

Dilution of contact frequency between superenhancers by loop extrusion at interfaces

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S1 Free energy of loop extruding polymer brush

S1.1 Short time scale

We treat chromatin as a polymer brush end-grafted to a surface with grafting density σ in an aqueous solution at a physiological salt concentration. The electric charges of chromatin are screened by salt ions in the solution. Each chain is much longer than the Kuhn length and thus is treated as a flexible chain composed of N Kuhn segments of length l_a . Cohesin is loaded at the grafted ends of the chains and extrudes these chains with a constant rate τ_s^{-1} .

Cohesin divides the chain into the loop subchain, which has been extruded, and the arm subchain, which has not been extruded, see fig. 1 in the main article. For short enough times, $t < t_{th}$, the height of the arm subchain is larger than the height of the loop subchain. A part of the arm subchain occupies the top layer above the loop subchain and the rest of the arm subchain coexists with the loop subchain in the bottom layer. We assume that the loop subchain, the arm subchain in the bottom layer, and the arm subchain in the top layer are composed of blobs of size R_{lp} , R_b , and R_t , each containing g_{lp} , g_b , and g_t Kuhn segments, respectively. Here and after, we use the subscripts 'lp', 't', and 'b' to represent the loop subchain in the bottom layer, the subchain in the top layer, and the arm subchain in the bottom layer. The free energy of each blob has the form

$$\frac{f_{lp}}{k_B T} = \frac{3}{2} \frac{R_{lp}^2}{g_{lp} l_a^2} + v g_{lp} \frac{g_{lp}}{R_{lp}^3} \quad (S1)$$

$$\frac{f_t}{k_B T} = \frac{3}{2} \frac{R_t^2}{g_t l_a^2} + v g_t \frac{g_t}{R_t^3} \quad (S2)$$

$$\frac{f_b}{k_B T} = \frac{3}{2} \frac{R_b^2}{g_b l_a^2} + v g_b \frac{g_b}{R_b^3}. \quad (S3)$$

The free energy per chain thus has the form

$$\frac{F}{k_B T} = \frac{N_{lp}}{g_{lp}} \left(\frac{3}{2} \frac{R_{lp}^2}{g_{lp} l_a^2} + v g_{lp} \frac{g_{lp}}{R_{lp}^3} \right)$$

$$\begin{aligned}
& + \frac{N_t}{g_t} \left(\frac{3}{2} \frac{R_t^2}{g_t l_a^2} + v g_t \frac{g_t}{R_t^3} \right) \\
& + \frac{N_b}{g_b} \left(\frac{3}{2} \frac{R_b^2}{g_b l_a^2} + v g_b \frac{g_b}{R_b^3} \right)
\end{aligned} \tag{S4}$$

where N_{lp} is the number of Kuhn segments of the loop subchain, N_t is the number of Kuhn segments of the arm subchain in the top layer, and N_b is the number of Kuhn segments of the arm subchain in the bottom layer.

The heights of the top layer and the bottom layer have the forms

$$h_t = R_t \frac{N_t}{g_t} \tag{S5}$$

$$h_b = R_b \frac{N_b}{g_b} = R_{lp} \frac{N_{lp}}{2g_{lp}}. \tag{S6}$$

For simplicity, we here treat a loop as two subchains that are connected at the top. This is taken into account by the factor 2 in the denominator of the rightmost term of eq. (S6). The size of the blobs is determined by the area per subchains [1] and this leads to the forms

$$\sigma_{lp} = R_{lp}^{-2} \tag{S7}$$

$$\sigma_b = R_b^{-2} \tag{S8}$$

$$\sigma_t = R_t^{-2}, \tag{S9}$$

where σ_{lp} is the surface density of loop subchains, σ_b is the surface density of arm subchains at the bottom layer, and σ_t is the surface density of arm subchains at the top layer. The surface densities, σ_{lp} , σ_b , and σ_t , are related by

$$\frac{1}{\sigma} = \frac{1}{\sigma_t} = \frac{2}{\sigma_{lp}} + \frac{1}{\sigma_b} \tag{S10}$$

to the grafting density σ of the chain.

Substituting eqs. (S5) - (S9) into eq. (S4) leads to

$$F = F_{lp} + F_{arm}, \tag{S11}$$

where the free energy (per chain) F_{lp} of the loop subchain and the free energy (per chain) F_{arm} of the arm subchain have the forms

$$\frac{F_{lp}}{k_B T} = \frac{3}{2} \frac{4h_{lp}^2}{N_{lp} l_a^2} + \frac{1}{2} v \frac{\sigma_{lp} N_{lp}^2}{h_{lp}} \tag{S12}$$

$$\frac{F_{arm}}{k_B T} = \frac{3}{2} \frac{h_b^2}{N_b l_a^2} + v \frac{\sigma_b N_b^2}{h_b} + \frac{3}{2} \frac{h_t^2}{N_t l_a^2} + v \frac{\sigma_t N_t^2}{h_t}. \tag{S13}$$

Substituting eqs. (10) and (11) in the main article into eqs. (S12) and (S13) leads to eqs. (5) and (6) in the main article. The first term of eq. (S12) accounts for the fact that the loop is composed of two subchains of length $N_{lp}/2$.

S1.2 Longer time scale

For longer time scales, $t_{\text{th}} < t < \tau_{\text{ex}}$, the height of the loop subchain is larger than the height of the arm subchain. The top layer is thus occupied by a part of the loop subchain. The rest of the loop subchain and the arm subchain coexist in the bottom layer. Eq. (S4) is still applicable to this time scale because it just represents the fact that the free energy per chain is the free energy of each blob multiplied by the number of blobs. The only difference between this time regime and the short time regime is the fact that the blobs in the top layer are those of the loop subchain.

