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International Centre for Theoretical Physics

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World Year of PHYSICS 2005

SMR.1670 - 18

INTRODUCTION TO MICROFLUIDICS

8 - 26 August 2005

Influence of Various Flows on Single Polymer Dynamics and Stretching

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Influence of various flows on single polymer dynamics and stretching

(polymer dynamics and stretching in simple flows,
and in a random flow –elastic turbulence
in micro-geometry)

Lecture 3

V. Steinberg

**Summer School in Microfluidics,
August 8-26, 2005, ICTP, Trieste, Italy**

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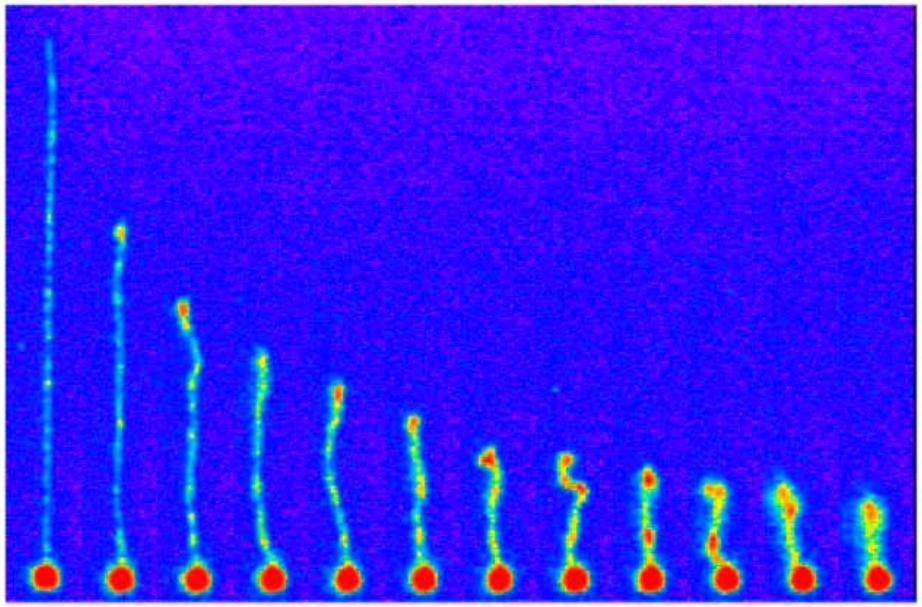
Some basic features

polymer coil

A polymer molecule consists of many monomers, $N = O(10^5)$; exists in coiled state in solution

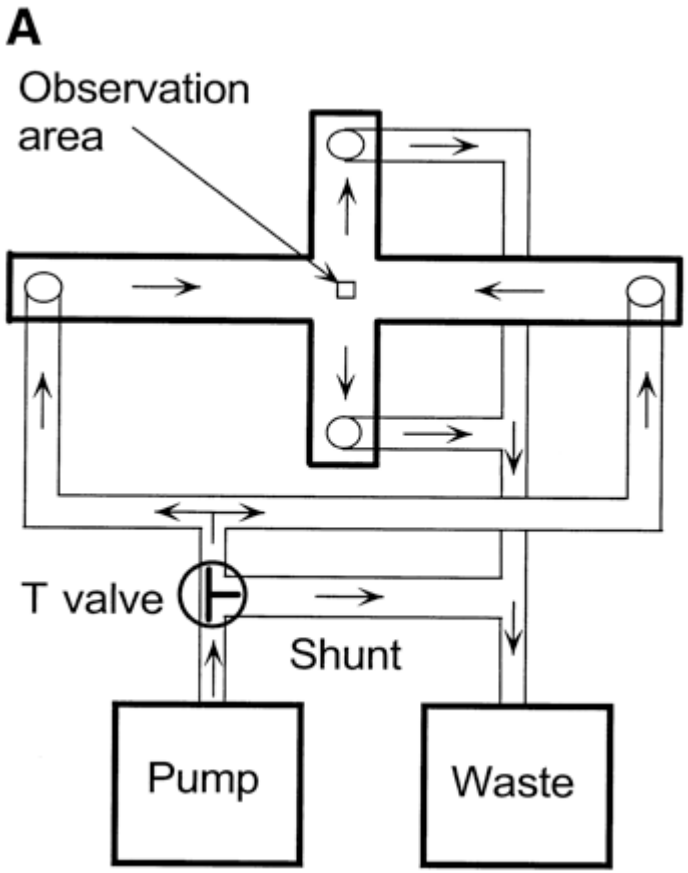
a, size of monomers = O(1Å); size of coil = radius of gyration, $R_g \sim aN^{3/5}$ (the so-called Flory radius for swollen coil)

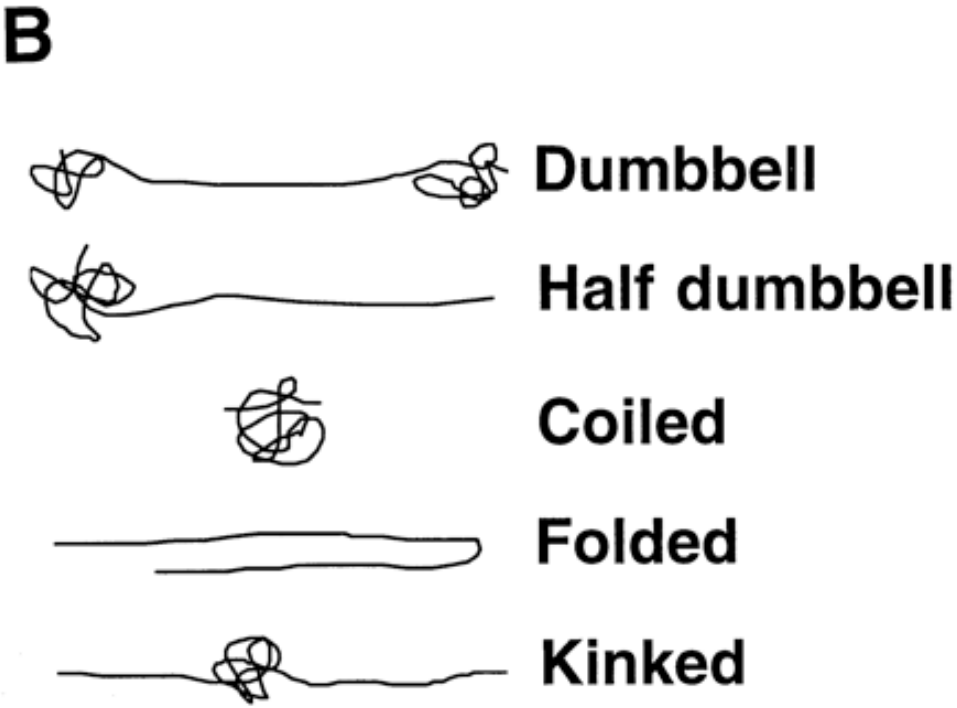
Zimm relaxation time $T_z = R_g^3 \mu_0 / kT$



Images of a single DNA molecule (~40 microns long) tethered to a 1 micron latex bead. The bead was trapped using optical tweezers and the DNA was labeled with a fluorescent dye. The DNA was stretched in a flow (far left) and its entropic relaxation was observed after the flow was turned off (left to right, 5 second intervals). From Perkins, Smith & Chu, *Science* 264, 819 (1994)

