Estudio de la dinámica de cadenas lineales por medio de un modelo discreto de reptación

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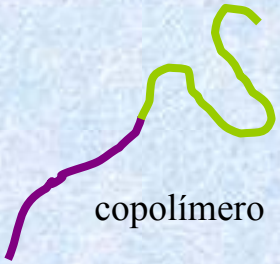
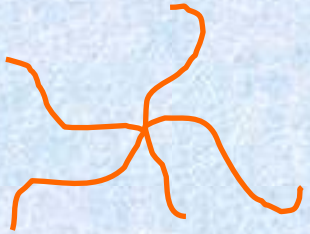
6° Biomat – La Falda, Córdoba. 4-7 de Agosto de 2014

Introducción

homopolímero



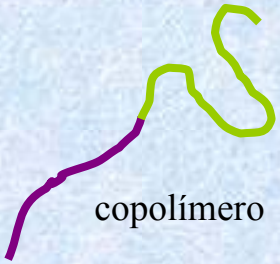
copolímero



polímero estrella

Introducción

homopolímero



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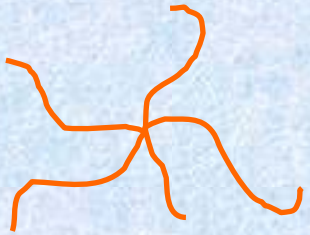
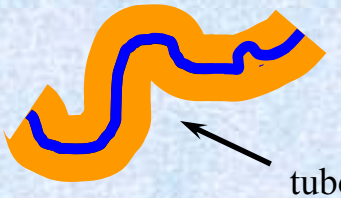


polímero estrella

polímero lineal
(*sin movimiento lateral*)