The heights of the top and bottom layers have the forms

$$h_t = \frac{N_t}{2g_t} R_t \quad (\text{S14})$$

$$h_b = \frac{N_b}{g_b} R_b = \frac{N_{\text{lp}}}{2g_{\text{lp}}} R_{\text{lp}}. \quad (\text{S15})$$

The fact that the size of each type of blob is determined by the area per subchain leads to the forms

$$\sigma_b = R_b^{-2} \quad (\text{S16})$$

$$\sigma_{\text{lp}} = R_{\text{lp}}^{-2} \quad (\text{S17})$$

$$\sigma_t = R_t^{-2}. \quad (\text{S18})$$

The surface densities, σ_b , σ_{lp} , and σ_t , obey the relationship

$$\frac{1}{\sigma} = \frac{2}{\sigma_t} = \frac{2}{\sigma_{\text{lp}}} + \frac{1}{\sigma_b}. \quad (\text{S19})$$

Substituting eqs. (S14) to (S18) into eq. (S4) leads to the form

$$F = F_{\text{lp}} + F_{\text{arm}}, \quad (\text{S20})$$

where the free energy (per chain) F_{lp} of the loop subchain and the free energy (per chain) F_{arm} of the arm subchain have the forms

$$\frac{F_{\text{lp}}}{k_{\text{B}}T} = \frac{3}{2} \frac{4h_{\text{lp}}^2}{N_{\text{lp}}l_{\text{a}}^2} + v \frac{\sigma_{\text{lp}}N_{\text{lp}}^2}{2h_{\text{lp}}} + \frac{3}{2} \frac{4h_t^2}{N_t l_{\text{a}}^2} + v \frac{\sigma_t N_t^2}{2h_t} \quad (\text{S21})$$

$$\frac{F_{\text{arm}}}{k_{\text{B}}T} = \frac{3}{2} \frac{h_b^2}{N_b l_{\text{a}}^2} + v \frac{\sigma_b N_b^2}{h_b}. \quad (\text{S22})$$

Substituting eqs. (10) and (11) in the main article into eqs. (S21) and (S22) leads to eqs. (14) and (15) in the main article.

S2 Dynamics of Alexander brush predicted by Onsager's principle

Here we use Onsager's principle to analyze the dynamics of a polymer brush. In the brush, flexible chains, each composed of N Kuhn segments of length l_{a} , are

end-grafted to a surface with grafting density σ . Onsager's principle predicts that the time evolution equation is derived by minimizing the Rayleighian

$$\mathcal{R} = \Phi + \dot{F}, \quad (\text{S23})$$

where Φ is the dissipation function and \dot{F} is the time derivative of the free energy F [3]. We use the Alexander approximation, which assumes that the concentration of chain segments in the brush is uniform [1, 2]. The dissipation function of the brush has the form

$$\Phi = \frac{1}{2} N \zeta \dot{h}^2(t), \quad (\text{S24})$$

where \dot{h} is the time derivative of the brush height h and ζ is the friction constant per Kuhn segment. The free energy of the Alexander brush has the form [1, 2]

$$F = \frac{3}{2} \frac{k_B T}{N l_a^2} h^2(t) + k_B T v \frac{\sigma N^2}{h(t)}. \quad (\text{S25})$$

With eqs. (S24) and (S25), we find for the Rayleighian

$$\begin{aligned} \mathcal{R} &= \frac{1}{2} N \zeta \dot{h}^2(t) + \left[\frac{3 k_B T}{N l_a^2} h(t) - k_B T v \frac{\sigma N^2}{h^2(t)} \right] \dot{h}(t) \\ &+ \left[-\frac{3}{2} \frac{k_B T}{N^2 l_a^2} h^2(t) + 2 k_B T v \frac{\sigma N}{h(t)} \right] \dot{N}(t). \end{aligned} \quad (\text{S26})$$

The last term of eq. (S26) is zero for the (usual) case in which the number N of Kuhn segments in each chain is constant. Minimizing the Rayleighian, eq. (S26), with respect to the velocity of the brush top \dot{h} leads to the equation

$$\frac{d}{dt} h(t) = -\frac{3 k_B T}{N^2 \zeta l_a^2} \left[h(t) - \frac{v \sigma N^3 l_a^2}{3} \frac{1}{h^2(t)} \right]. \quad (\text{S27})$$

For the case in which N is a constant N_0 , eq. (S27) can be rewritten in the form

$$\frac{d}{dt} h(t) = -\frac{1}{\tau_{N_0}} \left[h(t) - \frac{h_{\text{Alx}}^3}{h^2(t)} \right], \quad (\text{S28})$$

where τ_{N_0} denotes the longest relaxation time of the chain (Rouse time) given by

$$\tau_{N_0} = \frac{N_0^2 \zeta l_a^2}{3 k_B T} \quad (\text{S29})$$

and h_{Alx} is the brush height at equilibrium:

$$h_{\text{Alx}} = N_0 l_a \left(\frac{v \sigma}{3 l_a} \right)^{1/3}. \quad (\text{S30})$$

The solution of eq. (S28) has the form

$$h(t) = h_{\text{Alx}} \left[1 - (1 - \tilde{h}_0^3) e^{-3t/\tau_{N_0}} \right]^{1/3}, \quad (\text{S31})$$

where \tilde{h}_0 ($= h_0/h_{\text{Alx}}$) is the initial height h_0 of the brush, rescaled by the equilibrium value, see also eq. (32) in the main article. For short time scales, the height $h(t)$ has the asymptotic form

$$h(t) = h_{\text{Alx}} \left(\frac{3t}{\tau_{N_0}} \right)^{1/3}, \quad (\text{S32})$$

when the initial height h_0 is zero.

For the case in which the number $N(t)$ of Kuhn segments per chain is a function of time (such as the case of loop extruded chains), eq. (S27) can be rewritten in the form

$$\frac{d}{dt} \tilde{h}(t) = -\frac{1}{\tau_{N_0}} \frac{1}{\tilde{N}(t)} \left[\frac{\tilde{h}(t)}{\tilde{N}(t)} - \frac{\tilde{N}^2(t)}{\tilde{h}^2(t)} \right], \quad (\text{S33})$$

where $\tilde{N}(t)$ ($= N(t)/N_0$) is the number of Kuhn segments per chain, rescaled by the characteristic value N_0 . The general solution of eq. (S33) is given by

$$h(t) = h_{\text{Alx}} \left[\tilde{h}_0^3 + 3 \int_0^t \frac{dt'}{\tau_{N_0}} \tilde{N}(t') e^{3\kappa(t')} \right]^{1/3} e^{-\kappa(t)}, \quad (\text{S34})$$

where the exponent $\kappa(t)$ is given by

$$\kappa(t) = \frac{1}{\tau_{N_0}} \int_0^t dt' \frac{1}{\tilde{N}^2(t')}. \quad (\text{S35})$$

Eq. (S34) returns to eq. (S32) when $N(t)$ is the constant N_0 .

