SoftComp
SOFT MATTER COMPOSITES
Network of Excellence
www.eu-softcomp.net
news letter
No. 2 · June 2006

Editorial

This issue of the SoftComp Newsletter coincides with the beginning of the third SoftComp NoE year, June 1st 2006 to May 31st 2007.

Thus, the scientific contributions in this newsletter reflect the work of the past second SoftComp reporting period. While the popular scientific article *"Parachutes in the bloodstream"* offers an exciting inside view of SoftComp's simulation research activities and its potential biomedical applications, the articles *"Colloidal Glasses"* and *"Non-equilibrium Phase Behaviour and Vorticity Shear banding of Rod-like Colloids in Shear Flow"*, show two further highlights of SoftComp NoE research activities.

If you are interested in more details of the SoftComp research programme, its publications or educational activities, please have a look at the SoftComp web portal: www.eu-softcomp.net

Hugo Bohn & Dieter Richter

Latest News

New research school...
An International Helmholtz Research School of Biophysics and Soft Matter at the Forschungszentrum Jülich, Germany in cooperation with the Universities of Düsseldorf and Cologne has been approved by the Helmholtz Gemeinschaft. Starting date: fall 2006. www.ihrs-biosoft.de

Accepted new partners...
Farfield Scientific, Cheshire, UK
Imperial College, London, UK

In this issue

Parachutes in the bloodstream

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Haemoglobin in the blood cells colours the blood red; this has long been general knowledge. But the red blood cells also have a decisive influence on the flow properties of blood. In fluid flow, they change their normal discus shape, which means that blood can flow faster through the capillaries. The elasticity of the cell surface plays an important part in this process. Computer simulations – part of the SoftComp research programme on complex membranes – allow a detailed investigation of the flow behavior of red blood cells. The results have recently been published in the journal Proceedings of the National Academy of Sciences, USA. (www.pnas.org)

Red blood cells are not rigid. Their surface consists of a lipid membrane with properties similar to the skin of a soap bubble. But underneath there is a skeleton of rigid polymers: the spectrin network. Together they determine the bending and shear rigidity of the cell.

In a detailed computer simulation, both components of the skin of the cell with their different properties were studied. Equally important for the hydrodynamic behavior in flow is the modelling of the solvent. Since there is an enormous length-scale gap between the nanometer size of the solvent molecules and the micrometer scale of the red blood cell, a coarse-grained, mesoscopic description of the solvent is essential.

Fig. 2 – **Red blood cells have the form of a discus at rest and in slow flows – as observed in computer simulations.**

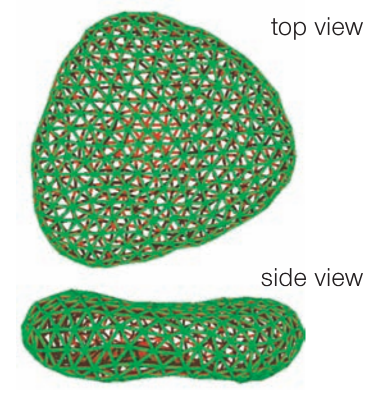
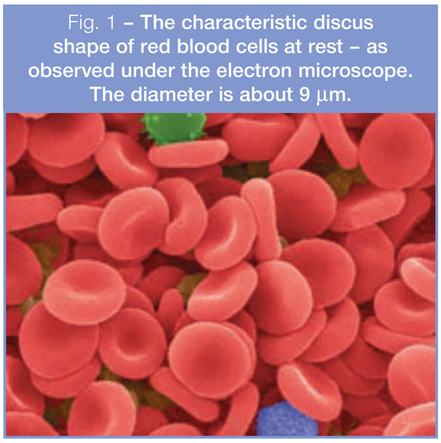


Fig. 1 – **The characteristic discus shape of red blood cells at rest – as observed under the electron microscope. The diameter is about 9 μm.**



The result: only the rigidity of the spectrin network enables the red blood cells to take on the shapes they do in flow experiments.