matriz de obstáculos fijos (medio poroso)
u otros polímeros

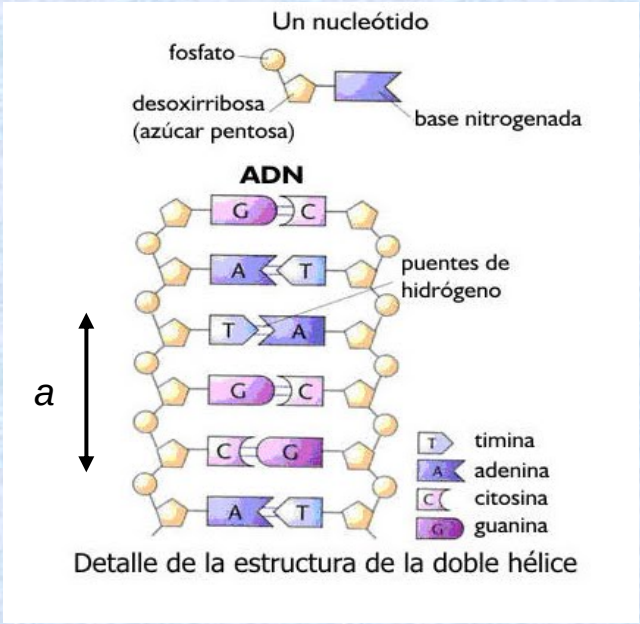


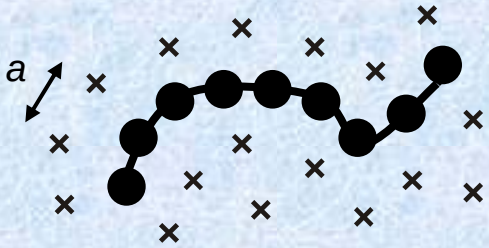
tubo

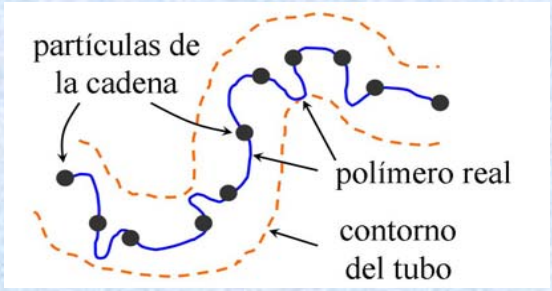
reptación

La cadena difunde unidimensionalmente a lo largo del tubo

Modelo en una dimensión







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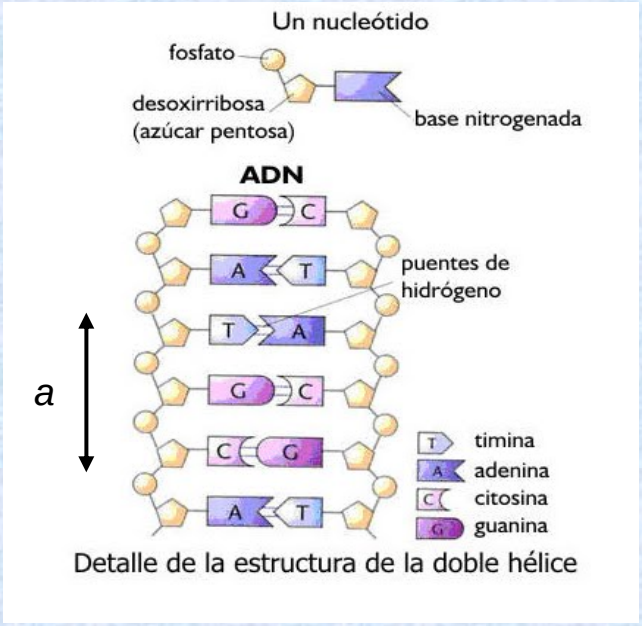
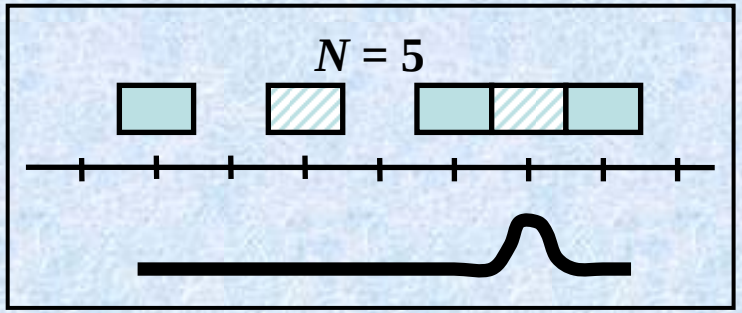
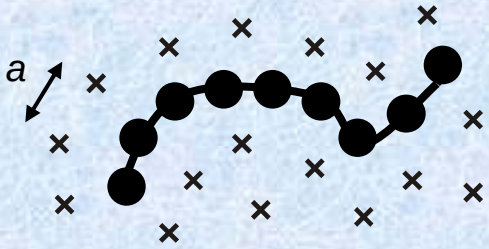
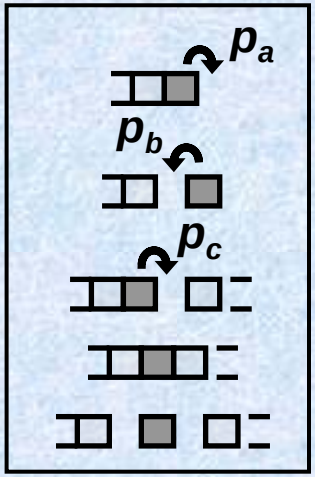
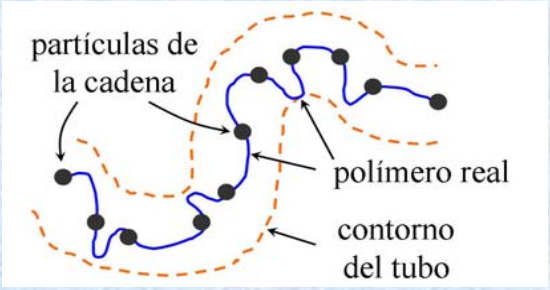








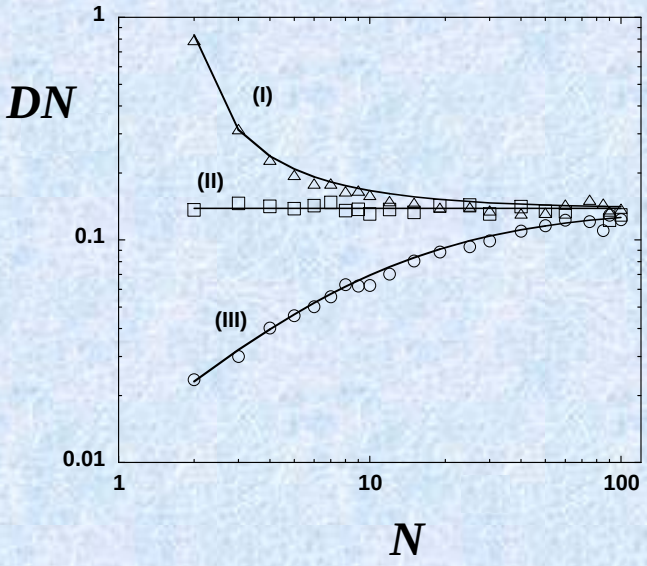
El modelo posee tres parámetros libres p_a, p_b y p_c