First, we consider the case in which chains are reeled from the grafted end with a constant rate, $N(t) = N_0 - t/\tau_s$, analogous to the situation of the arm subchain during the loop extrusion process. In this case, the height of the brush has the form

$$h(t) = h_{\text{Alx}} \left[\tilde{h}_0^3 + 3\alpha_0 \int_0^{t/\tau_{\text{ex}}} d\tilde{t}' (1 - \tilde{t}') e^{3\alpha_0 \tilde{t}' / (1 - \tilde{t}')} \right]^{1/3} e^{-\alpha_0 \tilde{t} / (1 - \tilde{t})}, \quad (\text{S36})$$

see fig. S1, where \tilde{t} ($= t/\tau_{\text{ex}}$) is the rescaled time and we define the time scale ratio in the form

$$\alpha_0 = \frac{\tau_{\text{ex}}}{\tau_{N_0}}. \quad (\text{S37})$$

Eq. (S36) has the asymptotic form

$$h(t) = h_0 e^{-\alpha_0 \tilde{t} / (1 - \tilde{t})} \quad (\text{S38})$$

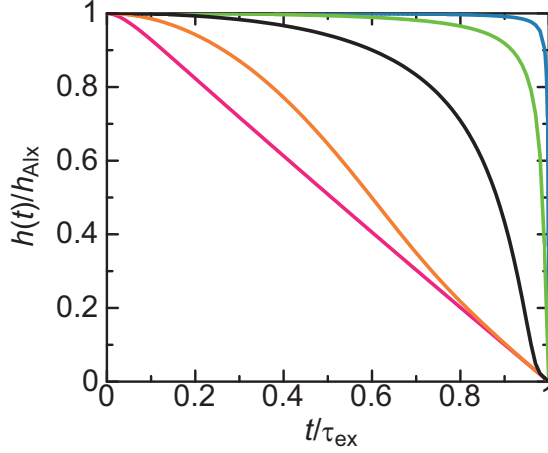


Figure S1: The brush height $h(t)$ (rescaled by the equilibrium value h_{Alx}) is shown as a function of time t (rescaled by the time scale τ_{ex}) when the chains are reeled from the grafted ends with a constant rate. τ_{ex} is the time scale of the reeling process. The curves are derived by using eq. (S36). The values of time scale ratio α_0 (defined by eq. (S37)) are 0.001 (cyan), 0.01 (light green), 0.1 (black), 1.0 (orange), 10.0 (magenta).

for small values of α_0 and

$$h(t) = \left[(1 - \tilde{t})^3 - (1 - \tilde{h}_0^3) e^{-3\alpha_0 \tilde{t}/(1-\tilde{t})} \right]^{1/3} \quad (\text{S39})$$

for large values of α_0 .

Second, we consider the case in which the number of Kuhn segments increases with a constant rate, $N(t) = t/\tau_s$, analogous to the situation of the loop subchain during the loop extrusion process. The initial height h_0 is zero because there are no Kuhn segments in the ‘chain’ at $t = 0$. In this case, the height of the brush has the form

$$h(t) = h_{\text{Alx}} \left[3\alpha_0 \int_0^{\tilde{t}} d\tilde{t}' \tilde{t}' e^{-3\alpha_0(1/\tilde{t}' - 1/\tilde{t})} \right]^{1/3}, \quad (\text{S40})$$

see fig. S2. The brush height $h(t)$ has the asymptotic form

$$h(t) = h_{\text{Alx}} \left(\frac{3}{2} \alpha_0 \tilde{t}^2 \right)^{1/3} \quad (\text{S41})$$

for small values of α_0 and

$$h(t) = h_{\text{Alx}} \tilde{t} \left(1 - \frac{\tilde{t}}{3\alpha_0} \right) \quad (\text{S42})$$

for large values of α_0 .

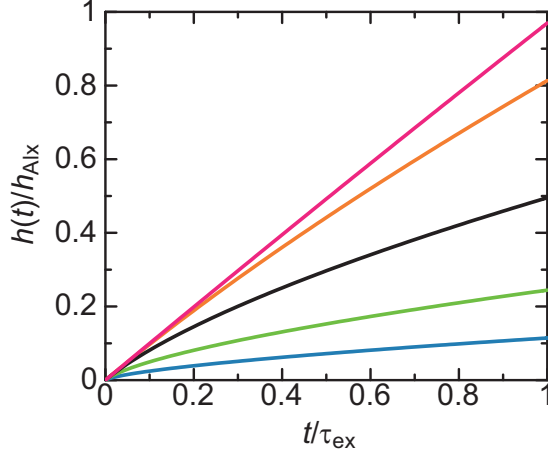


Figure S2: The brush height $h(t)$ (rescaled by the equilibrium value h_{Alx}) is shown as a function of time t (rescaled by the time scale τ_{ex}) when the number of Kuhn segments of the chain increases with a constant rate. τ_{ex} is the time scale with which the number of Kuhn segments becomes N_0 . These curves are derived by using eq. (S40). The values of time scale ratio α_0 (defined by eq. (S37)) are 0.001 (cyan), 0.01 (light green), 0.1 (black), 1.0 (orange), 10.0 (magenta).

S3 Asymptotic form for the short time regime

The dynamics of chains in the brush is determined by eqs. (9), (12), (13) in the main article. These equations are rewritten in the forms

$$\frac{d}{dt} \tilde{h} = -\alpha \frac{1}{\tilde{N}_t} \left(\frac{\tilde{h}_t}{\tilde{N}_t} - \frac{\tilde{N}_t^2}{\tilde{h}_t^2} \right) \quad (\text{S43})$$

$$\frac{d}{dt} \tilde{h}_b = -\alpha \left[\frac{4\tilde{h}_{\text{lp}}}{\tilde{N}_{\text{lp}}} + \frac{\tilde{h}_{\text{lp}}}{\tilde{N}_b} - \frac{(\tilde{N}_{\text{lp}} + \tilde{N}_b)^2}{\tilde{h}_{\text{lp}}^2} - \frac{\tilde{h}_t}{\tilde{N}_t} + \frac{\tilde{N}_t^2}{\tilde{h}_t^2} \right] \quad (\text{S44})$$