Only at rest does the cell adopt its characteristic shape, the discus, with depressions on both sides (Figs. 1 and 2). In the computer simulations, this shape is obtained by minimizing the bending and stretching energy at a fixed surface

Parachutes in the bloodstream (continued)

Fig. 3 – **Red blood cells change their shape in fluid flows. In faster flows they adopt the shape of a parachute. Blue arrows indicate the parabolic velocity profile of the solvent.**

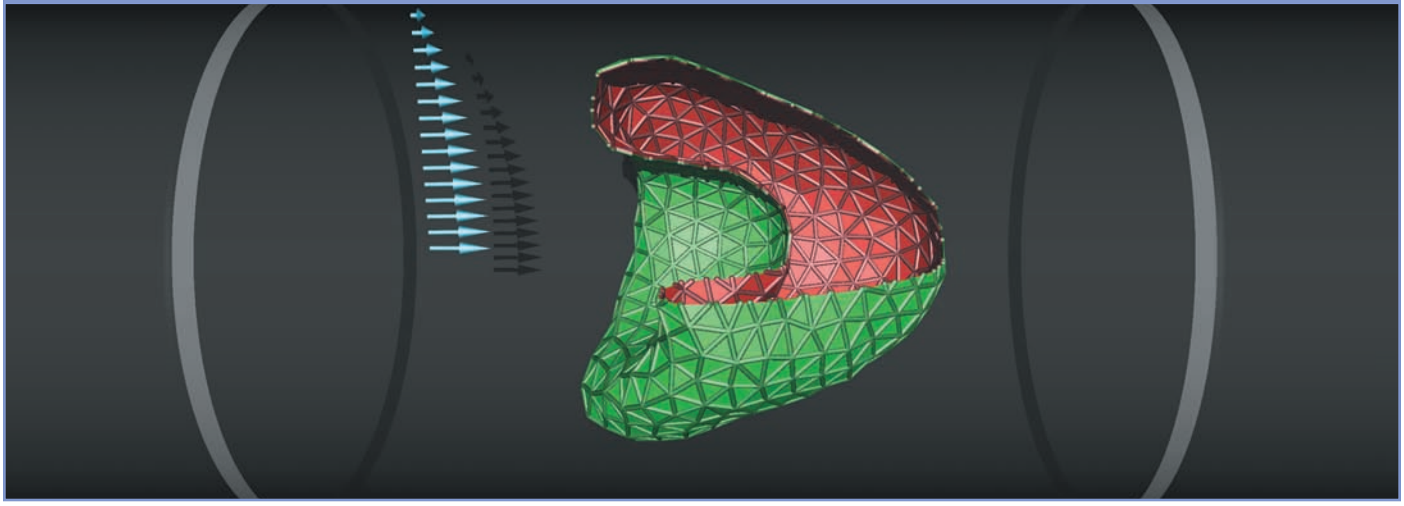
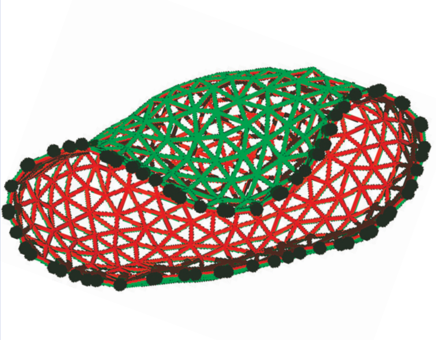


Fig. 4 – **Red blood cells during the transition assume the shape of slipper.**



area and the proper internal volume. Interestingly, the cells are found to orient their axis of rotational symmetry perpendicular to the capillary axis for slow flows. Above a certain flow velocity, this changes dramatically (Fig. 3). The cell bends back so strongly that it resembles a parachute. In contrast, droplets that only have a fluid lipid layer tend to deform into the elongated shape of a rugby ball. The reason is that fluid vesicles can deform quite easily, and minimize the flow forces by elongating in the center of the parabolic flow profile. The shear elasticity of the spectrin network prohibits such elongated shapes – the fast flow in the center of the capillary and the slow flow near the walls then induces the parachute shape.

And yet another cell shape is observed. During the transition, a transient asymmetrical entity is formed, which resembles a slipper (Fig. 4).

Of particular interest was the flow velocity at which the transition from discus to parachute shape occurs. The more rigid the cell becomes, the faster the required fluid flow (Fig. 5). Some metabolic disorders, such as diabetes mellitus, change the material properties of the cell membrane and may influence the blood circulation via this mechanism. However, it is suspected that only the appropriate shapes of the red blood cells ensure that the blood flows with relatively low resistance and the heart can work at low pumping pressures.