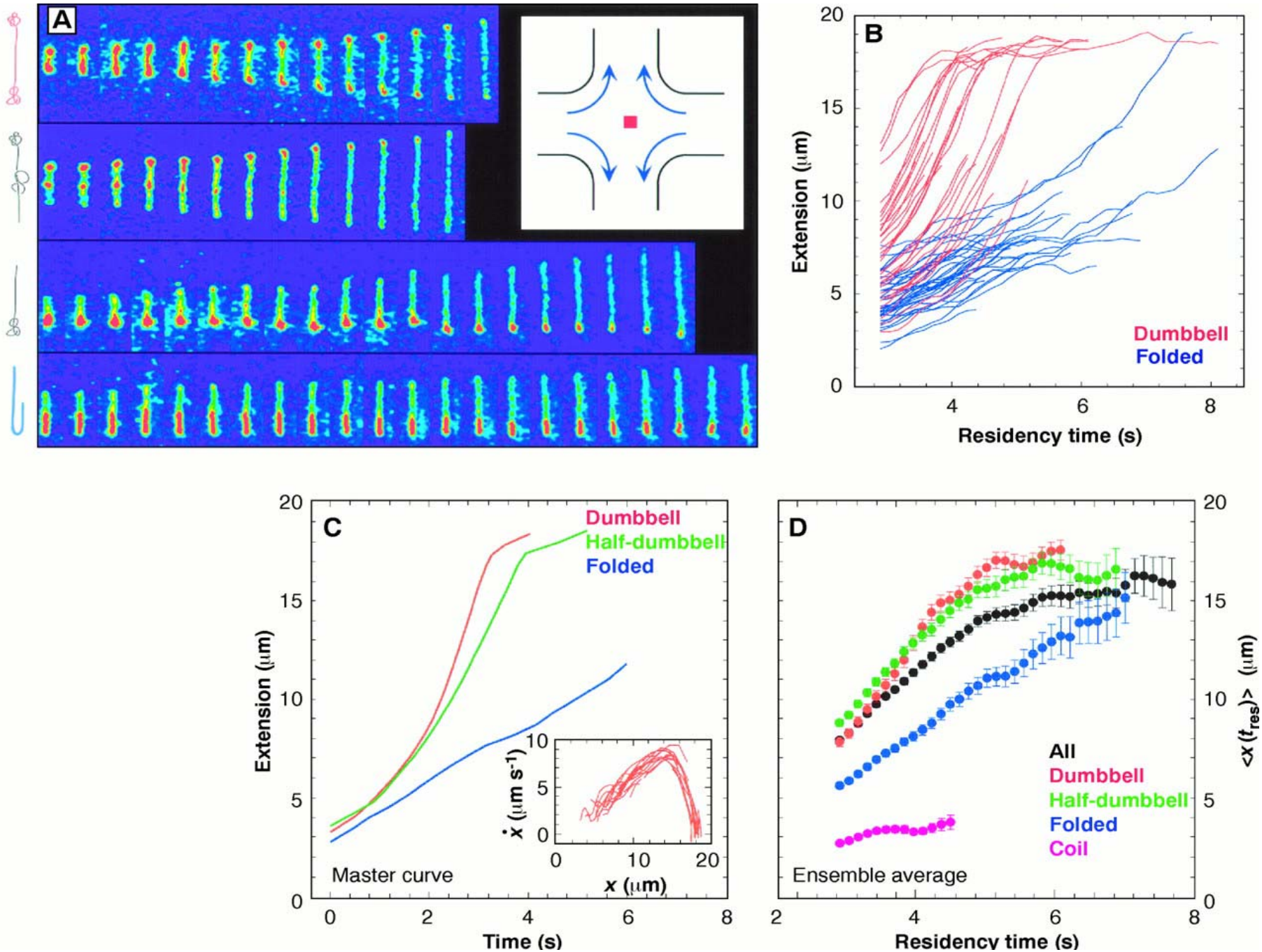
Single-Polymer Dynamics in simple stationary flows (elongational, shear, and mixed)

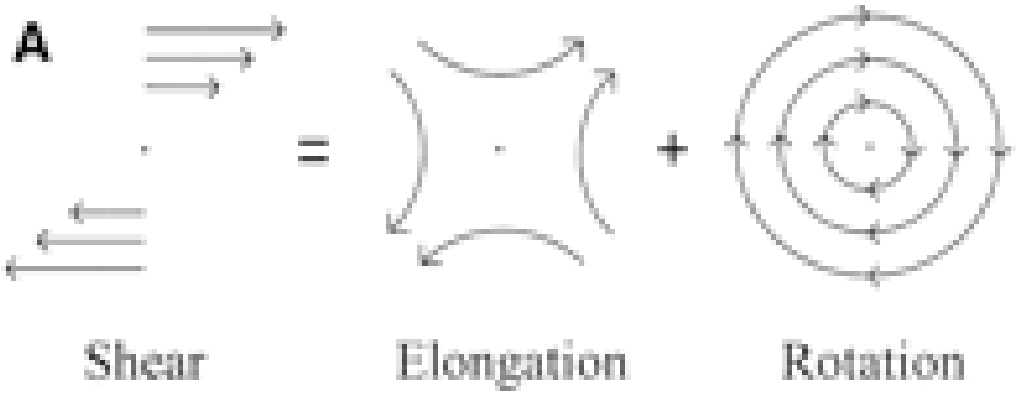




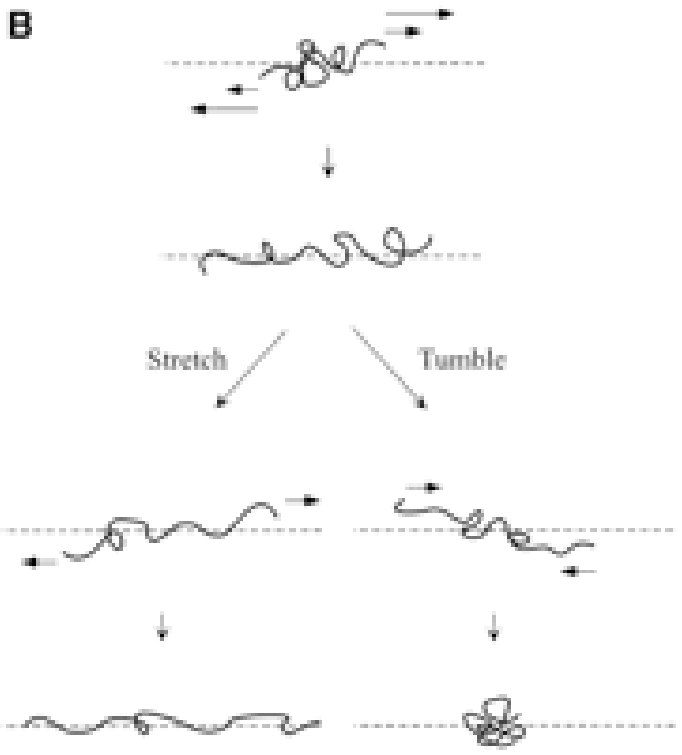
Schematic drawings of the different transient polymer conformations observed during stretching

Coil-Stretch transition in elongational flow (T. Perkins, D. Smith, S. Chu (1997)).

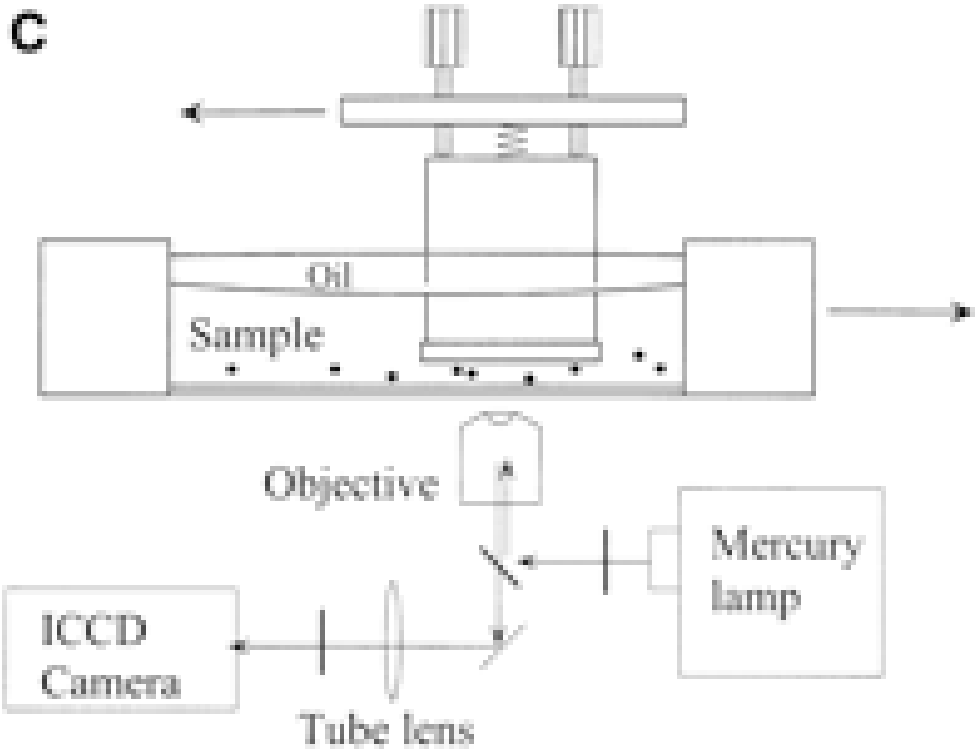

A
B
Extension (μm)
Residency time (s)
Dumbbell
Folded
C
Dumbbell
Half-dumbbell
Folded
Extension (μm)
Time (s)
Master curve
ẋ (μm s⁻¹)
x (μm)
D
All
Dumbbell
Half-dumbbell
Folded
Coil
Ensemble average
Residency time (s)
<x(t_res)> (μm)