$$-\frac{3}{2} \frac{\tilde{h}_t^2}{\tilde{N}_t} + 6 \frac{\tilde{N}_t}{\tilde{h}_t} = -\frac{3}{2} \frac{\tilde{h}_b^2}{\tilde{N}_b} + 6 \frac{\tilde{N}_{\text{lp}} + \tilde{N}_b}{\tilde{h}_b}, \quad (\text{S45})$$

where $\tilde{h}_t (= h_t/h_{\text{Alx}})$ and $\tilde{h}_b (= h_b/h_{\text{Alx}})$ are the brush heights of the top and bottom layers, rescaled by the equilibrium brush height h_{Alx} . $\tilde{h} (= \tilde{h}_t + \tilde{h}_b)$ is the height of the chain, rescaled by the equilibrium brush height h_{Alx} . $\tilde{N}_t (= N_t/N)$, $\tilde{N}_b (= N_b/N)$, and $\tilde{N}_{\text{lp}} (= N_{\text{lp}}/N)$ are the number of Kuhn segments of the arm subchain in the top layer, the arm subchain in the bottom layer, and the loop subchain, rescaled by the number N of Kuhn segments of each chain. $\tilde{t} (= t/\tau_{\text{ex}})$ is the time rescaled by the time scale τ_{ex} of the loop extrusion process. α is the

ratio of time scales

$$\alpha = \frac{\tau_{\text{ex}}}{\tau_N}, \quad (\text{S46})$$

where τ_{ex} is the time scale of the loop extrusion process and τ_N is the longest relaxation time (Rouse time). The rescaled numbers \tilde{N}_t and \tilde{N}_{lp} of Kuhn segments have the form

$$\tilde{N}_t = 1 - \tilde{t} - \tilde{N}_b \quad (\text{S47})$$

$$\tilde{N}_{\text{lp}} = \tilde{t}. \quad (\text{S48})$$

We solve eqs. (S43) - (S45) for the short time regime using the ansatz

$$\tilde{h}_t = \tilde{h}_0 + b_1 \tilde{t} + b_2 \tilde{t}^2 \quad (\text{S49})$$

$$\tilde{h}_b = a_1 \tilde{t} + a_2 \tilde{t}^2 \quad (\text{S50})$$

$$\tilde{N}_b = c_1 \tilde{t} + c_2 \tilde{t}^2. \quad (\text{S51})$$

We substitute eqs. (S49) to (S51) into eq. (S43) and expand this equation in the power series of \tilde{t} up to linear order. This leads to the relations

$$a_1 + b_1 = -\alpha \left(\tilde{h}_0 - \frac{1}{\tilde{h}_0^2} \right) \quad (\text{S52})$$

$$a_2 + b_2 = -\frac{1}{2}\alpha \left[(1 + c_1) \left(2\tilde{h}_0 + \frac{1}{\tilde{h}_0^2} \right) + \frac{b_1}{\tilde{h}_0} \left(\tilde{h}_0 + \frac{2}{\tilde{h}_0^2} \right) \right]. \quad (\text{S53})$$

In a similar manner, we substitute eqs. (S49) to (S51) into eq. (S44) and expand this equation in a power series of \tilde{t} up to linear order. We obtain

$$a_1 = -\alpha \left[4a_1 + \frac{a_1}{c_1} - \frac{(1 + c_1)^2}{a_1^2} - \left(\tilde{h}_0 - \frac{1}{\tilde{h}_0^2} \right) \right] \quad (\text{S54})$$

$$a_2 = -\frac{1}{2}\alpha \left[4a_2 + \frac{a_1}{c_1} \left(\frac{a_2}{a_1} - \frac{c_2}{c_1} \right) - \frac{(1 + c_1)^2}{a_1^2} \left(\frac{2c_2}{1 + c_1} - \frac{2a_2}{a_1} \right) - \left(\tilde{h}_0 + \frac{2}{\tilde{h}_0^2} \right) \left(1 + c_1 + \frac{b_1}{\tilde{h}_0} \right) \right]. \quad (\text{S55})$$

We substitute eqs. (S49) - (S51) into eq. (S45) and expand this equation in a power series of \tilde{t} up to linear order. This leads to the forms

$$-\frac{1}{2}\tilde{h}_0^2 + \frac{2}{\tilde{h}_0} = -\frac{1}{2}\frac{a_1^2}{c_1^2} + 2\frac{1 + c_1}{a_1} \quad (\text{S56})$$

$$-\left(1 + c_1 + \frac{b_1}{\tilde{h}_0} \right) \left(\tilde{h}_0^2 + \frac{2}{\tilde{h}_0} \right) = -\frac{a_1^2}{c_1^2} \left(\frac{a_2}{a_1} - \frac{c_2}{c_1} \right) + 2\frac{1 + c_1}{a_1} \left(\frac{c_2}{1 + c_1} - \frac{a_2}{a_1} \right). \quad (\text{S57})$$

The constants a_1 and c_1 are derived by using eqs. (S54) and (S56). Eq. (S54) is rewritten as

$$\left(\frac{1}{\alpha} + 4 + \frac{1}{c_1}\right) a_1^3 - (1 + c_1)^2 - \left(\tilde{h}_0 - \frac{1}{\tilde{h}_0^2}\right) a_1^2 = 0. \quad (\text{S58})$$

In the limit of $\alpha \rightarrow 0$, \tilde{h}_b is zero, see eq. (S44) and thus $a_1 = 0$ and $c_1 = 0$. For small time scale ratio α , the solution of eq. (S58) thus has the form

$$a_1^3 = \frac{\alpha}{1 + \alpha/c_1}. \quad (\text{S59})$$

We used $c_1 < 1$ and $a_1 < 1$ to derive eq. (S59). In the same limit, the solution of eq. (S56) has the asymptotic form

$$a_1^3 = 4c_1^2. \quad (\text{S60})$$

Eqs. (S59) and (S60) lead to

$$\begin{aligned} c_1 &= \frac{-\alpha + \sqrt{\alpha^2 + \alpha}}{2} \\ &\simeq \frac{1}{2}\alpha^{1/2}. \end{aligned} \quad (\text{S61})$$

Substituting eq. (S61) into eq. (S60) we find

$$a_1 = \alpha^{1/3}. \quad (\text{S62})$$

By using eq. (S52), the constant b_1 can be derived:

$$a_1 + b_1 = \frac{\alpha}{\tilde{h}_0^2}(1 - \tilde{h}_0^3). \quad (\text{S63})$$

We retained the right hand side of eq. (S63), even though it is smaller than a_1 , because it is the leading order term of the brush height h .

