<u>Supplementary Information</u>

In-Situ Temperature-Controllable Shear Flow Device for Neutron Diffraction or SANS Measurement – An Example of Aligned Bicellar Mixtures (Derivation of Sample Transmissivity)

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The rocking curve [obtained as a scattering intensity detected at the fixed detector angle $2\theta_B$ that satisfies the Bragg condition while sample angle θ varies around θ_B] is presumably symmetric with respect to $\theta=\theta_B$. Therefore, the correction factors are derived only for half of the rocking curve (i.e. $\theta > \theta_B$) which can be directly applied to the other half at the corresponding angles (i.e., $\theta_B - \theta$).

We define x and y according to the sample coordinates, i.e., along the sample thickness (gap) and width, respectively (Fig. S1 – the top view of the sample). As θ varies, the incident and diffracted beam can enter and exit through different sides of the sample, leading to different calculation of the path length, L. We define the surface of sample width closest to the source to be "1" as shown in Fig. S1. Then surfaces 2, 3, and 4 are defined following the counter-clockwise direction.

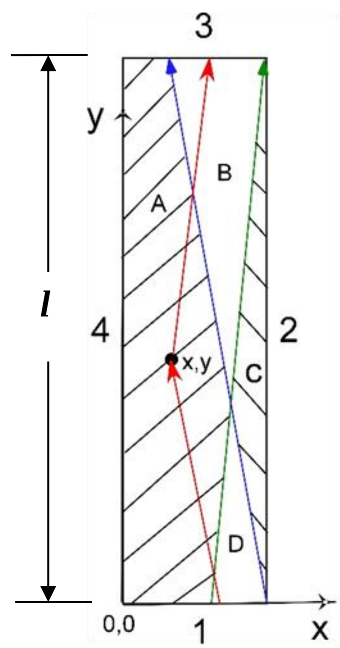

Figure S1 Scattering scheme in the case $\theta_B \leq \theta < 2\theta_B$

The calculation of L will be derived in 5 different angular considerations of θ, namely, $\theta_B \leq \theta < 2\theta_B$, $\theta = 2\theta_B$, $2\theta_B < \theta < \theta'$, $\theta' \leq \theta < \theta''$, and $\theta > \theta''$, where θ' and θ'' will be defined later in the following sections. It should be noted that all incident paths are assumed to be parallel and so are the diffracted paths due to small thickness of the sample.

1. $\theta_B \leq \theta < 2\theta_B$

In this case, the entrance surfaces can be either 1 or 2, while the exit surfaces can be 2 or 3. As a result, L in the four regions of A, B, C, and D as shown in Fig S1, and identified by 'entrance surface → exit surface' nomenclature as '1→3', '2→3', '2→2' and '1→2', respectively, should be calculated differently.

a) In region A (1→3), L for a scatterer at location (x,y) can be calculated via Eq (S1) as indicated by the red line in Fig. S1.

$$L_A(x,y) = \frac{y}{\cos(\theta)} + \frac{l-y}{\cos(2\theta_B-\theta)}, \tag{S1}$$

where l is the width of the sample. The integration of $(\frac{I}{I_0})$ over region A should be separated into two parts through the line $y = \frac{l*\cot(\theta)}{\cot(\theta)+\cot(2\theta_B-\theta)}$ (the intersection point of incident beam and the diffracted beam). Therefore, the integration of the transmissivity with respect to the scattering volume at region A is

$$\frac{I}{I_{0A}}(\theta) = \int_{\frac{l*\cot(\theta)}{\cot(\theta)+\cot(2\theta_B-\theta)}}^{l} \int_0^{w'-\frac{y}{\cot(\theta)}} exp - [\mu k(\frac{y}{\cos(\theta)} + \frac{l-y}{\cos(2\theta_B-\theta)})]dxdy + \int_0^{\frac{l*\cot(\theta)}{\cot(\theta)+\cot(2\theta_B-\theta)}} \int_0^{\frac{y-l}{\cot(2\theta_B)}+w'} \exp[-\mu k\left(\frac{y}{\cos(\theta)} + \frac{l-y}{\cos(2\theta_B-\theta)}\right)]\, dxdy, \tag{S2}$$

where w' is the total thickness of the sample, i.e., the length of surface 1 or 3.