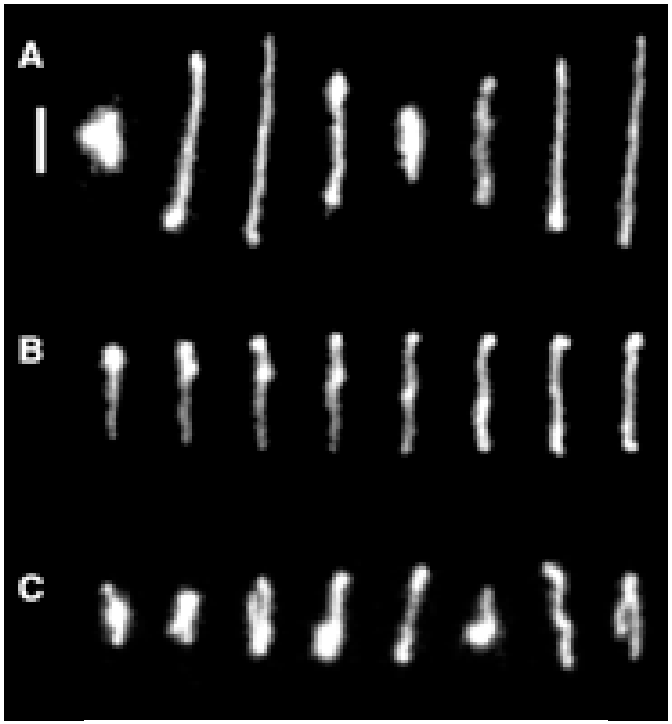
Simple shear flow

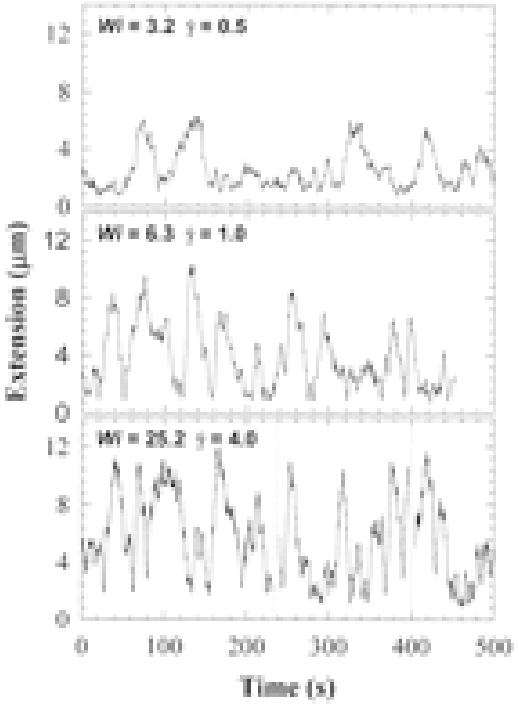


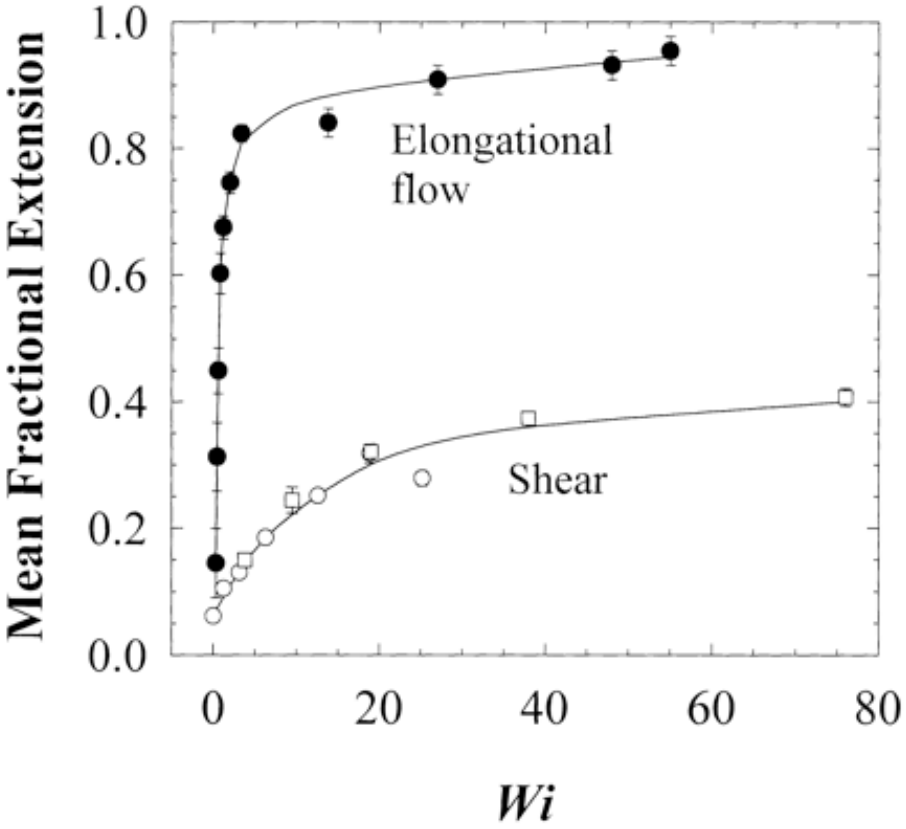
Flexible polymer stretching in a shear flow: stretch and tumble



Schematic diagram of set-up



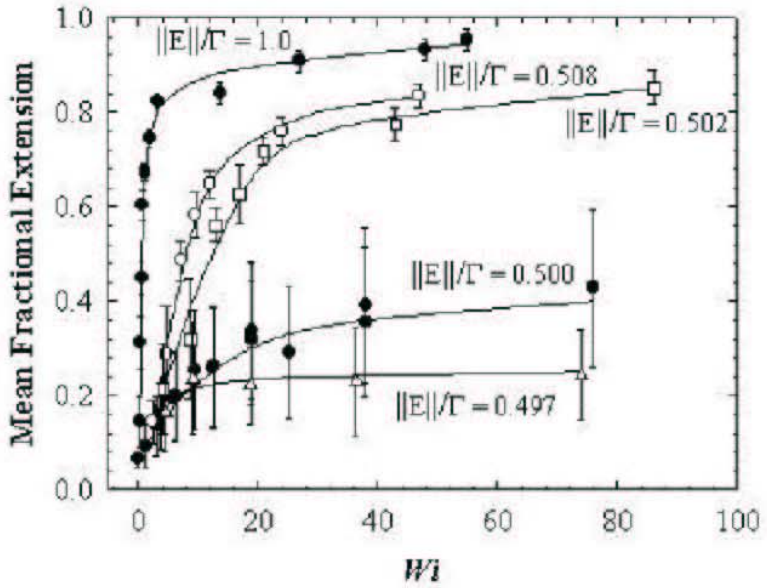




D. Smith, H. Babcock, S. Chu (1999).

Coil-stretch transition

(data from S. Chu's lab, Stanford)



DNA stretching by pure strain and mixed rotational strain

$$\eta = \eta_0(1+\alpha c R_{eff}^3)$$

R_{eff} = effective dimension of the suspended object;
c = concentration (objects/volume)

H. Babcock, R. Teixera, J. Hur, E. Shaqfeh, S. Chu (2003).

Single Polymer Dynamics: coil-stretch transition in a random flow.