Substituting eqs. (S61) and (S62) into eqs. (S55) and (S57) and omitting the higher order terms with respect to α , we arrive at

$$-\frac{6}{\alpha^{2/3}}a_2 + \frac{8}{\alpha^{5/6}}c_2 = -\left(1 + c_1 + \frac{b_1}{\tilde{h}_0}\right)\left(\tilde{h}_0^2 + \frac{2}{\tilde{h}_0}\right) \quad (\text{S64})$$

$$\frac{4}{\alpha}a_2 - \frac{6}{\alpha^{2/3}}c_2 = \left(1 + c_1 + \frac{b_1}{\tilde{h}_0}\right)\left(\tilde{h}_0 + \frac{2}{\tilde{h}_0^2}\right). \quad (\text{S65})$$

By solving eqs. (S64) and (S65), the constants a_2 and c_2 are derived:

$$c_2 = -\frac{1}{4}\frac{\alpha^{5/6}}{\tilde{h}_0}\left(1 + \frac{\tilde{h}_0^3}{2}\right) \quad (\text{S66})$$

$$a_2 = \frac{\alpha}{2\tilde{h}_0^2}\left(1 + \frac{\tilde{h}_0^3}{2}\right). \quad (\text{S67})$$

Substituting eqs. (S61) and (S63) into eq. (S53) we obtain

$$a_2 + b_2 = -\frac{1}{2} \frac{\alpha}{\tilde{h}_0^2} (1 + 2\tilde{h}_0^3). \quad (\text{S68})$$

For the short time regime, the rescaled height \tilde{h}_b of the bottom layer has the form

$$\tilde{h}_b = \alpha^{1/3} \tilde{t}, \quad (\text{S69})$$

which is derived by substituting eq. (S62) into eq. (S50). Eq. (S69) is equal to eq. (28) in the main article. The rescaled height \tilde{h} ($= \tilde{h}_t + \tilde{h}_b$) of the arm subchain has the form

$$\tilde{h} = \tilde{h}_0 + \frac{\alpha}{\tilde{h}_0^2} (1 - \tilde{h}_0^3) \tilde{t} - \frac{1}{2} \frac{\alpha}{\tilde{h}_0^2} (1 + 2\tilde{h}_0^3) \tilde{t}^2, \quad (\text{S70})$$

which we derived by using eqs. (S63) and (S68). We retained the second order term with respect to the power of \tilde{t} because the first order term is zero for $\tilde{h}_0 = 1$. Eq. (S70) is equal to eq. (29) in the main article. Finally, the rescaled number \tilde{N}_b of chain segments of the arm subchain in the bottom layer has the form

$$\tilde{N}_b = \frac{1}{2} \alpha^{1/2} \tilde{t}. \quad (\text{S71})$$

Including the second order term, the rescaled number \tilde{N}_b we find

$$\tilde{N}_b = \frac{1}{2} \alpha^{1/2} \tilde{t} - \frac{1}{4} \frac{\alpha^{5/6}}{\tilde{h}_0} \left(1 + \frac{\tilde{h}_0^3}{2} \right) \tilde{t}^2. \quad (\text{S72})$$

S4 Approximate solution for $t \sim t_{\text{th}}$

We here derive approximate solutions of eqs. (S43) to (S45) for the short time regime. At the beginning of the loop extrusion process, $t \sim 0$, the loop subchain that has been extruded is confined in a space of height $h_b \sim 0$. The dynamics of the loop subchain is thus governed by the excluded volume interactions, the third term of eq. (S44). Retaining only that third term, the approximate solution of eq. (S44) follows to be

$$\tilde{h}_p(t) = \alpha^{1/3} \tilde{t}. \quad (\text{S73})$$

Eq. (S73) is indeed equal to eq. (S69), derived by the power expansion with respect to the rescaled time \tilde{t} , and is effective for a long period of time, see the blue curves in fig. 2 of the main article.

The subchain in the top layer is stretched by the loop extrusion process and thus, for $t \sim t_{\text{th}}$, the entropic elasticity of the subchain dominates the excluded

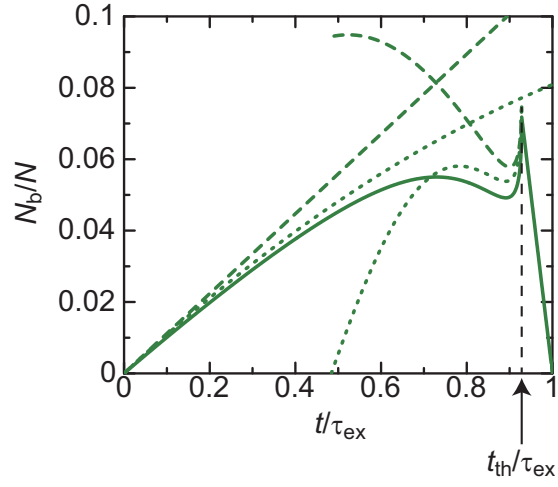


Figure S3: The number N_b of Kuhn segments of the arm subchain in the bottom layer (rescaled by the total number N of Kuhn segments of the chain) is shown as a function of time t (rescaled by the time scale τ_{ex} of the loop extrusion process). We used $\alpha = 0.05$ for the time scale ratio α (defined by eq. (S46)). The broken curve in the short time regime is derived by using eq. (S71). The dotted curve in the same regime is derived by using eq. (S72). The broken curve at $t \sim t_{\text{th}}$ ($= 0.9282$) is derived by using eq. (S75). The dotted curve in the same regime is derived by using eq. (S76).