b) The path length in region B (2→3) can be expressed as

$$L_B(x,y) = \frac{w'-x}{\sin(\theta)} + \frac{l-y}{\cos(2\theta_B-\theta)}, \tag{S3}$$

and the integrated transmitted intensity is

$$\frac{I}{I_{0B}}(\theta) = \int_{\frac{l*\cot(\theta)}{\cot(\theta)+\cot(2\theta_B-\theta)}}^{l} \int_{w'-y/\cot(\theta)}^{\frac{y-l}{\cot(2\theta_B-\theta)}+w'} \exp[-\mu k\left(\frac{w'-x}{\sin(\theta)} + \frac{l-y}{\cos(2\theta_B-\theta)}\right)]dxdy, \tag{S4}$$

c) The path length in region C (2→2) can be expressed as

$$L_C(x,y) = \frac{w'-x}{\sin(\theta)} + \frac{w'-x}{\sin(2\theta_B-\theta)}, \tag{S5}$$

and the integrated transmissivity is

$$\frac{I}{I_{0C}}(\theta) = \int_{w'-\frac{l}{\cot(\theta)+\cot(2\theta_B-\theta)}}^{w'} \int_{(w'-x)*\cot(\theta)}^{l+(x-w')*\cot(2\theta_B-\theta)} \exp[-\mu k(\frac{w'-x}{\sin(\theta)} + \frac{w'-x}{\sin(2\theta_B-\theta)})]\, dxdy, \tag{S6}$$

d) The path length in region D (1→2) is

$$L_D(x,y) = \frac{y}{\cos(\theta)} + \frac{w'-x}{\sin(2\theta_B-\theta)}, \quad \text{(S7)}$$

and the integrated transmissivity is

$$\frac{I}{I_0}_D(\theta) = \int_0^{\frac{l*\cot(\theta)}{\cot(\theta)+\cot(2\theta_B-\theta)}} \int_{\frac{y-l}{\cot(2\theta_B-\theta)}+w'}^{w'-\frac{y}{\cot(\theta)}} \exp[-\mu k(\frac{y}{\cos(\theta)} + \frac{w'-x}{\sin(2\theta_B-\theta)})]\, dxdy, \quad \text{(S8)}$$

As a result, the average transmitted intensity normalized by the total area is

$$\frac{I}{I_0}_{ave} = \frac{\frac{I}{I_0}_A(\theta)+\frac{I}{I_0}_B(\theta)+\frac{I}{I_0}_C(\theta)+\frac{I}{I_0}_D(\theta)}{w'l}, \quad \text{(S9)}$$

2. $\theta = 2\theta_B$

As $\theta = 2\theta_B$, y-axis is parallel with the sample-to-detector line. The entrance surfaces can be 1 or 2 but exit surface can only be 3. Thus only two regions need to be considered in order to calculate L (Fig. S2). In region A (1 → 3), L can be calculated from

$$L_A(x,y) = \frac{y}{\cos(\theta)} + l - y, \quad \text{(S10)}$$

and the integrated transmissivity is

$$\frac{I}{I_0}_A(\theta) = \int_0^l \int_0^{w'-\frac{y}{\cot(\theta)}} \exp[-\mu k(\frac{y}{\cos(\theta)} + l - y)]dxdy \quad \text{(S11)}$$

In region B (2→3), L can be obtained from

$$L_B(x,y) = \frac{w'-x}{\sin(\theta)} + l - y, \quad \text{(S12)}$$

and the integrated transmitted intensity is

$$\frac{I}{I_0}_B(\theta) = \int_0^l \int_{w'-\frac{y}{\cot(\theta)}}^{w'} \exp[-\mu k(\frac{w'-x}{\sin(\theta)} + l - y)]\, dxdy, \quad \text{(S13)}$$

Finally, the average transmissivity can be obtained through

$$\frac{I}{I_0}_{ave} = \frac{\frac{I}{I_0}_A(\theta)+\frac{I}{I_0}_B(\theta)}{w'l}, \quad \text{(S14)}$$