S. Geraschenko, C. Chevallard, V. Steinberg, Europhys. Lett. **71**, 221 (2005)

Theory of Polymers Dynamics in Turbulent Flow: long-standing problem

(Lumley (1971),

E. Balkovsky, A. Fouxon, V. Lebedev, ***PRL* 84,** 4765 (2000)

M. Chertkov, ***PRL* 84**, 4761 (2000)

A. Celani, S. Musacchio, D. Vincenzi, ***J. Stat. Mech***. **118**, 529 (2005)

M. Chertkov, I. Kolokolov, V. Lebedev, K. Turitsyn, accepted to ***J. Fluid Mech.*** (2005)

K. Turitsyn, submitted to ***PRE*** (2005)

M. Martins, D. Vincenze, submitted to ***J. Fluid Mech***. (2005)

Polymer molecule in turbulent or chaotic flow

R<η-dissipation length.

So a polymer molecule is immersed into spatially smooth and temporally random velocity field (similar to Batchelor problem of passive scalar mixing).

Thus, dynamics of stretching is governed by the velocity gradient only

$$\vec{V}(r,t) = \frac{\partial V_i}{\partial r_j}(t)\cdot\vec{r}$$

$\frac{\partial V_i}{\partial r_j}$ -rate of deformation in Lagrangian coordinates randomly varies in time.

Two nearby fluid elements diverge exponentially on average:

$$\langle R(t)\rangle = R(0)\exp(\gamma t)$$

Since polymer molecule follows deformation of a fluid element, it can be stretched significantly even in a random flow (γ is the Lyapunov exponent and defines the rate of stretching of a fluid element)

Elastic turbulence and statistics of polymer molecules extension.

$R_0 << R << R_{max}$

Dynamic equation for the end-to-end vector **R=Rn:**

$$\frac{d}{dt}R_i = R_j \nabla_j V_i - \frac{R_i}{\tau}$$

Probability distribution function of the molecule size R:

$$P(R_i) \propto R_0^{\alpha} R_i^{-\alpha-1} \quad \text{where} \quad \alpha \propto (\tau^{-1} - \gamma)$$

At $\alpha<0$ the majority of molecules is strongly stretched.
At $\alpha>0$ the majority of molecules has nearly equilibrium size.

α changes sign at $\gamma\tau=1$. At $\gamma\tau<1 \Rightarrow \alpha>0$; at $\gamma\tau>1 \Rightarrow \alpha<0$.

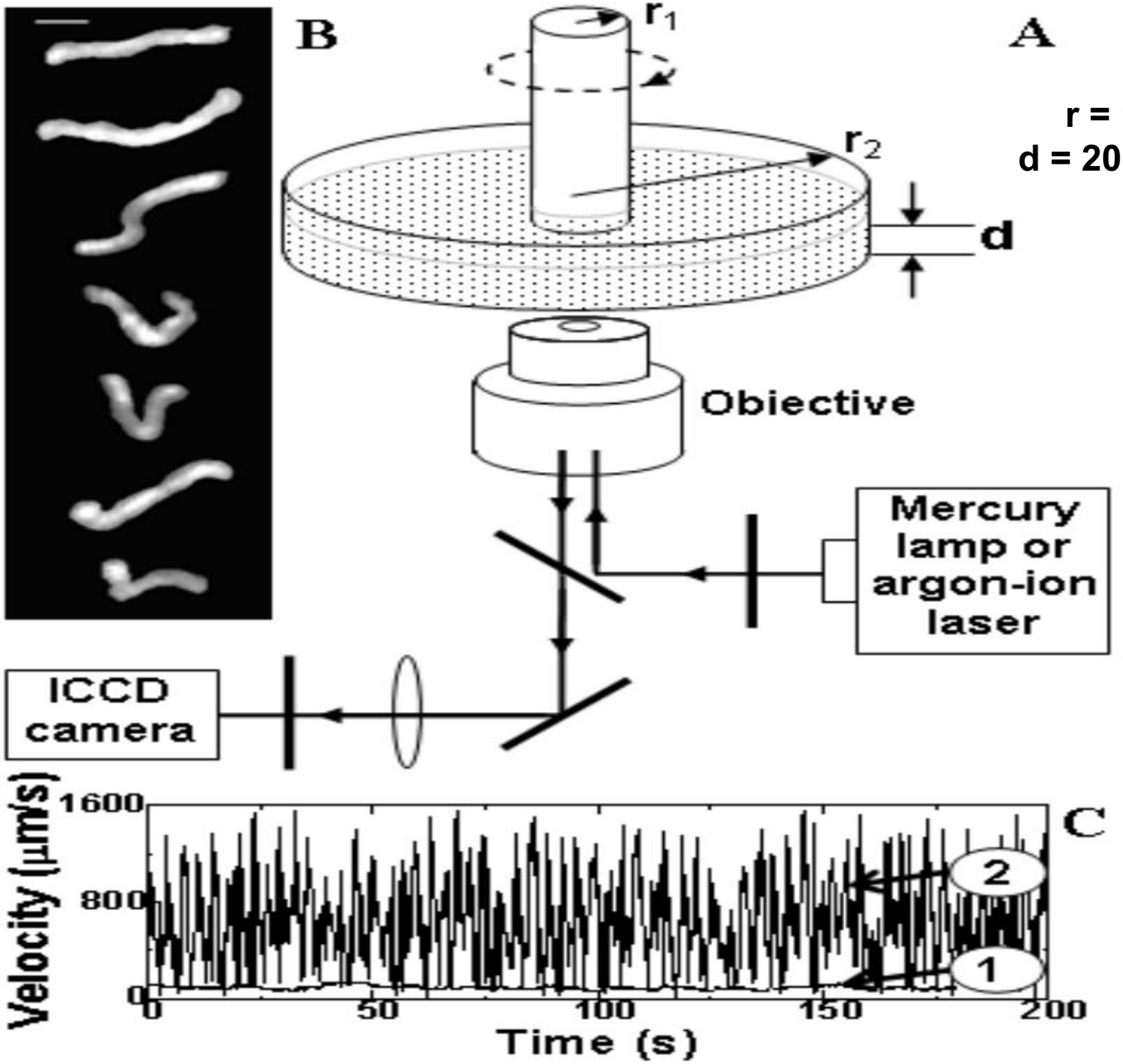
*Thus, Wi'=$\gamma\tau$ plays a role of a local Weissenberg number for a random flow and the condition $\alpha=0$ can be interpreted as the criterion for the coil-stretch transition in a random flow that occurs at **Wi'=1**.*