volume interactions in the top layer. With this approximation, eq. (S45) is rewritten in the form

$$-\frac{3}{2} \frac{h_t^2}{N_t^2} \simeq -\frac{3}{2} \frac{h_b^2}{N_b^2} + \frac{6}{\alpha^{1/3}}, \quad (\text{S74})$$

where we used eq. (S73) and $N_{lp} \gg N_b$. For $t \sim t_{th}$, we assume that the arm chain in the bottom layer is stretched and the entropic elasticity of this subchain dominates the excluded volume interactions in the bottom layer. With this assumption, the solution of eq. (S74) is given by

$$\tilde{N}_b = \frac{\alpha^{1/3} \tilde{t}(1-\tilde{t})}{\tilde{h}}, \quad (\text{S75})$$

see the broken curve at $t \sim t_{th}$ in fig. S3. We used eq. (S73) and $\tilde{N}_t = 1 - \tilde{t} - \tilde{N}_b$ to derive eq. (S75). Taking into account the second term of the right hand side of eq. (S74) by the first order perturbation leads to the form

$$\tilde{N}_b = \frac{\alpha^{1/3} \tilde{t}(1-\tilde{t})}{\tilde{h}} - \frac{2\tilde{t}(1-\tilde{t})^3}{\tilde{h}^3} \left(1 - \frac{\alpha^{1/3} \tilde{t}}{\tilde{h}}\right) \left(1 - \frac{\alpha^{1/3}(1-\tilde{t})}{\tilde{h}}\right), \quad (\text{S76})$$

see the dotted curve at $t \sim t_{th}$ in fig. S3. At the crossover time t_{th} , the height of the arm subchain is equal to the height of the loop subchain, $\tilde{h} = \tilde{h}_b (\simeq \alpha^{1/3} \tilde{t})$, and the number \tilde{N}_b of Kuhn segments of the arm chain in the bottom layer is $1 - \tilde{t}$. Both eqs. (S75) and (S76) satisfy these conditions. Although eq. (S76) is the better approximation, we use eq. (S75) for its simplicity.

Substituting eq. (S75) into eq. (S43) leads to

$$\frac{d}{dt} \tilde{h}(\tilde{t}) = -\alpha \frac{1}{(1-\tilde{t})^2} \frac{\tilde{h}}{1 - \alpha^{1/3} \tilde{t}/\tilde{h}}, \quad (\text{S77})$$

where we neglected the second term of eq. (S43). Eq. (S77) is rewritten in the form

$$\frac{d}{dt} y(\tilde{t}) + \frac{y(\tilde{t})}{\tilde{t}} + \alpha \frac{1}{(1-\tilde{t})^2} \frac{y^2(\tilde{t})}{y(\tilde{t}) - 1} = 0, \quad (\text{S78})$$

where we used the variable transformation $y(\tilde{t}) = h(t)/(\alpha^{1/3} \tilde{t})$. By solving eq. (S78) for $y(\tilde{t}) > 1$, we arrive at

$$h(t) = h_0 e^{-\alpha \tilde{t}/(1-\tilde{t})}. \quad (\text{S79})$$

Eq. (S79) is equal to eq. (29) in the main article and is indeed equal to the case in which we neglect the distinction between the top and bottom layers and the excluded volume interactions, see eq. (S38). This is not surprising as the only difference between the subchains in the top and bottom layers is that they experience different magnitudes of the excluded volume interactions due to the loop subchain in the bottom layer.

S5 Approximate solution for the long time regime

For longer time scales, $t_{\text{th}} < t < \tau_{\text{ex}}$, the dynamics of the brush is determined by eqs. (16) to (18) in the main article. These equations are rewritten as

$$\frac{d}{d\tilde{t}}\tilde{h} = -\frac{\alpha}{\tilde{N}_t} \left(\frac{4\tilde{h}_t}{\tilde{N}_t} - \frac{\tilde{N}_t^2}{\tilde{h}_t^2} \right) \quad (\text{S80})$$

$$\frac{d}{d\tilde{t}}\tilde{h}_b = -\alpha \left[\frac{\tilde{h}_b}{\tilde{N}_b} + \frac{4\tilde{h}_b}{\tilde{N}_{\text{lp}}} - \frac{(\tilde{N}_{\text{lp}} + \tilde{N}_b)^2}{\tilde{h}_b^2} - \frac{4\tilde{h}_t}{\tilde{N}_t} + \frac{\tilde{N}_t^2}{\tilde{h}_t^2} \right] \quad (\text{S81})$$

$$-\frac{\tilde{h}_b^2}{\tilde{N}_{\text{lp}}^2} + \frac{\tilde{N}_{\text{lp}} + \tilde{N}_b}{\tilde{h}_b} = -\frac{\tilde{h}_t^2}{\tilde{N}_t^2} + \frac{\tilde{N}_t}{\tilde{h}_t}, \quad (\text{S82})$$

see the discussion below eqs. (S43) to (S45) for the scheme of rescaling. In this time regime, the rescaled number of the Kuhn segments of the arm subchain has the form $\tilde{N}_b = 1 - \tilde{t}$ and the rescaled number of the loop subchain in the bottom layer has the form $\tilde{N}_{\text{lp}} = \tilde{t} - \tilde{N}_t$.

The arm subchain is strongly stretched in the long time regime and thus the first term of eq. (S81), the elastic force generated by the arm subchain, dominates over the other terms on the right hand side of this equation. Retaining only that term, the approximate solution of eq. (S81) has the form

$$h_{\text{lp}}(\tilde{t}) = h_{\text{th}} \left(\frac{1 - \tilde{t}}{1 - \tilde{t}_{\text{th}}} \right)^\alpha, \quad (\text{S83})$$

where h_{th} is the height of the chains at $t = t_{\text{th}}$. Eq. (S83) is indeed equal to eq. (30) in the main article.

In contrast to the arm subchain, the loop subchain is still compressed. The number of Kuhn segments of the arm subchain is thus smaller than the number of Kuhn segments of the loop subchain in the bottom layer, $\tilde{N}_b < \tilde{N}_{\text{lp}}$. Eq. (S82) is approximated by

$$-\frac{\tilde{h}_b^2}{\tilde{N}_{\text{lp}}^2} + \frac{\tilde{N}_{\text{lp}}}{\tilde{h}_b} \simeq -\frac{\tilde{h}_t^2}{\tilde{N}_t^2} + \frac{\tilde{N}_t}{\tilde{h}_t}. \quad (\text{S84})$$

Eq. (S84) has the solution

$$\frac{\tilde{h}_{\text{lp}}}{\tilde{N}_{\text{lp}}} = \frac{\tilde{h}_t}{\tilde{N}_t}. \quad (\text{S85})$$

By using the relationship $\tilde{N}_{\text{lp}} = \tilde{t} - \tilde{N}_t$, eq. (S85) is rewritten as

$$\tilde{N}_t = \frac{\tilde{h}_t}{\tilde{h}} \tilde{t}. \quad (\text{S86})$$

Substituting eq. (S86) into eq. (S80) leads to

$$\frac{d}{d\tilde{t}}\tilde{h} = -\alpha \frac{\tilde{h}}{\tilde{h} - \tilde{h}_{\text{lp}}} \frac{1}{\tilde{t}} \left[\frac{4\tilde{h}}{\tilde{t}} - \frac{\tilde{t}^2}{\tilde{h}^2} \right]. \quad (\text{S87})$$

The rescaled height \tilde{h} of the chain is derived as a function of \tilde{t} and α by using eq. (S87).

