Supplementary Material: Segregation in binary mixture with differential contraction among active rings

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A - BOUNDARY CONDITIONS - REPULSIVE CIRCULAR WALLS

We configure the system as a binary mixture of N active rings confined within a circular arena of radius R_0. The force exerted by the wall on a specific particle within a ring is given by

$$\vec{F}_w = -F_w \left(\frac{|\vec{r}_{i,j} - \vec{r}_{cm}|}{R_0} - 1 \right) \frac{(\vec{r}_{i,j} - \vec{r}_{cm})}{|\vec{r}_{i,j} - \vec{r}_{cm}|} \tag{1}$$

where $\frac{(\vec{r}i,j-\vec{r}cm)}{|\vec{r}i,j-\vec{r}cm|}$ is the unit vector connecting the center of particle i within ring j to the center of mass, and F_w is the characteristic force exerted by the wall on the particle.

B - FORCES

We derive the analytical expressions for the forces acting on each particle i within a ring j. These particles are subjected to forces resulting from both shape and interaction energies, which are determined by the area, perimeter, differential line tension, particle-particle overlap, and adhesion terms as defined in the main text. The force on particle i in ring j is obtained by taking the vector derivative of the total energy E with respect to its coordinates.

$$\vec{r}_{i,j} = x_{i,j}\hat{e}_x + y_{i,j}\hat{e}_y, \tag{2}$$

$$\vec{F}_{i,j} = -\frac{\partial E}{\partial \vec{r}_{i,j}} \equiv -\frac{\partial E}{\partial x_{i,j}}\hat{e}_x - \frac{\partial E}{\partial y_{i,j}}\hat{e}_y. \tag{3}$$

Perimeter force

The perimeter energy, as defined in the main text for a configuration of N rings labeled by $j = 1, \ldots, N$, with n particles labeled $i = 1, \ldots, n$, is given by

$$E_P = \frac{\epsilon_P}{2} \sum_{j=0}^{N} \sum_{i=0}^{n} \left(\frac{|\vec{l}_{i,j}|}{l_0} - 1 \right)^2 . \tag{4}$$

The force on particle i due to deviations in the segment length $|\vec{l}_{i,j}| = |\vec{r}_{i,j} - \vec{r}_{i-1,j}|$ from its preferred value l_0 is given by

$$\vec{F}_P^{i,j} = -\frac{\partial E_P}{\partial \vec{r}_{i,j}} = -\frac{\partial E_P}{\partial x_{i,j}}\hat{e}_x - \frac{\partial E_P}{\partial y_{i,j}}\hat{e}_y, \tag{5}$$

$$\vec{F}_P^{i,j} = -\frac{\epsilon_P}{l_0} \left[\left(\frac{|\vec{l}_{i,j}|}{l_0} - 1 \right) \frac{\partial |\vec{l}_{i,j}|}{\partial \vec{r}_{i,j}} - \left(\frac{|\vec{l}_{i+1,j}|}{l_0} - 1 \right) \frac{\partial |\vec{l}_{i+1,j}|}{\partial \vec{r}_{i+1,j}} \right], \tag{6}$$

$$\vec{F}_P^{i,j} = \frac{\epsilon_P}{l_0} \left[\left(\frac{|\vec{l}_{i+1,j}|}{l_0} - 1 \right) \frac{\vec{l}_{i+1,j}}{|\vec{l}_{i+1,j}|} - \left(\frac{|\vec{l}_{i,j}|}{l_0} - 1 \right) \frac{\vec{l}_{i,j}}{|\vec{l}_{i,j}|} \right], \tag{7}$$

where we use the following relations:

$$\frac{\partial|\vec{l}_{i,j}|}{\partial\vec{r}_{i,j}} = \frac{\partial|\vec{l}_{i,j}|}{\partial x_{i,j}}\hat{e}_x + \frac{\partial|\vec{l}_{i,j}|}{\partial y_{i,j}}\hat{e}_y = -\frac{\vec{l}_{i,j}}{|\vec{l}_{i,j}|}, \tag{8}$$

$$\frac{\partial|\vec{l}_{i+1,j}|}{\partial\vec{r}_{i+1,j}} = \frac{\partial|\vec{l}_{i+1,j}|}{\partial x_{i+1,j}}\hat{e}_x + \frac{\partial|\vec{l}_{i+1,j}|}{\partial y_{i+1,j}}\hat{e}_y = \frac{\vec{l}_{i+1,j}}{|\vec{l}_{i+1,j}|}. \tag{9}$$