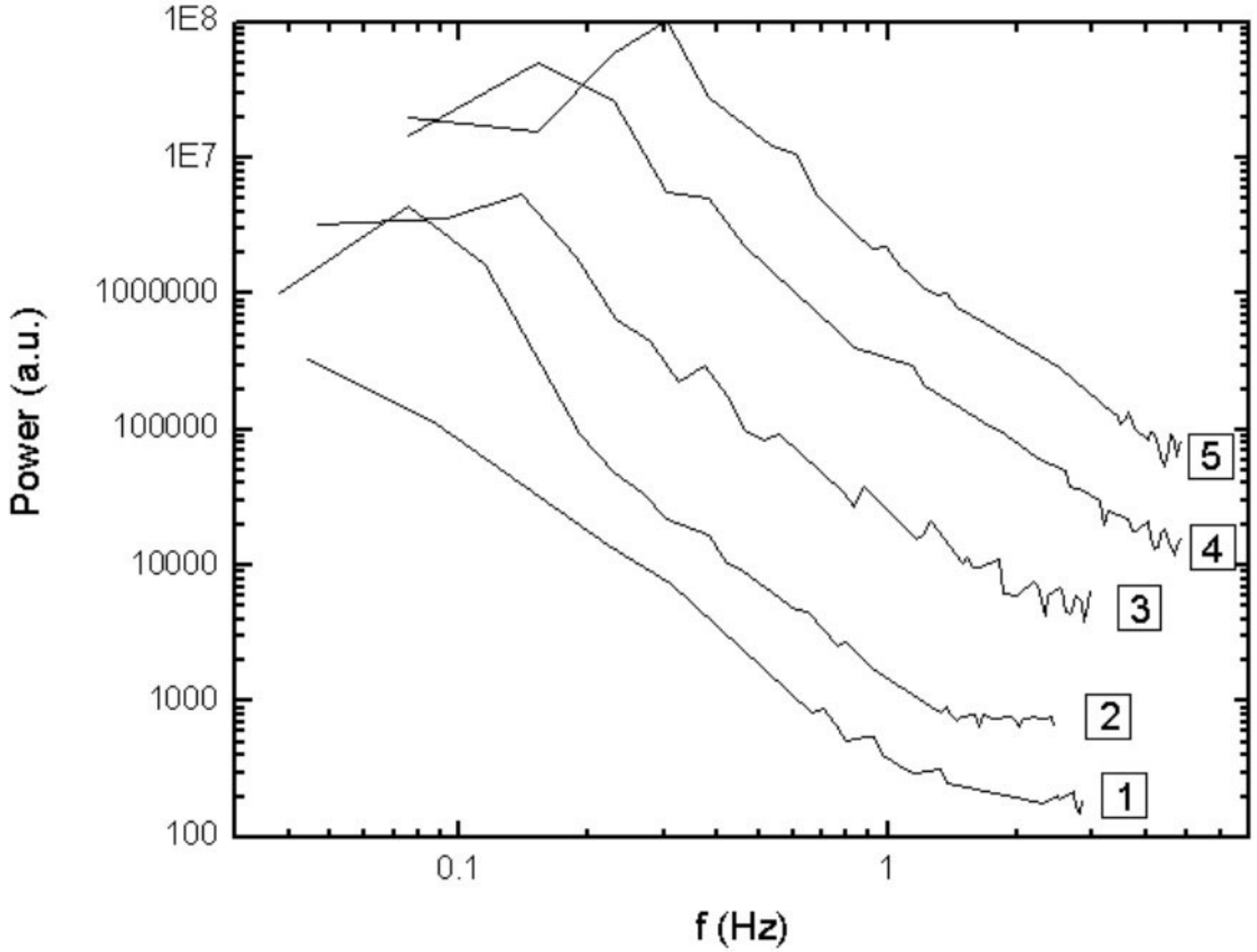
Numerical Simulations

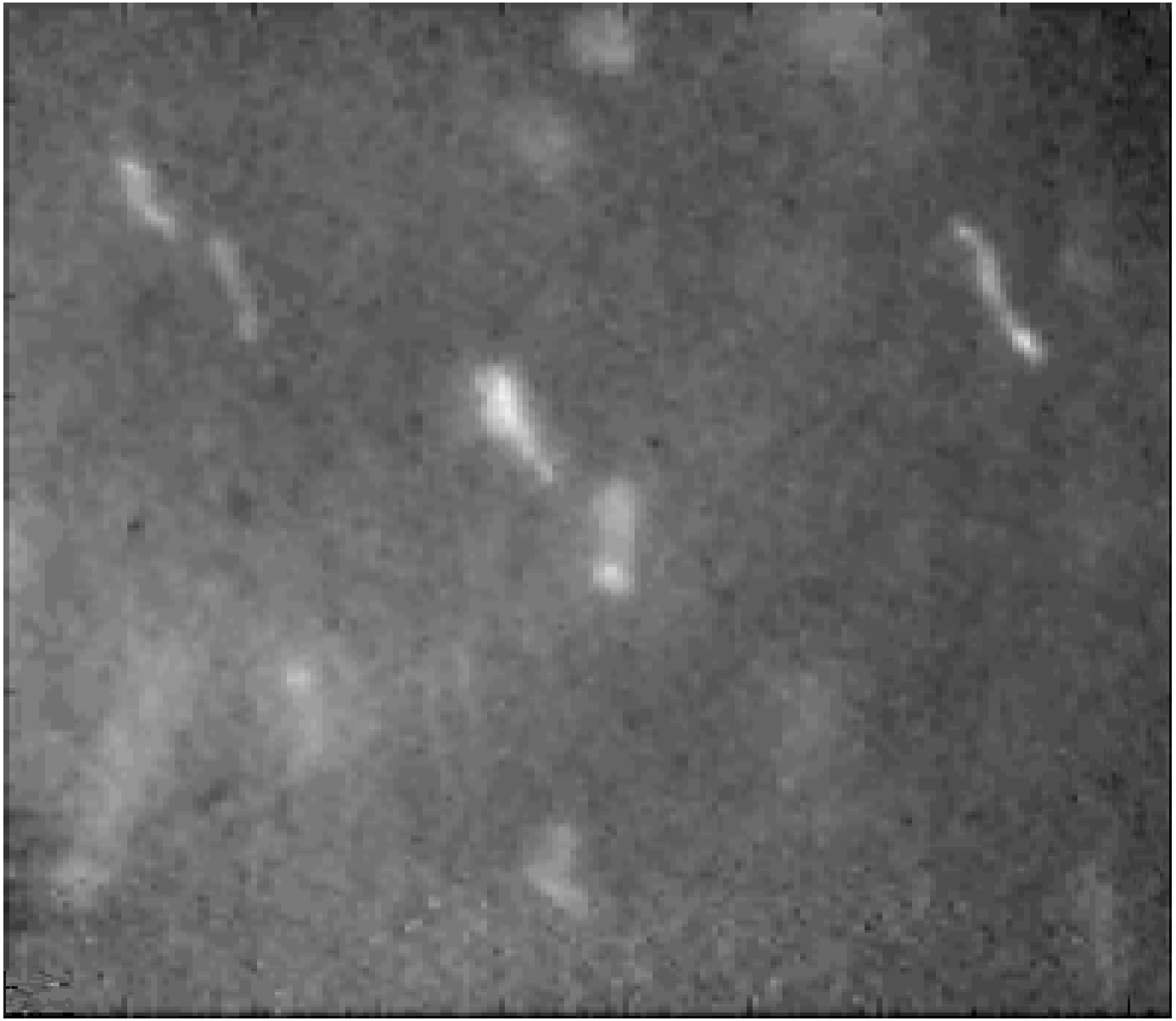
B. Eckhardt, J.Kronjager, J.Schumacher, ***Comput. Phys. Commun.*** **147**, 538 (2002)

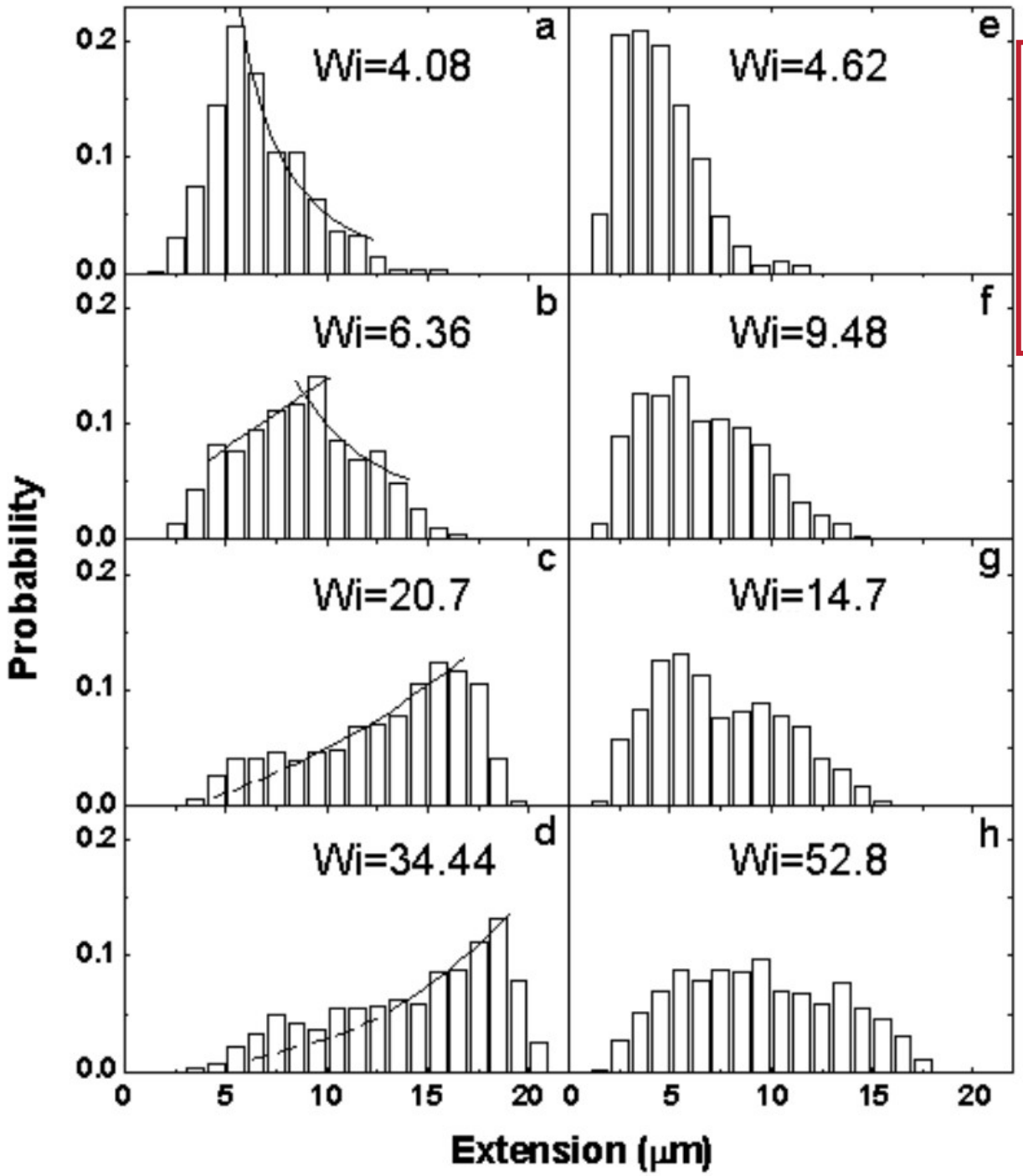
G. Boffetta, A. Celani, S. Musacchio, ***PRL*** **91**, 034501 (2003)