Coeficiente de difusión en una dimensión

$$D = \frac{p_a p_b p_c}{(p_a + p_b)\left[(N-2)(p_a + p_b) + 2p_c\right]}$$

$$\langle x^2 \rangle = 2\,D\,t$$



(p_a, p_b, p_c)	
(1, 1/5, 1/5)	(I)
(5/6, 1/6, 1)	(II)
(5/36, 1/36, 1)	(III)

$p_a + p_b = p_c$

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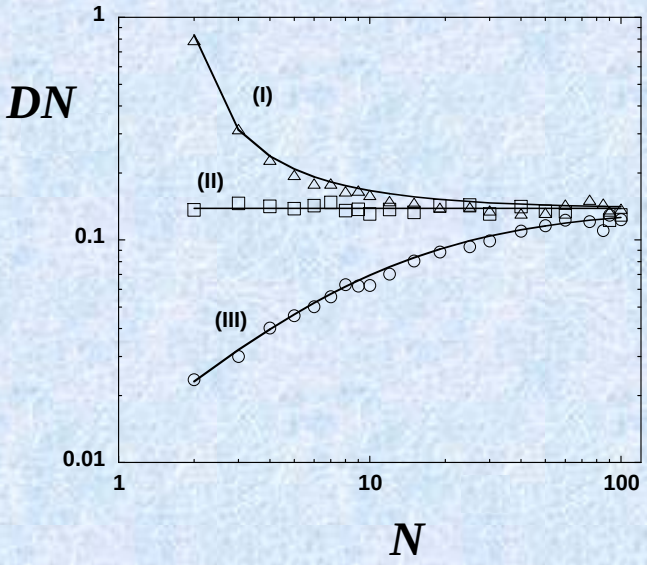


(p_a, p_b, p_c)	
(1, 1/5, 1/5)	(I)
(5/6, 1/6, 1)	(II)
(5/36, 1/36, 1)	(III)

$\leftarrow p_a + p_b = p_c$

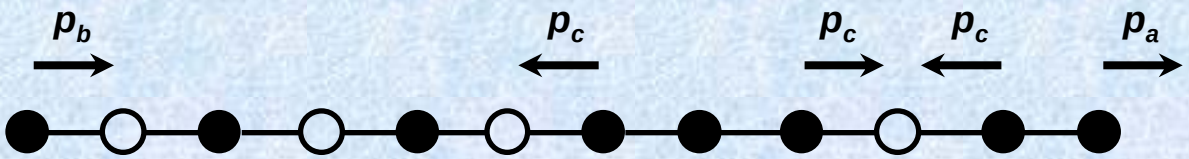
$$D = \frac{p_{a1} p_{bN} p'_c}{(p_{aN} + p_{bN})\left[\left(1 + \frac{p_{b1}}{p_{bN}}\right) p'_c + (p_{a1} + p_{b1})\right]}, \qquad \frac{1}{p'_c} = \sum_i \frac{1}{p_{ci}}$$

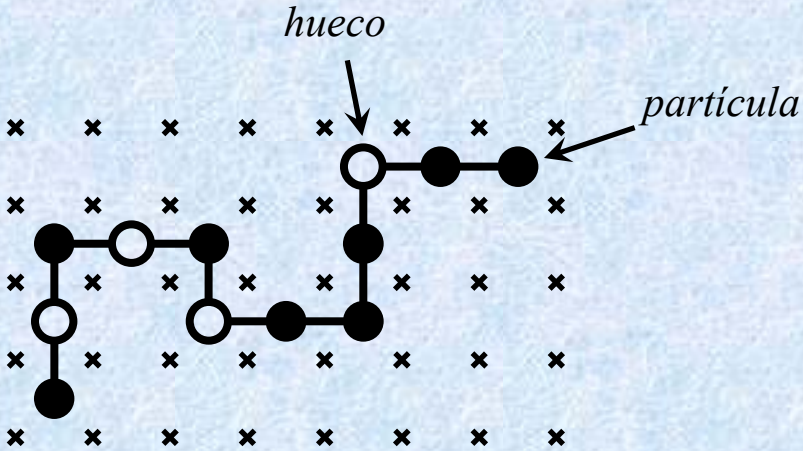
Terranova, Mártin, Aldao. Phys. Rev. E. 72, 61108 (2005).