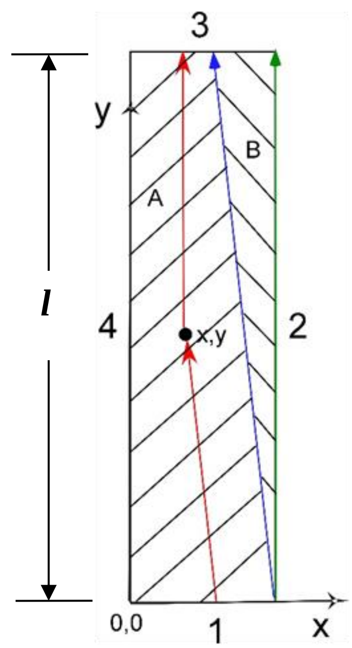

Figure S2 Scattering scheme in the case of $\theta=2\theta_B$

3. $2\theta_B < \theta \leq \theta'$

New formula for calculating transmissivity are derived as the θ rotates from $2\theta_B$ to θ', which is defined as the angle of the sample at which its diagonal line is parallel with the incident beam. The possible combinations of entrance and exit surfaces are '1→4', '1→3', and '2→3' combinations, resulting in three different regions: A, B, and C, respectively as shown in Fig. S3.

In region A (1→4), L is calculated as

$$L_A(x,y) = \frac{y}{\cos(\theta)} + \frac{x}{\sin(\theta-2\theta_B)}, \tag{S15}$$

and the integrated transmissivity is

$$\frac{I}{I_0}_A(\theta) = \int_0^l \int_0^{\frac{l-y}{\cot(\theta-2\theta_B)}} \exp[-\mu k(\frac{y}{\cos(\theta)} + \frac{x}{\sin(\theta-2\theta_B)})]dxdy. \tag{S16}$$

In region B (1→3), L and the integrated transmissivity are calculated as

$$L_B(x,y) = \frac{l-y}{\cot(\theta-2\theta_B)} + \frac{y}{\cos(\theta)}, \tag{S17}$$

$$\frac{I}{I_0}_B(\theta) = \int_0^l \int_{\frac{l-y}{\cot(\theta-2\theta_B)}}^{w'-\frac{y}{\cot(\theta)}} \exp[-\mu k(\frac{l-y}{\cot(\theta-2\theta_B)} + \frac{y}{\cos(\theta)})]dxdy. \tag{S18}$$

In region C (2→3),

$$L_C(x,y) = \frac{w'-x}{\sin(\theta)} + \frac{y}{\cos(\theta-2\theta_B)}, \tag{S19}$$

$$\frac{I}{I_0}_C(\theta) = \int_0^l \int_{w'-\frac{y}{\cot(\theta)}}^{w'} \exp[-\mu k(\frac{w'-x}{\sin(\theta)} + \frac{y}{\cos(\theta-2\theta_B)})]. \tag{S20}$$

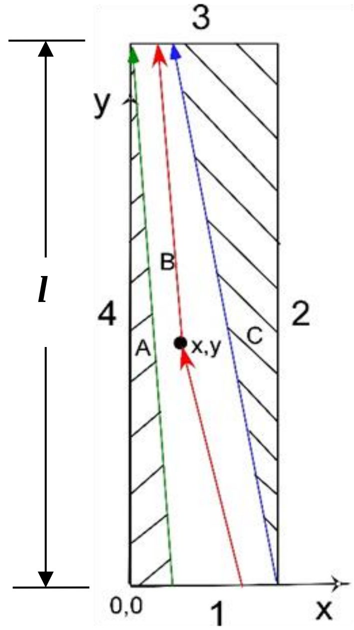

Figure S3 Scattering scheme in the case of $2\theta_B < \theta < \theta'$

The final average transmissivity in this case is

$$\frac{I}{I_0}_{ave} = \frac{\frac{I}{I_0}_A(\theta) + \frac{I}{I_0}_B(\theta) + \frac{I}{I_0}_C(\theta)}{A}. \tag{S21}$$

4. $\theta' < \theta \leq \theta'$

Another special angle, θ'' is defined as the sample diagonal line being parallel with the diffracted beam (Fig. S4). In this case, the scattering volume is divided into 4 regions. A, B, C, and D corresponding to '1→4', '1→3', '2→3', and '2→4', respectively.

