathbf{r}_3)^\perp$, $\mathbf{u}_2 = -\mathbf{u}_1^\perp + \mathbf{u}_1^\parallel$, $\mathbf{u}_3 = \mathbf{u}_1^\perp - \mathbf{u}_1^\parallel$ and $\mathbf{u}_4 = -\mathbf{u}_1^\perp - \pm\mathbf{u}_1^\parallel$, where $\mathbf{v}^\parallel$ and $\mathbf{v}^\perp$ are the projections of a vector $\mathbf{v}$ on $\mathbf{c}$ and the plane perpendicular to $\mathbf{c}$ respectively. We have chosen not to make use of these relations, but instead quote all lattice parameters, to allow straightforward use of the lattice parameters to construct an overlap-free initial condition. For the same reason, we quote values with considerably more precision than the statistical error. From the results of multiple pressure annealing simulations, the IB seems to be the optimum packed crystal in a whole range of similar crystal structures that differ by the "intra-braid" structure, *i.e.* $\mathbf{r}_2 - \mathbf{r}_1$ and $\mathbf{u}_1$. This means that even if the remaining independent "inter-braid" lattice parameters ($\mathbf{r}_3 - \mathbf{r}_1$ and a) could be

[†]Supporting information for *Phase behavior and structure of a new colloidal model system of bowl-shaped particles* by Matthieu Marechal, Ahmet Faik Demirörs, Arnout Imhof, Rob J. Kortschot and Marjolein Dijkstra

calculated analytically, the resulting complicated packing fraction would need to be minimized with respect to $\mathbf{r}_2 - \mathbf{r}_1$ and $\mathbf{u}_1$ to get the optimal packing IB phase. It is unlikely that this minimization can be done analytically, so there is no clear advantage of such an approach over the pressure annealing simulations.

Lattice parameters of the IB crystal for $D = 0.3\sigma$

a	1.13586197	0	-0.00003361
b	-0.72221419	1.74575009	-0.00000447
c	0	0	0.48778705

i	$\mathbf{r}_i$			$\mathbf{u}_i$		
1	0	0	0	-0.44310914	-0.20392779	0.87296492
2	0.16946163	0.08134674	0.24389181	0.44302984	0.20410954	0.87296269
3	-0.36110276	0.87287720	0.32817667	-0.44311007	-0.20392295	-0.87296558
4	-0.19163763	0.95422020	0.08428280	0.44302336	0.20407540	-0.87297396

Lattice parameters of the IB crystal for $D = 0.4\sigma$

a	1.22872695	0	0.00000422
b	-0.40560941	1.81922681	0.00000520
c	0	0	0.53502404

i	$\mathbf{r}_i$			$\mathbf{u}_i$		
1	0	0	0	-0.47929206	-0.23375651	0.84595332
2	0.29418699	0.23467723	0.26751527	0.47931080	0.23371489	0.84595420
3	-0.20280562	0.90961486	0.36260283	-0.47928418	-0.23376167	-0.84595636
4	0.09137928	1.14428875	0.09509094	0.47930254	0.23373779	-0.84595255

Lattice parameters of the IB crystal for $D = 0.45\sigma$

a	1.24543545	0	0
b	-0.22453231	1.83301385	0.00001114
c	-0.00000138	0	0.55602668

i	$\mathbf{r}_i$			$\mathbf{u}_i$		
1	0	0	0	-0.48428597	-0.21505414	0.84806770
2	0.33904189	0.31806276	0.27801634	0.48427764	0.21505358	0.84807260
3	-0.11226153	0.91650883	0.38395744	-0.48426627	-0.21506780	-0.84807548
4	0.22677388	1.23456487	0.10594466	0.48424986	0.21509406	-0.84807819

4 Paired face centered cubic crystal (fcc^2)

For completeness, we list the lattice parameters of the fcc^2 phase, which is a face centered cubic crystal of spheres that are made up of two anti-parallel hemispheres. The cubic unit cell has an edge length of $a = \sqrt{2}\sigma$ at close packing and pairs of particles are located at the centers of the

faces of this cubic unit cell:

$$\mathbf{r}_1 = \mathbf{0}, \qquad \mathbf{u}_1 = \mathbf{e}_1^R \tag{9}$$
$$\mathbf{r}_2 = \mathbf{r}_1, \qquad \mathbf{u}_2 = -\mathbf{u}_1 \tag{10}$$
$$\mathbf{r}_3 = \tfrac{1}{2}(\mathbf{a}+\mathbf{b}), \qquad \mathbf{u}_3 = \mathbf{e}_2^R \tag{11}$$
$$\mathbf{r}_4 = \mathbf{r}_3, \qquad \mathbf{u}_4 = -\mathbf{u}_3 \tag{12}$$
$$\mathbf{r}_5 = \tfrac{1}{2}(\mathbf{b}+\mathbf{c}), \qquad \mathbf{u}_5 = \mathbf{e}_3^R \tag{13}$$
$$\mathbf{r}_6 = \mathbf{r}_5, \qquad \mathbf{u}_6 = -\mathbf{u}_5 \tag{14}$$
$$\mathbf{r}_7 = \tfrac{1}{2}(\mathbf{c}+\mathbf{a}), \qquad \mathbf{u}_7 = \mathbf{e}_4^R \tag{15}$$
$$\mathbf{r}_8 = \mathbf{r}_7, \qquad \mathbf{u}_8 = -\mathbf{u}_7, \tag{16}$$

where $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ are the cubic lattice vectors with length a and $\mathbf{e}_i^R$ is a random unit vector, that is different for each pair i in the rotator crystal.