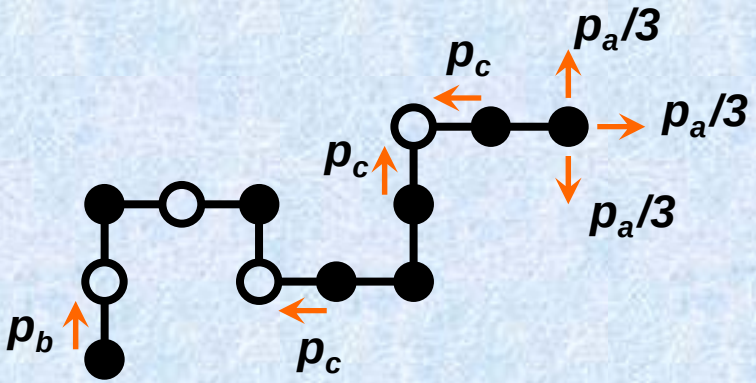
A. Buhot, Eur. Phys. J. E **18**, 239 (**2005**).

A. Drzewinski y J. M. J. van Leeuwen, Phys. Rev. E **73**, 051801 (**2006**).

Modelo en dos dimensiones



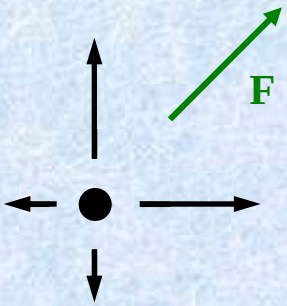


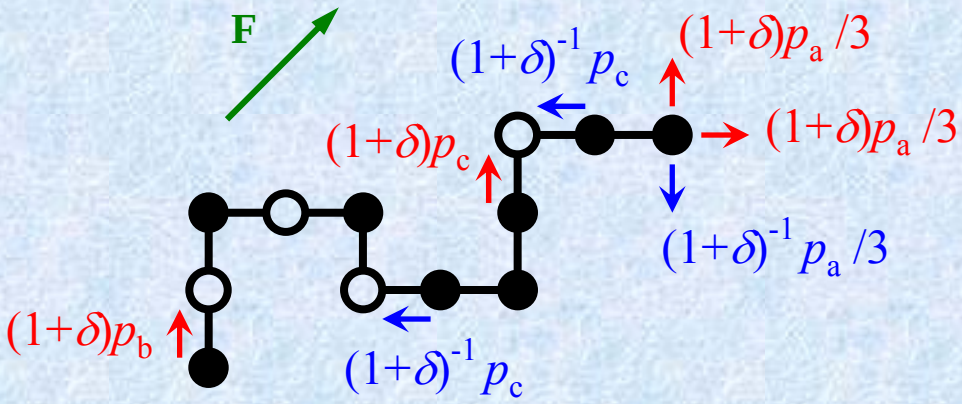


$$D_{2d} = A\frac{p_a p_b p_c}{[(N-2)(p_a+p_b)+2p_c][N(p_a+p_b)+(N-1)p_a]}$$

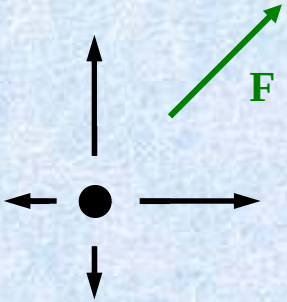
Terranova, Mártin, Aldao. Phys. Rev. E. 76, 31111 (2007).