Area force

The force related to area energy on particle i in ring j is given by

$$\vec{F}_A^{i,j} = -\frac{\partial E_A}{\partial\vec{r}_{i,j}} = -\frac{\epsilon_A}{A_0}\left(\frac{A_j}{A_0} - 1\right)\frac{\partial A_j}{\partial\vec{r}_{i,j}}, \tag{10}$$

being E_A the area energy defined by

$$E_A = \frac{\epsilon_A}{2}\sum_{j=0}^{N}\left(\frac{A_j}{A_0} - 1\right)^2. \tag{11}$$

The ring area A_j is calculated using the vector product property, given by

$$A_j = \frac{1}{2}\sum_{j}^{n}|(\vec{r}_{i,j} - \vec{r}_{cm}) \times \vec{l}_{i,j}| = \frac{1}{2}\sum_{j}^{n}(x_{i,j} - x_{cm})(y_{i,j} - y_{i-1,j}) - (y_{i,j} - y_{cm})(x_{i,j} - x_{i-1,j}), \tag{12}$$

where the factor 1/2 is included to avoid double-counting the area. Therefore, we obtain:

$$\frac{\partial A_j}{\partial x_{i,j}} = \frac{(y_{i+1,j} - y_{i-1,j})}{2}, \tag{13}$$

$$\frac{\partial A_j}{\partial y_{i,j}} = \frac{(x_{i-1,j} - x_{i+1,j})}{2}, \tag{14}$$

thus,

$$\vec{F}_A^{i,j} = -\frac{\partial E_A}{\partial\vec{r}_{i,j}} = -\frac{\epsilon_A}{2A_0}\left(\frac{A_j}{A_0} - 1\right)\left[(x_{i+1,j} - x_{i-1,j})\,\hat{e}_x - (y_{i+1,j} - y_{i-1,j})\,\hat{e}_y\right]. \tag{15}$$

Interaction forces

The core repulsion for non-neighboring particles within the same ring and the adhesion between particles of different rings are accounted for by the interaction energy E_{int}, which is described by a truncated harmonic potential,

$$E_{int} = \begin{cases} \frac{\epsilon_c}{2}\left(\frac{r_{ik}}{\sigma} - 1\right)^2, & r_{ik} \leq \sigma \\ \frac{\epsilon_{adh}}{2}\left(\frac{r_{ik}}{\sigma} - 1\right)^2, & l_{adh} \geq r_{ik} > \sigma \\ 0, & r_{ik} > l_{adh}. \end{cases} \tag{16}$$

Therefore, the corresponding force

$$\vec{F}^{i,j}_{int} = -\frac{\partial E_{int}}{\partial \vec{r}_{i,j}}, \tag{17}$$

$$\vec{F}^{i,j}_{int} = \hat{r}_{ik} \begin{cases} -\frac{\epsilon_c}{\sigma}\left(\frac{r_{ik}}{\sigma} - 1\right), & r_{ik} \leq \sigma \\ -\frac{\epsilon_{adh}}{\sigma}\left(\frac{r_{ik}}{\sigma} - 1\right), & l_{adh} \geq r_{ik} > \sigma \\ 0, & r_{ik} > l_{adh} \end{cases} \tag{18}$$

where $\hat{r}_{ik} = \frac{\vec{r}_{ik}}{r_{ik}}$ is a unit vector connecting particle i and k.

Differential line tension (contraction)

The contraction energy represents a line tension that acts between two particles from different rings when they are within a distance cutoff l_Λ. This energy term is given by

$$E_\Lambda = \sum_{j=0}^{N}\sum_{i=0}^{n} \Lambda_{\alpha\beta}|\vec{l}_{i,j}|. \tag{19}$$

The force acting on particle i inside ring j is

$$\vec{F}^{i,j}_{\Lambda} = -\frac{\partial E_\Lambda}{\partial \vec{r}_{i,j}}, \tag{20}$$

$$\vec{F}^{i,j}_{\Lambda} = \Lambda_{\alpha\beta}\left[\frac{\vec{l}_{i+1,j}}{|\vec{l}_{i+1,j}|} - \frac{\vec{l}_{i,j}}{|\vec{l}_{i,j}|}\right]. \tag{21}$$

Therefore, the force $\vec{F}^{i,j}_{\Lambda}$ on particle i within ring j depends on the type α of its ring and the type β of the ring of the particle it interacts with. If the particle is within the cutoff distance and interacts with multiple particles from other rings, the tension value will be the mean of all the individual tensions. Specifically, this mean is given by

$$\Lambda_{\alpha\beta} = \frac{1}{n_c}\sum_k \Lambda_{\alpha k}, \tag{22}$$

where the sum k runs over all contacts (both $\alpha - \alpha$ and $\alpha - \beta$ interactions) and n_c represents the total number of contacts.