A. Celani and A. Puliafito, private communication and to be published (2005)

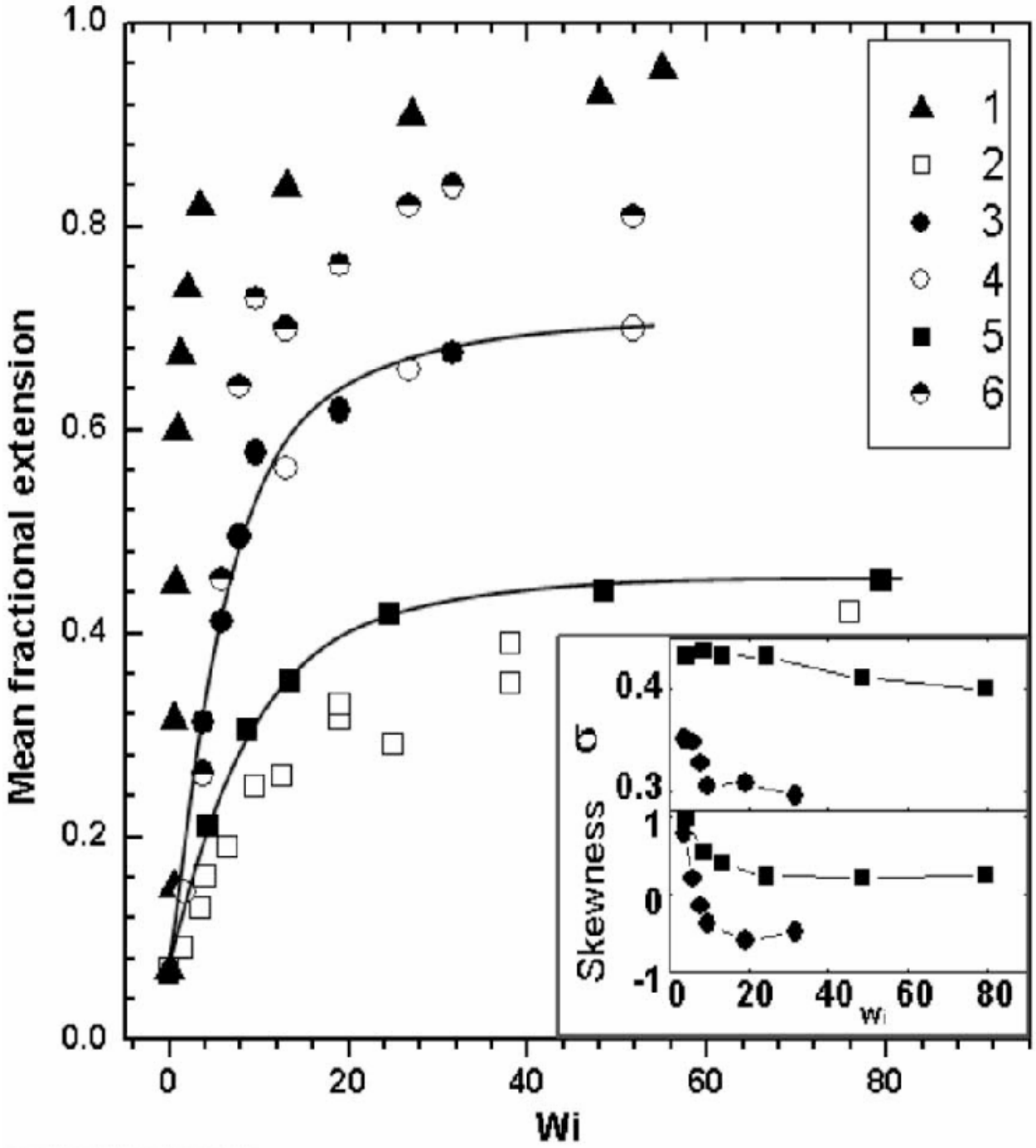

B
A
r1
r2
d
r = 1mm
d = 200 μm
Objective
Mercury lamp or argon-ion laser
ICCD camera
C
Velocity (μm/s)
1600
800
0
0
50
100
150
200
Time (s)
2
1