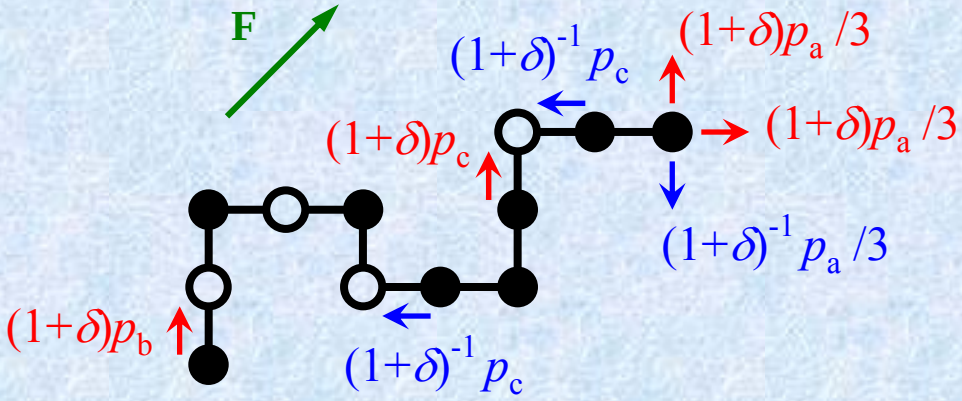
Velocidad de arrastre en dos dimensiones

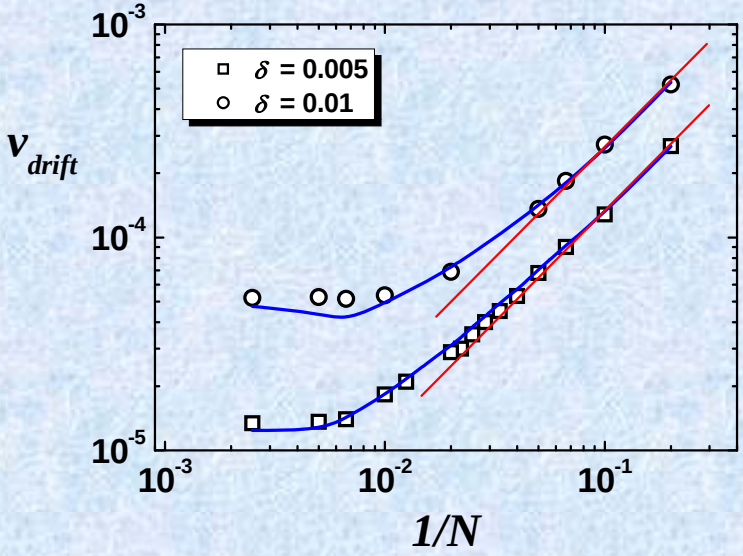


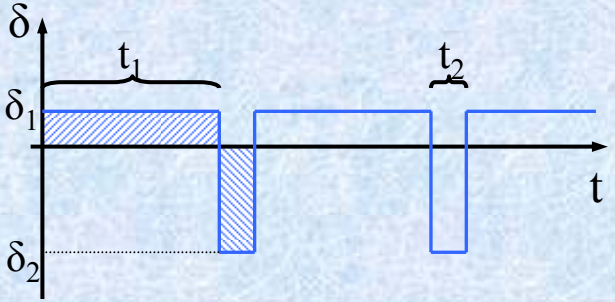


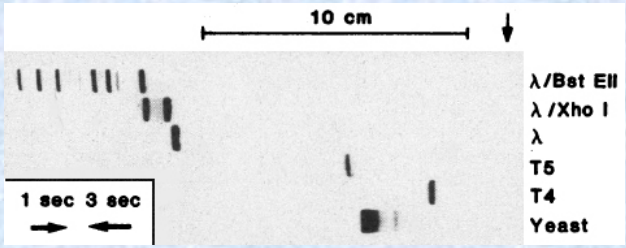
Velocidad de arrastre en dos dimensiones