C - CONTROL PARAMETERS

The value of the total equilibrium area A_r is the sum of the equilibrium area imposed by the area elastic energy term plus half the area of each particle composing the ring,

$$A_r = A_0 + \frac{n\pi\sigma^2}{8}. \tag{23}$$

We define a packing fraction ϕ for the system, relative to a circular region of radius R_0, through the relation

$$\phi = \frac{NA_r}{\pi R_0^2}. \tag{24}$$

We fix $\phi = 0.895$ allowing for neighbor exchange and neighbor interaction simultaneously and we use a fixed dimensionless perimeter-area equilibrium ratio $p_0 = P_0/\sqrt{A_0} = 4$, where $P_0 = nl_0$ is the equilibrium perimeter. The shape parameter p_0 defines the degree of stiffness of the ring. The choice of this value is based on previous works with Vertex

[? ? ?], Voronoi [?], and ring models [?], where an excess of cell perimeter is found for $p_0 > 3.81$ as well as the emergence of a liquid-like behavior. To prevent overlap among rings, we reached a compromise by setting comparable values for ϵ_c, ϵ_P and ϵ_A/n, while assigning a much lower value to ϵ_{adh}. So, we simulate the ring system keeping the following parameters fixed: $\epsilon_c/\epsilon_P = 1$, $\epsilon_A/\epsilon_P = 35$, $(F_w\sigma)/\epsilon_P = 1$, $\epsilon_{adh}/\epsilon_P = 5.10^{-4}$, $n = 10$, $l_0 = 1$, $\sigma = l_0$, $l_\Lambda = l_{adh} = 1.5\, l_0$ and $\mu = 1$. This choice of parameters ensures that ϵ_P and ϵ_A are sufficiently large to maintain the bond length close to l_0 and the equilibrium area close to A_0. The adhesion forces between different rings are kept equal for all rings. Furthermore, to emphasize the effects of differential contractions, we adopted an adhesion value that is considerably lower compared to the other energy terms involved. We integrate the equations of motion, using the Euler-Maruyama algorithm with a time step $\Delta t = 0.01$.

D - Neighbors criterion for measurements

In this work, we use the criterion for defining whether two rings are neighbors based on the distance between their centers of mass, $d_{jk} = |\vec{R}_j - \vec{R}_k| \leq \frac{P_0}{2} = 5\sigma$. This relation ensures that even two completely flattened rings in contact will be considered neighbors.

VIDEOS CAPTIONS

- Video 1: Simulation of a binary mixture of rings with differential membrane contraction. Time is in log scale. Set parameters: $N = 1000$, $Pe = 0.3$, $\Lambda = 0.1$ and Ring type ratio: (30:70). → Fig 2a
- Video 2: Simulation of a binary mixture of rings with differential membrane contraction. Time is in log scale. Set parameters: $N = 1000$, $Pe = 0.3$, $\Lambda = 1.5$ and Ring type ratio: (30:70). → Fig 2a
- Video 3: Simulation of a binary mixture of rings with differential membrane contraction. Time is in log scale. Set parameters: $N = 1000$, $Pe = 0.3$, $\Lambda = 10$ and Ring type ratio: (30:70). → Fig 2a
- Video 4: Simulation of a binary mixture of rings with differential membrane contraction. Time is in log scale. Set parameters: $N = 10000$, $Pe = 0.4$, $\Lambda = 10$ and Ring type ratio: (10:90). → Fig 4c-d
- Video 5: Simulation of a binary mixture of rings with differential membrane contraction. Time is in log scale. Set parameters: $N = 10000$, $Pe = 0.4$, $\Lambda = 10$ and Ring type ratio: (30:70). → Fig 4
- Video 6: Simulation of a binary mixture of rings with differential membrane contraction. Time is in log scale. Set parameters: $N = 10000$, $Pe = 0.4$, $\Lambda = 10$ and Ring type ratio: (50:50). → Fig 4c-d