In region A (1→4), L_A(x,y) can be expressed as Eq. (S15) while the integrated transmissivity is described as

$$\frac{I}{I_0}_A(\theta) = \int_{\frac{w'*\cot(\theta)*\cot(\theta-2\theta_B)-l*\cot(\theta)}{\cot(\theta-2\theta_B)-\cot(\theta)}}^{w'*\cot(\theta)} \int_0^{w'-\frac{y}{\cot(\theta)}} \exp[-\mu k\left(\frac{y}{\cos(\theta)} + \frac{x}{\sin(\theta-2\theta_B)}\right)]dxdy + \int_0^{\frac{w'*\cot(\theta)*\cot(\theta-2\theta_B)-l*\cot(\theta)}{\cot(\theta-2\theta_B)-\cot(\theta)}} \int_0^{\frac{l-y}{\cot(\theta-2\theta_B)}} \frac{y}{\cos(\theta)} + \frac{x}{\sin(\theta-2\theta_B)} dxdy, \tag{S22}$$

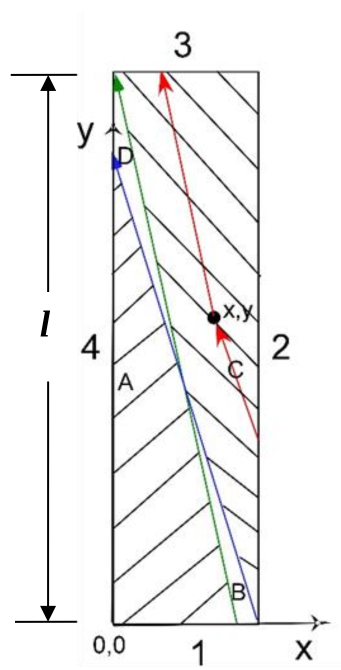

Figure S4 Scattering scheme in the case of $\theta' < \theta < \theta''$

In region B (1→3), L_B(x,y) can be expressed as Eq. (S17) and the integrated transmitted intensity is

$$\frac{I}{I_{0_B}}(\theta) = \int_{\frac{l-y}{\cot(\theta-2\theta_B)}}^{w'-\frac{y}{\cot(\theta)}} \int_0^{\frac{w'*\cot(\theta)*\cot(\theta-2\theta_B)-l*\cot(\theta)}{\cot(\theta-2\theta_B)-\cot(\theta)}} \exp[-\mu k(\frac{y}{\cos(\theta)} + \frac{l-y}{\cos(\theta-2\theta_B)})]\, dxdy. \quad \text{(S23)}$$

In region C (2→3), L_C(x,y) can be expressed as Eq. (S19) and the integrated transmitted intensity is

$$\frac{I}{I_{0_C}}(\theta) = \int_{\frac{w'*\cot(\theta)*\cot(\theta-2\theta_B)-l*\cot(\theta)}{\cot(\theta-2\theta_B)-\cot(\theta)}}^{l} \int_{\frac{l-y}{\cot(\theta-2\theta_B)}}^{w'} \exp[-\mu k(\frac{w'-x}{\sin(\theta)} + \frac{l-y}{\cos(\theta-2\theta_B)})]\, dxdy + \int_0^{\frac{w'*\cot(\theta)*\cot(\theta-2\theta_B)-l*\cot(\theta)}{\cot(\theta-2\theta_B)-\cot(\theta)}} \int_{w'-\frac{y}{\cot(\theta)}}^{w'} \exp\left[-\mu k\left(\frac{w'-x}{\sin(\theta)} + \frac{l-y}{\cos(\theta-2\theta_B)}\right)\right] dxdy. \quad \text{(S24)}$$