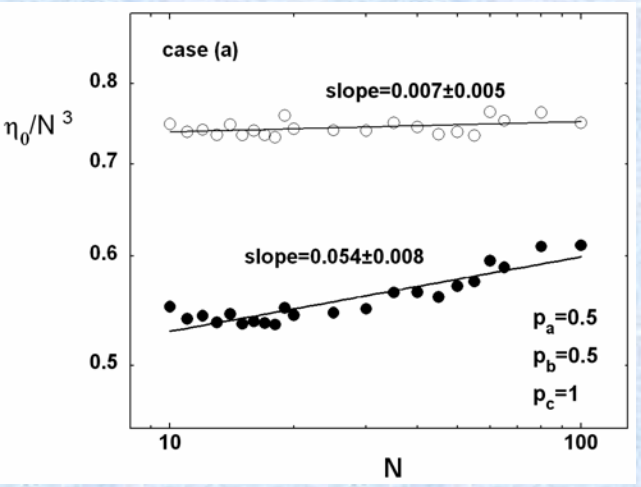


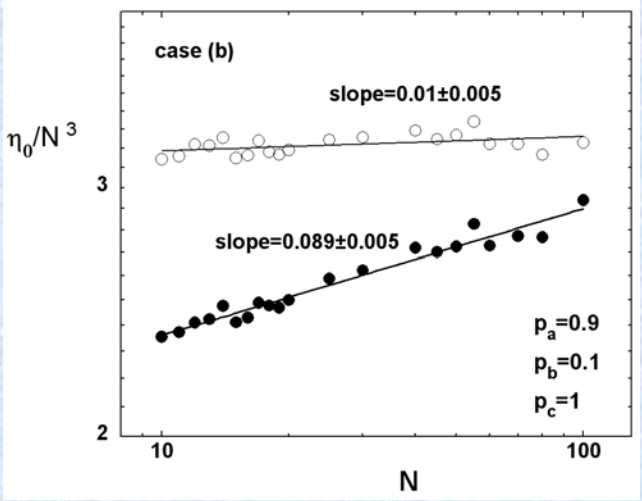
Viscosidad

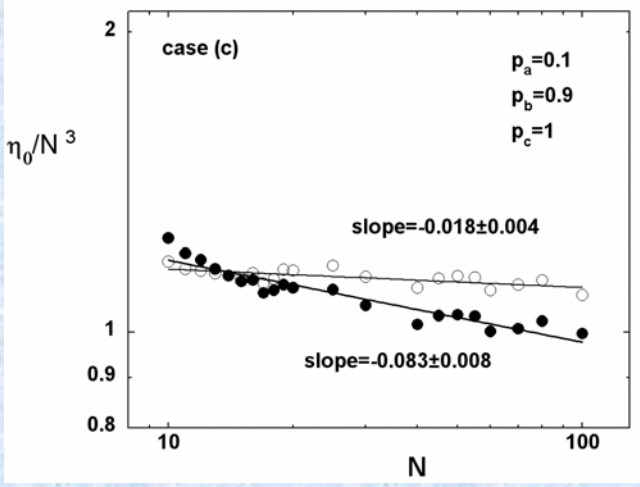
Efecto de las fluctuaciones de las longitudes de las cadenas.

Teóricamente se espera que $\eta_0 \sim N^3$ (de Gennes)

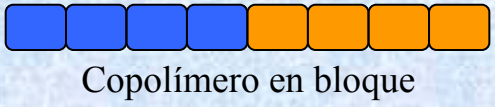
$\eta_{\text{experimental}} \sim N^{\beta}, \beta > 3$