Eq. (S83) implies that the height of the bottom layer changes only at $t \sim \tau_{\text{ex}}$ when the time scale ratio α is small. We thus solve eq. (S87) by using $h_{\text{lp}}(\tilde{t}) \simeq \tilde{h}_{\text{th}}$. The loop subchain is still compressed and thus the excluded volume interactions, the second term of eq. (S87), dominates the entropic elasticity of the chain, the first term of the same equation. With this approximation, the solution of eq. (S87) is given by

$$\frac{1}{3}\tilde{h}^3 - \frac{1}{2}\tilde{h}_{\text{th}}\tilde{h}^2 + \frac{1}{6}\tilde{h}_{\text{th}}^3 = \frac{1}{2}\alpha(\tilde{t}^2 - \tilde{t}_{\text{th}}^2). \quad (\text{S88})$$

For small time scale ratio α , the rescaled height \tilde{h} has the approximate form

$$\tilde{h}(\tilde{t}) = \tilde{h}_{\text{th}} + \sqrt{\frac{\alpha}{\tilde{h}_{\text{th}}}}(\tilde{t}^2 - \tilde{t}_{\text{th}}^2). \quad (\text{S89})$$

S6 Approximate solution for the relaxation process

During the relaxation process, $t > \tau_{\text{ex}}$, the height of the chain has the form

$$\tilde{h}(t) = \left[1 - \left(1 - \tilde{h}_{\text{ex}}^3\right) e^{-3(t - \tau_{\text{ex}})/\tau_N}\right]^{1/3}, \quad (\text{S90})$$

where $\tilde{h}_{\text{ex}} (= h(\tau_{\text{ex}})/h_{\text{Alx}})$ is the height of the chain at $t = \tau_{\text{ex}}$, rescaled by the equilibrium brush height h_{Alx} , see also eq. (31) in the main article. The lateral pressure generated by the chain is given by eq. (22) in the main article. For small time scale ratio α , the height of the brush at the end of the loop extrusion process has the form

$$\tilde{h}_{\text{ex}} \simeq \alpha^{1/3}, \quad (\text{S91})$$

where we used eq. (S73) and the fact that the period of the time regime, $t_{\text{th}} < t < \tau_{\text{ex}}$, is negligible for small α . The brush height $h(\tau_{\text{on}}) = h_0$ at which cohesin is loaded onto the chain has the form

$$\tilde{h}_0 = \left[1 - (1 - \alpha) e^{-3(\tau_{\text{on}}/\tau_N - \alpha)}\right]^{1/3}, \quad (\text{S92})$$

which is derived by substituting eq. (S91) into eq. (S90). Eq. (S92) is equal to eq. (32) in the main article.

S7 Lateral pressure generated by the brush

The forms of the lateral pressure, $\Pi_{\text{t}}(t)$ and $\Pi_{\text{b}}(t)$, generated by the subchains in the top and bottom layers are shown in eqs. (7) and (8) in the main article. In

the steady state, the lateral pressure generated by the brush can be calculated from

$$\bar{\Pi}_{\parallel} = \frac{1}{\tau_{\text{on}}} \int_0^{\tau_{\text{on}}} dt' \Pi_{\parallel}(t'), \quad (\text{S93})$$

where $\Pi_{\parallel}(t)$ has the form

$$\Pi_{\parallel}(t) = \Pi_{\text{t}}(t) + \Pi_{\text{b}}(t). \quad (\text{S94})$$

For small rescaled time ratio α , the period of the time regime, $t_{\text{th}} < t < \tau_{\text{ex}}$, is negligible. The rescaled lateral pressure, $\tilde{\Pi}_{\text{t}}(\tilde{t})$ ($= \Pi_{\text{t}}(t)/\Pi_{\text{Alx}}$), generated in the top layer has the approximate form

$$\tilde{\Pi}_{\text{t}}(\tilde{t}) = \frac{\tilde{N}_{\text{t}}^2}{\tilde{h}_{\text{t}}} = \frac{(1 - \tilde{t})^2}{\tilde{h}} \left(1 - \frac{\alpha^{1/3} \tilde{t}}{\tilde{h}} \right). \quad (\text{S95})$$

We used eq. (S75) to derive eq. (S95). In steady state, the lateral pressure $\bar{\Pi}_{\text{t}}$ generated by the top layer during the loop extrusion process follows to be

$$\begin{aligned} \frac{\bar{\Pi}_{\text{t}}}{\bar{\Pi}_{\text{Alx}}} &= \frac{\tau_{\text{ex}}}{\tau_{\text{on}}} \int_0^{\tilde{t}_{\text{th}}} d\tilde{t}' \tilde{\Pi}_{\text{t}}(\tilde{t}') \\ &= \frac{\tau_{\text{ex}}}{\tau_{\text{on}}} \int_0^{\tilde{t}_{\text{th}}} d\tilde{t}' \frac{(1 - \tilde{t}')^2}{\tilde{h}_0} e^{\alpha \tilde{t}' / (1 - \tilde{t}')} \left(1 - \frac{\alpha^{1/3} \tilde{t}'}{\tilde{h}} \right) \\ &\simeq \frac{\tau_{\text{ex}}}{\tau_{\text{on}}} \int_0^1 d\tilde{t}' \frac{(1 - \tilde{t}')^2}{\tilde{h}_0} \\ &\simeq \frac{1}{3} \frac{\tau_{\text{ex}}}{\tau_{\text{on}}} \frac{1}{\tilde{h}_0}. \end{aligned} \quad (\text{S96})$$