In region D (2→4),

$$L_D(x,y) = \frac{w'-x}{\sin(\theta)} + \frac{x}{\sin(\theta-2\theta_B)}, \quad \text{(S25)}$$

and

$$\frac{I}{I_{0_D}}(\theta) = \int_{(w'-x)*\cot(\theta)}^{l-x*\cot(\theta-2\theta_B)} \int_0^{\frac{l-w'*\cot(\theta)}{\cot(\theta-2\theta_B)-\cot(\theta)}} \exp[-\mu k(\frac{w'-x}{\sin(\theta)} + \frac{x}{\sin(\theta-2\theta_B)})]\, dxdy, \quad \text{(S26)}$$

Therefore, the average transmitted intensity is

$$\frac{I}{I_{0_{ave}}} = \frac{\frac{I}{I_{0_A}}(\theta)+\frac{I}{I_{0_B}}(\theta)+\frac{I}{I_{0_C}}(\theta)+\frac{I}{I_{0_D}}(\theta)}{A}. \quad \text{(S27)}$$

5. $\theta \geq \theta'$

As the sample angle $\theta \geq \theta''$, the scattering volume can be divided into three regions A, B, and C corresponding to the '1→4', '2→4' and '2→3' combinations, respectively (Fig. S5).

In region A (1→4), L_A(x,y) can be calculated from Eq. (S15) and

$$\frac{I}{I_{0_A}}(\theta) = \int_0^{w'} \int_0^{(w'-x)*\cot(\theta)} \exp[-\mu k(\frac{y}{\cos(\theta)} + \frac{x}{\sin(\theta-2\theta_B)})]dxdy, \quad \text{(S28)}$$

In region B (2→4), $L_{\boldsymbol{B}}$(x,y) can be calculated by Eq (S25), the same as region D in the previous section and

$$\frac{I}{I_{0_B}}(\theta) = \int_0^{w'} \int_{(w'-x)*\cot(\theta)}^{l-x*\cot(\theta-2\theta_B)} \exp[-\mu k(\frac{w'-x}{\sin(\theta)} + \frac{x}{\sin(\theta-2\theta_B)})]\, dxdy, \qquad \text{(S29)}$$

In region C (2→3), $L_{\boldsymbol{C}}$(x,y) can be calculated by Eq (S19) and

$$\frac{I}{I_{0_C}}(\theta) = \int_0^{w'} \int_{l-x*\cot(\theta-2\theta_B)}^{l} \exp[-\mu k(\frac{w'-x}{\sin(\theta)} + \frac{l-y}{\cos(\theta-2\theta_B)})]\, dxdy, \quad \text{(S30)}$$

Therefore, the final average transmissivity is

$$\frac{I}{I_{o_{ave}}} = \frac{\frac{I}{I_{0_A}}(\theta)+\frac{I}{I_{0_B}}(\theta)+\frac{I}{I_{0_C}}(\theta)}{A}. \qquad \text{(S31)}$$

It should be noted that all the above mathematical calculations have been derived based on the assumption that the whole sample area is within the scattering volume (i.e., the cross-section area of beam width and detector width is larger than the sample area at all considered angles). However, the derivation can be extended to the sample area protruding from the scattering volume. The solutions will become more complicated in that case as more scenarios will have to be included.

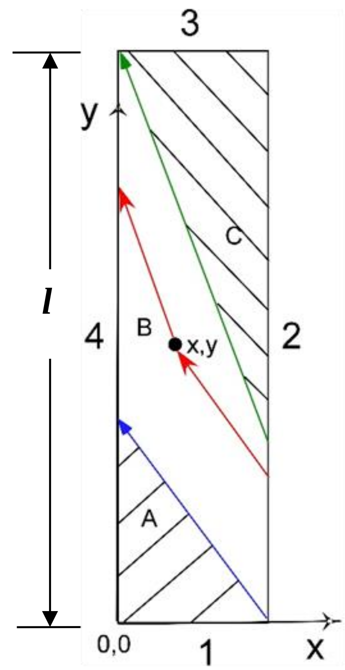

Figure S5 Scattering scheme in the case of $\theta > \theta''$