Fig. 5 – **The flow velocity V_m required to induce the discus-to-parachute transition for red blood cells increases linearly with increasing bending rigidity κ (full line). For fluid vesicles transition from discus to prolate ellipsoid is found (dashed line).**

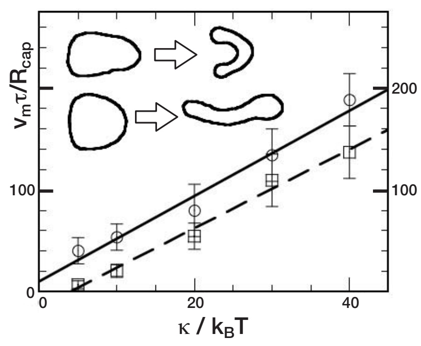
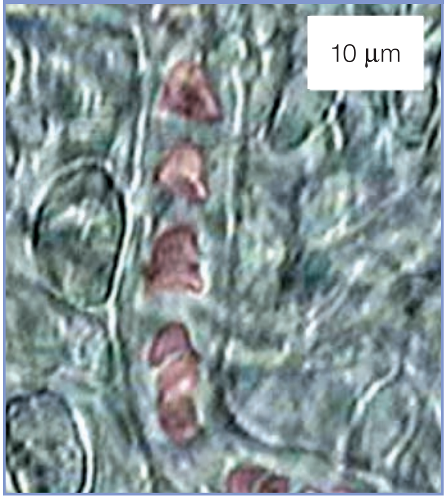


Fig. 6 – **Experiments on red blood cells in micro vessels show parachute shapes at physiological flow rates, but also clustering of several cells. (http://www.ncvc.go.jp/res-old/Microcir.html)**



Optical microscopy of micro vessels shows that red blood cells do indeed form parachute shapes at physiological flow rates (Fig. 6). In addition, cells seem to move in small clusters. Therefore, simulations in the future, will be extended from individual cells to whole groups of blood cells. Attention will be focused on the connection between the material properties of the cells and the flow properties of blood as a whole.

Colloidal Glasses

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Summary

Colloidal glasses are amorphous, metastable, solid states of concentrated suspensions of particles in which formation of the expected equilibrium colloidal crystal is prevented by **structural arrest.** Structural arrest can be caused simply by crowding, so that repulsive particles are permanently trapped within **cages** formed by their neighbours (repulsive glasses), or by attractive forces between the particles which lead to permanent clustering (attractive glasses). After reviewing early work on repulsive glasses composed of **hard-sphere** PMMA colloids suspended in organic liquids, this paper [1] emphasised more recent studies of the re-entrant transition - repulsive glass ⇨ liquid ⇨ attractive glass (see below) - predicted by mode-coupling theory when an increasingly strong narrow attraction is added to the hard-sphere repulsion. Recent rheological measurements on the two types of glass were summarised briefly.

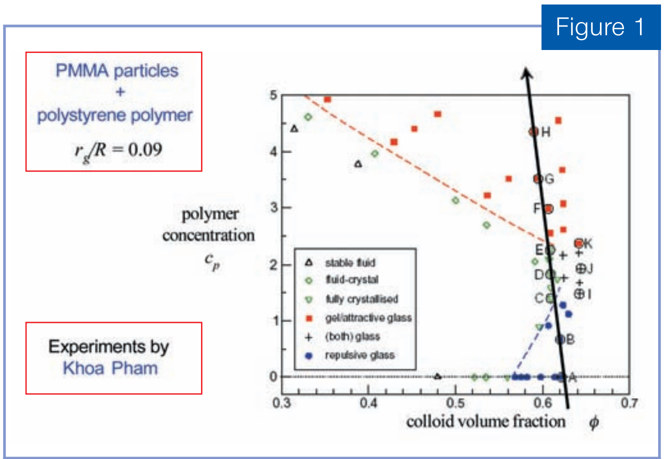
Repulsive glasses

An assembly of hard spheres at equilibrium is expected to show liquid-like behaviour for volume fraction $\phi \leq 0.494$, liquid-crystal coexistence for $0.494 \leq \phi \leq 0.545$, and crystal for $\phi \geq 0.545$ up to close packing at $\phi = 0.74$. In fact, samples of hard-sphere colloids, mixed by thorough shaking, do not crystallize at $\phi \geq 0.58$ but remain as amorphous repulsive glasses [2]. Dynamic light scattering (DLS) measurements [3,4] on metastable, shear-melted fluids show a dramatic slowing down of particle diffusion with increasing concentration, and the emergence of a non-decaying **plateau** in the intermediate scattering function (ISF), signalling structural arrest, at the glass transition concentration $\phi_G \approx 0.58$. The ISFs measured by DLS are in good agreement with the predictions of mode coupling theory (MCT) for the hard-sphere glass transition [4].