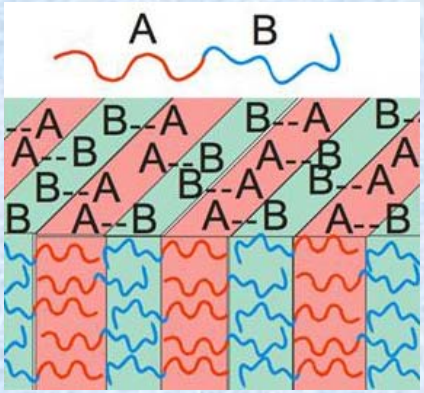
Copolímeros lineales

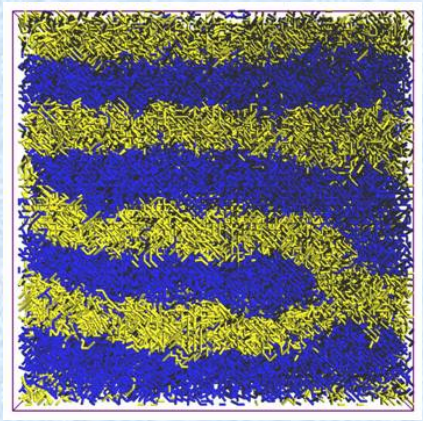


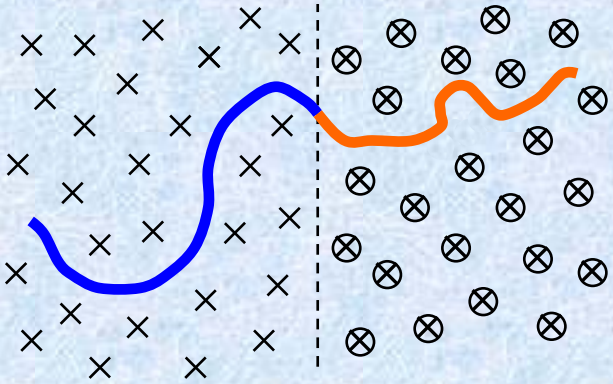
Copolímero en bloque

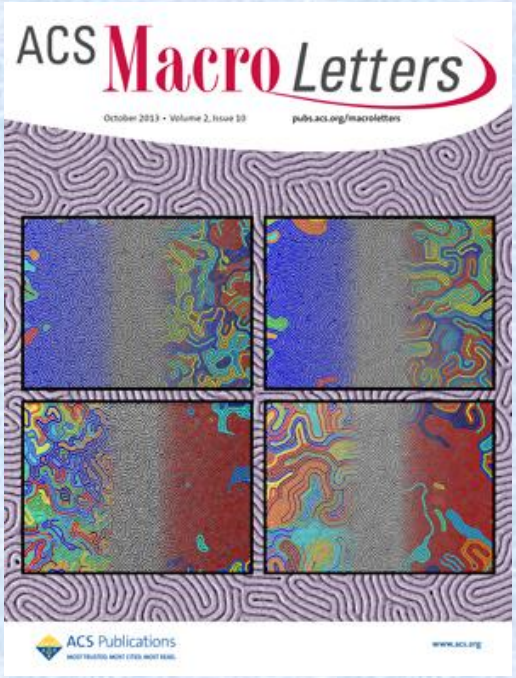
Copolímero alternado

Copolímero al azar

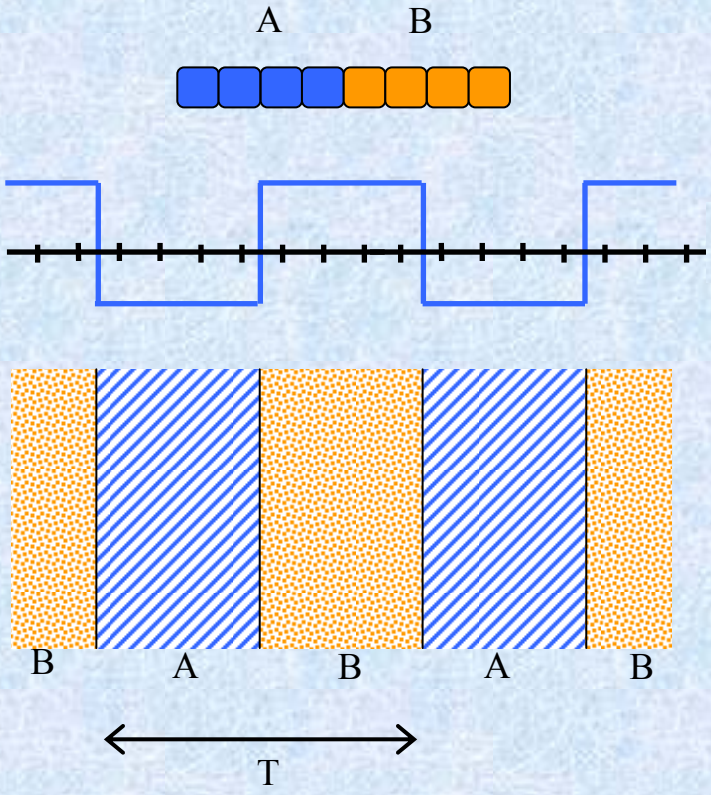


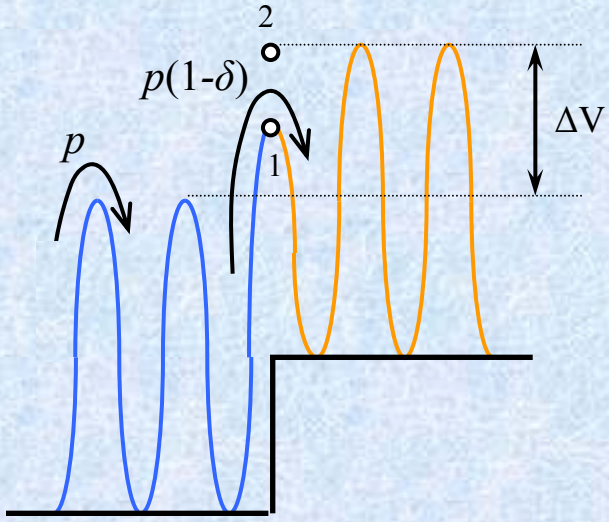






Modelo en una dimensión