1E8
1E7
1000000
100000
10000
1000
100
Power (a.u.)
0.1
1
f (Hz)
5
4
3
2
1

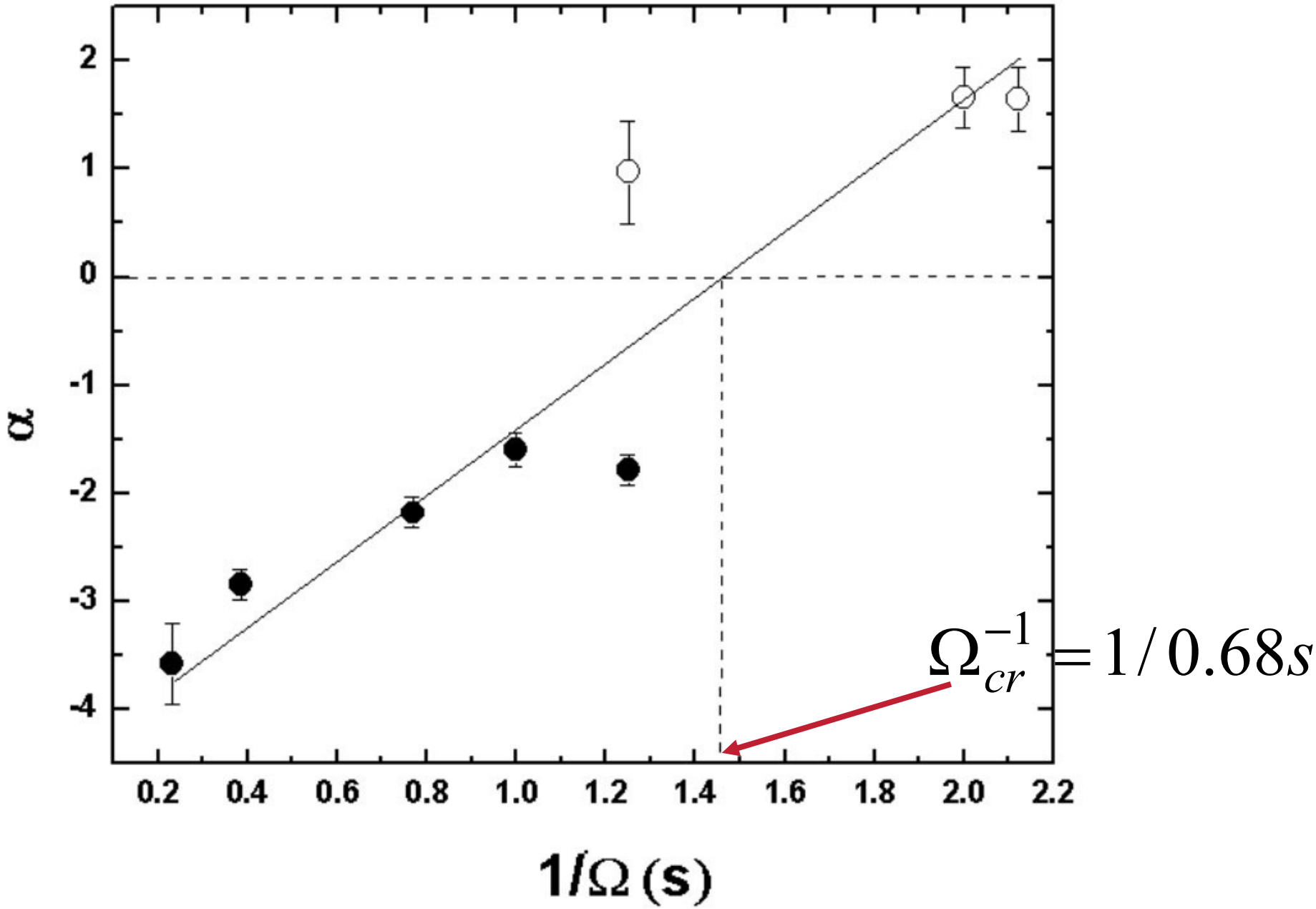




PDF of polymer extension at various Wi in random (left) and shear (right) flows
Solid lines are fits by power law $P(R_i) \propto R_i^{-\alpha-1}$ ***with*** α ***defined from the fits.***



(1)-elongational flow (S.Chu et al, (1997));
(2)-plane shear flow (S.Chu et al, (1999));
(3,4)-random flow in λ-DNA and PAAm solutions;
(5)-shear flow in both solutions
(6)-fractional extensions in random flow corresponding to PDF's maximum



Black dots are the data above the coil-stretch transition, open circles- below

Finite-time Lyapunov exponents

- Probability of finite-time Lyapunov exponents (FTLE) is defined as

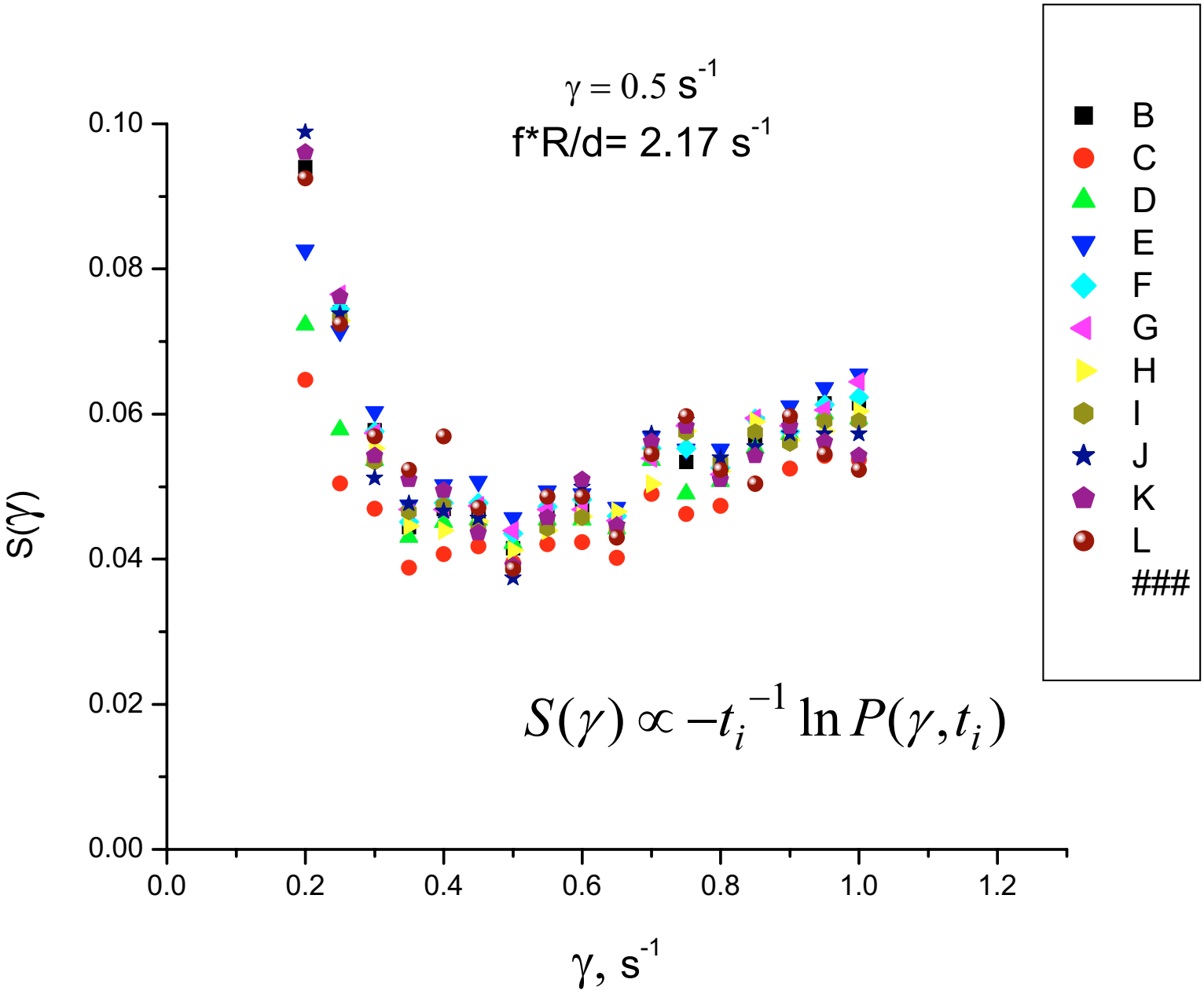
$$P(\gamma, t_i) \propto \exp[-t_i S(\gamma)]$$