We neglected the higher order terms with respect to α to derive the last form of eq. (S96). The rescaled lateral pressure, $\tilde{\Pi}_{\text{b}}(\tilde{t})$ ($= \Pi_{\text{b}}(t)/\Pi_{\text{Alx}}$), generated in the bottom layer has the approximate form

$$\begin{aligned} \tilde{\Pi}_{\text{b}}(\tilde{t}) &= \frac{(\tilde{N}_{\text{lp}} + \tilde{N}_{\text{b}})^2}{\tilde{h}_{\text{lp}}} \\ &\simeq \alpha^{-1/3} \tilde{t}. \end{aligned} \quad (\text{S97})$$

We used $\tilde{N}_{\text{b}} < \tilde{N}_{\text{lp}}$ and eq. (S73) to derive the last form of eq. (S97). In steady state, the lateral pressure generated by the bottom layer is approximately given by

$$\begin{aligned} \frac{\bar{\Pi}_{\text{b}}}{\bar{\Pi}_{\text{Alx}}} &= \frac{\tau_{\text{ex}}}{\tau_{\text{on}}} \int_0^{\tilde{t}_{\text{th}}} d\tilde{t}' \tilde{\Pi}_{\text{b}}(\tilde{t}') \\ &\simeq \frac{\tau_{\text{ex}}}{\tau_{\text{on}}} \int_0^1 d\tilde{t}' \alpha^{-1/3} \tilde{t}' \\ &\simeq \frac{1}{2} \frac{\tau_{\text{ex}}}{\tau_{\text{on}}} \alpha^{-1/3}. \end{aligned} \quad (\text{S98})$$

The rescaled lateral pressure $\tilde{\Pi}_{\text{rex}}(\tilde{t})$ during the relaxation process has the form

$$\tilde{\Pi}_{\text{rex}}(\tilde{t}) = \frac{1}{\tilde{h}(\tilde{t})}, \quad (\text{S99})$$

see eq. (22) in the main article. In steady state, the lateral pressure $\bar{\Pi}_{\text{rex}}$ is given by

$$\begin{aligned} \frac{\bar{\Pi}_{\text{rex}}}{\Pi_{\text{Alx}}} &= \frac{1}{\alpha} \frac{\tau_{\text{ex}}}{\tau_{\text{on}}} \int_1^{\tilde{\tau}_{\text{on}}} d\tilde{t} \frac{1}{\tilde{h}(\tilde{t})} \\ &= \frac{1}{\alpha} \frac{\tau_{\text{ex}}}{\tau_{\text{on}}} \int_{u(1)}^{u(\tilde{\tau}_{\text{on}})} du \frac{1}{(u^3 - 1)^{1/3}}, \end{aligned} \quad (\text{S100})$$

where $\tilde{\tau}_{\text{on}} (= \tau_{\text{on}}/\tau_{\text{ex}})$ is the average loading time rescaled by the time scale τ_{ex} of the loop extrusion process. The new variable $u(\tilde{t})$ is defined by

$$u(\tilde{t}) = \frac{1}{(1 - \alpha)^{1/3}} e^{\alpha(\tilde{\tau}_{\text{on}} - 1)}. \quad (\text{S101})$$

Using eqs. (S96), (S98), and (S100), we find for the lateral pressure $\tilde{\Pi}_{\parallel}$ in steady state:

$$\tilde{\Pi}_{\parallel} = \Pi_{\text{Alx}} \frac{\tau_{\text{ex}}}{\tau_{\text{on}}} \left[\frac{1}{3} \frac{1}{\tilde{h}_0} + \frac{1}{2} \alpha^{-1/3} + \frac{1}{\alpha} \int_{u(0)}^{u(\tilde{\tau}_{\text{on}})} du \frac{1}{(u^3 - 1)^{1/3}} \right]. \quad (\text{S102})$$

For large values of the time scale ratio $\alpha\tilde{\tau}_{\text{on}} (= \tau_{\text{on}}/\tau_N)$, the lateral pressure $\bar{\Pi}_{\text{rex}}$ for the relaxation process has the asymptotic form

$$\bar{\Pi}_{\text{rex}} = \Pi_{\text{Alx}} \left[1 + \frac{1}{\alpha\tilde{\tau}_{\text{on}}} \left(\frac{\log 3}{2} - \frac{\pi}{6\sqrt{3}} \right) \right]. \quad (\text{S103})$$

The lateral pressure $\tilde{\Pi}_{\parallel}$ is thus given by

$$\tilde{\Pi}_{\parallel} = \Pi_{\text{Alx}} \left[1 + \frac{1}{\alpha\tilde{\tau}_{\text{on}}} \left(\frac{\log 3}{2} - \frac{\pi}{6\sqrt{3}} \right) \right] \quad (\text{S104})$$

for small time scale ratio α , because the first and second terms in the square bracket of eq. (S102) are higher order terms with respect to α . Eq. (S104) is equal to eq. (34) in the main article. For small values of the time scale ratio $\alpha\tilde{\tau}_{\text{on}}$, the lateral pressure $\bar{\Pi}_{\text{rex}}$ for the relaxation process has the asymptotic form

$$\begin{aligned} \bar{\Pi}_{\text{rex}} &= \frac{1}{2} \Pi_{\text{Alx}} \left[(3u(\tilde{\tau}_{\text{on}}) - 3)^{2/3} - (3u(1) - 3)^{2/3} \right] \\ &\simeq \frac{1}{2} \Pi_{\text{Alx}} \left[(3\alpha\tilde{\tau}_{\text{on}} - 2\alpha)^{2/3} - \alpha^{2/3} \right]. \end{aligned} \quad (\text{S105})$$

The asymptotic form of the lateral pressure Π_{\parallel} is given by

$$\frac{\Pi_{\parallel}}{\Pi_{\text{Alx}}} = \frac{1}{3} \frac{1}{\tilde{\tau}_{\text{on}}} (3\alpha\tilde{\tau}_{\text{on}} - 2\alpha)^{-1/3} + \frac{1}{2} \frac{1}{\alpha\tilde{\tau}_{\text{on}}} (3\alpha\tilde{\tau}_{\text{on}} - 2\alpha)^{2/3}, \quad (\text{S106})$$

which follows from substituting eqs. (S92) and (S105) into eq. (S102) and omitting the higher order terms with respect to α . Eq. (S106) is equal to eq. (35) in the main article.

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