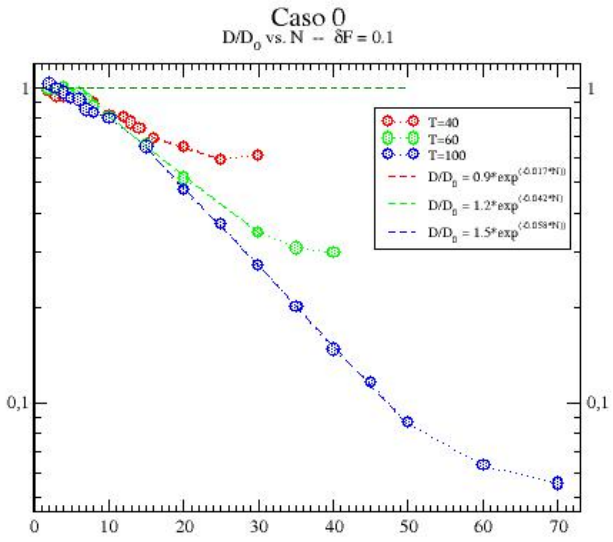


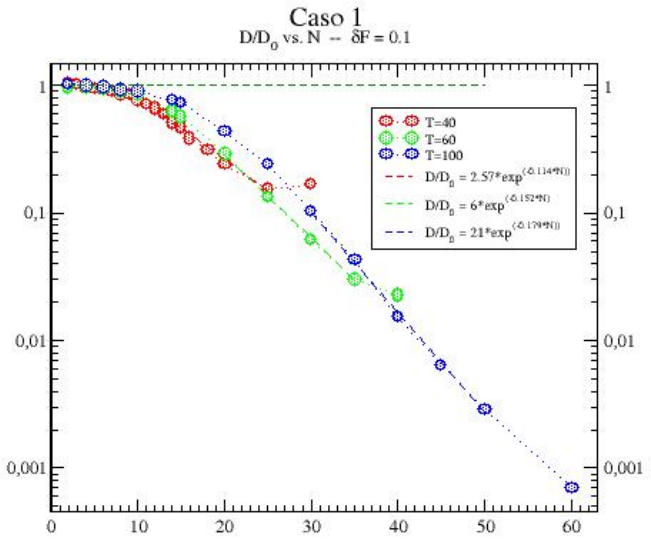
$$p(1\pm\delta) = \underbrace{Ae^{-(E/kT)}}_{p}\underbrace{e^{\pm(\Delta V/2kT)}}_{p(1\pm\delta)}$$

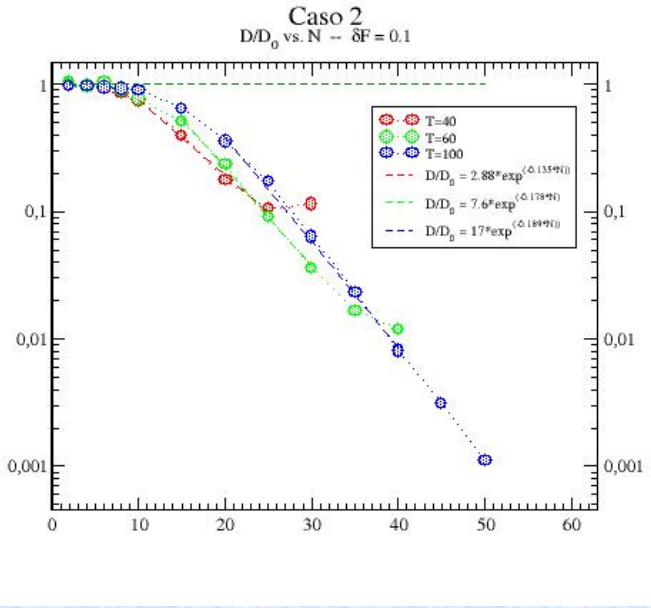
$$\delta = \Delta V/2kT$$

Resultados preliminares

$p_a + p_b = p_c$







El decaimiento de D/D_0 con N es debido a la estructura lamelar del medio.

Gracias
por su atención