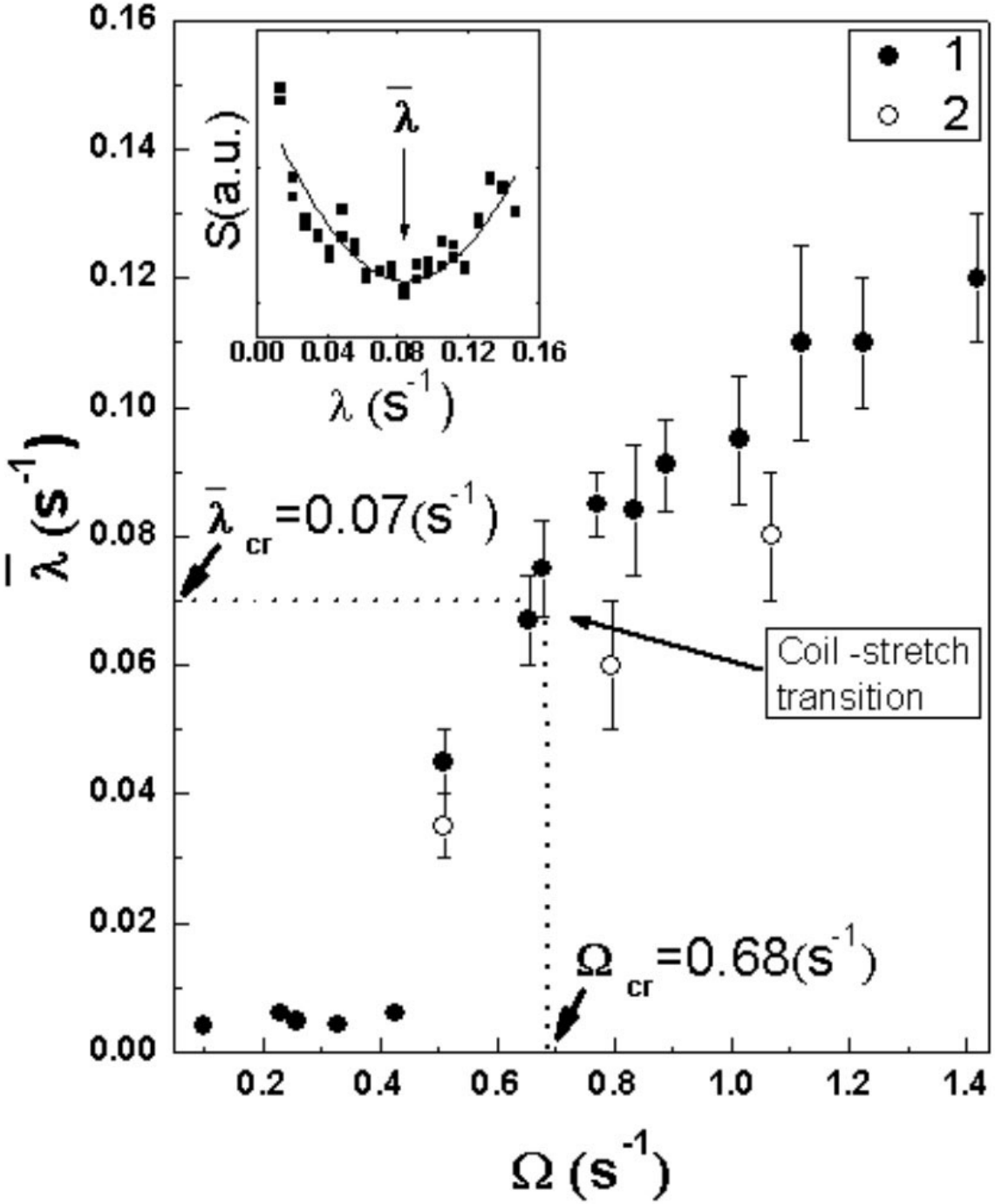
- By rescaling one can collapse the probability distribution functions for different $t_i < t_{corr}$ on one curve

$$S(\gamma) \propto -\frac{\ln P(\gamma, t_i)}{t_i}$$

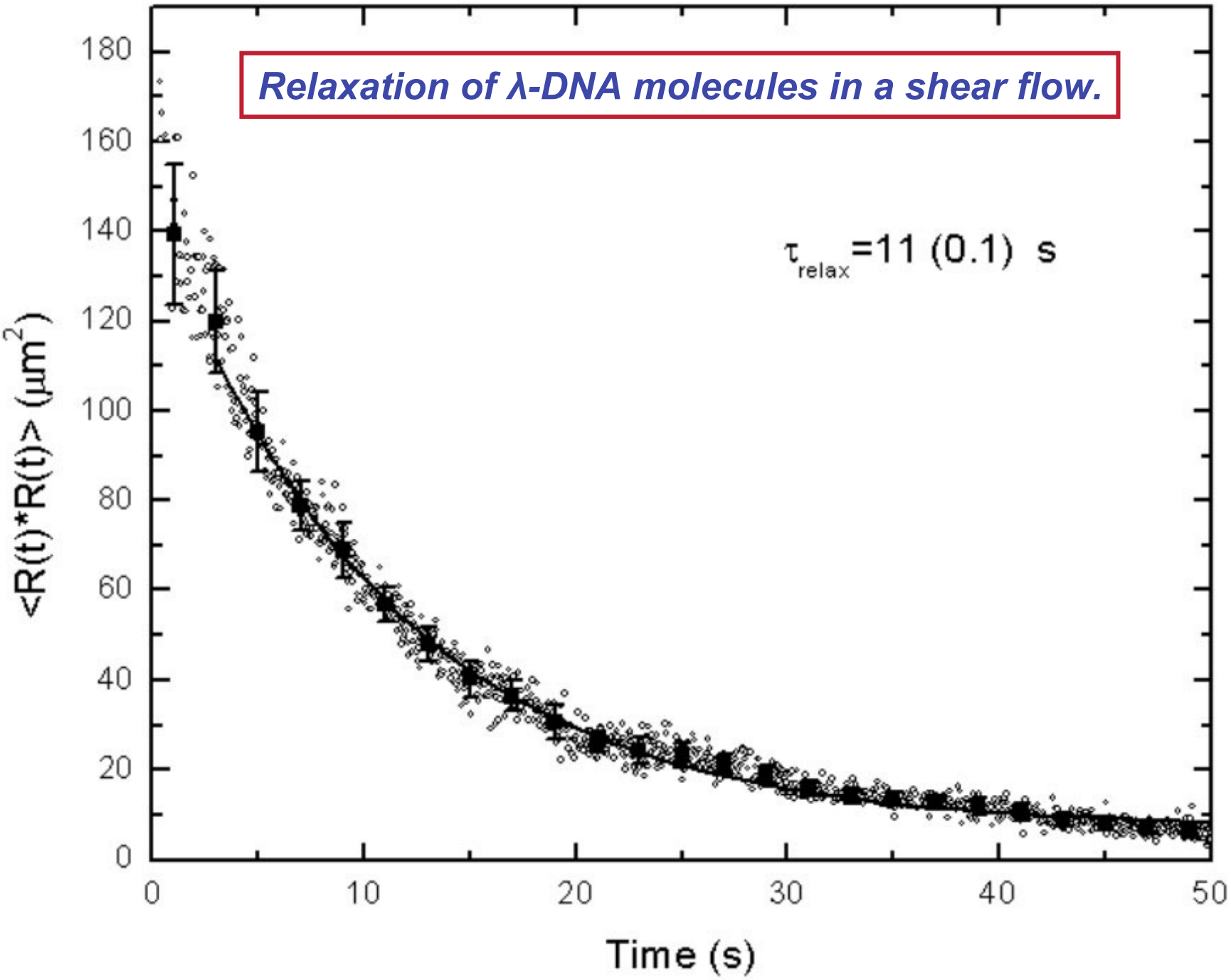
where S(λ) is the Cramer rate function.

- Minimum of $S(\gamma)$ determines the average Lyapunov exponent $\overline{\lambda}$ for a given rotation rate (i.e. $\overline{\lambda}(t_i) \cong const$ for all PDFs scaled).


$\gamma = 0.5\ s^{-1}$
f*R/d= 2.17 s^{-1}
$S(\gamma) \propto -t_i^{-1} \ln P(\gamma, t_i)$
S(γ)
γ, s^{-1}
0.00
0.02
0.04
0.06
0.08
0.10
0.0
0.2
0.4
0.6
0.8
1.0
1.2
B
C
D
E
F
G
H
I
J
K
L
###



Average Lyapunov exponent $\bar{\lambda}$ *as a function of Ω for (1) PAAm and (2) λ-DNA solutions. Inset: Cramer rate function at Ω=0.83 1/s.*


Relaxation of λ-DNA molecules in a shear flow.
τrelax=11 (0.1) s
<R(t)*R(t)> (μm2)
Time (s)
0
20
40
60
80
100
120
140
160
180
0
10
20
30
40
50

Criterion of the coil-stretch transition:

$$\overline{\lambda}_{cr} = 0.07 \pm 0.015 \quad 1/\text{sec}$$

$$\tau = 11 \pm 0.1 \ \text{sec}$$

The experimental value for the critical Weissenberg number

$$\widetilde{Wi} \equiv \overline{\lambda}_{cr}\tau = 0.77 \pm 0.2$$

and should be compared with theoretical prediction:

$$\widetilde{\mathrm{Wi}} = \mathbf{1}$$

Conclusions

- *Elastic turbulence is rather general dynamic phenomenon, which can occur in any system having first normal stress difference.*
- *Elastic turbulence can be reached in very viscous polymer solutions and in very small containers.*
- *Random 3D flow with steeply decaying power spectrum of the velocity fluctuations is an ideal experimental realization of the Batchelor regime of mixing in a broad range of scales.*
- *Efficient mixing in an open flow at arbitrarily low Re, at polymer concentration as low as 7ppm is obtained in macro- and microfluidic devices.*
- *Direct relation between statistics of stretched polymer molecules and statistics of a turbulent flows is found.*
- *The criterion of coil-stretch transition in a turbulent flow is quantitatively verified.*