Attractive glasses

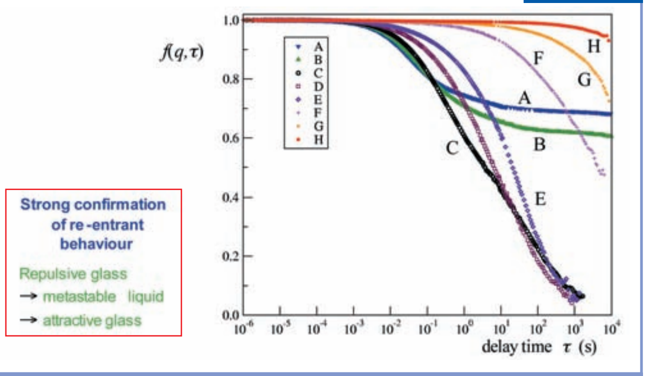
In 1999, MCT was applied to particles interacting through a potential with a hard core, followed by a narrow attraction [5]. These calculations predicted a detailed and complex scenario of behaviour, as the strength of the attraction was varied. Subsequent experiments by various groups, including experiments in Edinburgh, soon verified many of these predictions. Figure 1 shows Edinburgh results for PMMA colloids where the attraction was induced through the depletion effect of added small polymers, its strength being (approximately) proportional to the polymer concentration $\mathbf{c_p}$ [6]. Without attraction, $\mathbf{c_p} = 0$, the normal hard-sphere glass is found, e.g. sample A. Samples C-E, with a moderate amount of added polymer (moderate attraction), were metastable fluids, which crystallised in time. However, more polymer (samples F-H) led to samples, which again did not crystallise.

Figure 1



Phase Diagram

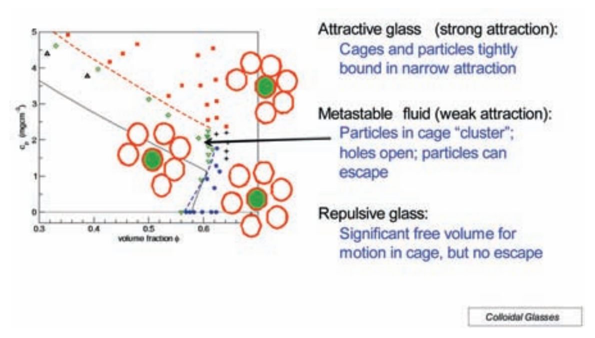
Figure 2



DLS results at $qR = 1.5$

These macroscopic observations were supplemented by DLS measurements of the microscopic dynamics (Fig. 2) [7]. Samples A and B show the usual behaviour of hard-sphere glasses, an initial decay of the ISF, $f(q,\tau)$, associated with **rattling** of the particles in their neighbour cages, followed by a plateau indicating structural arrest, the suppression of long-distance diffusion and of crystal nucleation. However, with moderate attractions (samples C-E) the ISFs decay completely to zero, consistent with long-distance diffusion – the glasses have been melted to metastable fluids which subsequently crystallise. Strong attractions (samples F-H) again give ISFs which do not decay completely – attractive glasses. Indeed the particles in sample H, for which $f(q,\tau) \approx 1$ at all times, hardly move at all, being tightly bound by the strong attraction to their neighbours. A schematic representation of the processes leading to the re-entrant transition from caged repulsive glasses, through melting, to bonded attractive glasses is given in Fig. 3. Much more data and detail can be found in Refs. 6 and 7.

Figure 3



Attractive glass (strong attraction):
Cages and particles tightly bound in narrow attraction

Metastable fluid (weak attraction):
Particles in cage "cluster"; holes open; particles can escape

Repulsive glass:
Significant free volume for motion in cage, but no escape

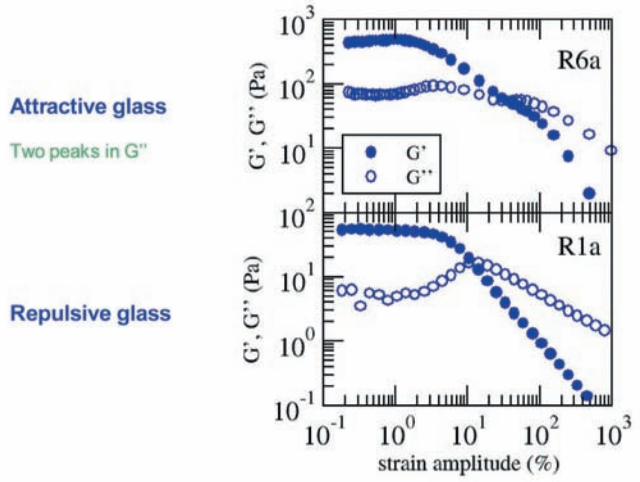
Simple-minded interpretation

Although it remains controversial, mainly because of the lack of a simple physical picture of its content, MCT has received renewed support from this and other recent work on attractive glasses, where theory motivated experiment.

Rheology

Although relatively weak applied stresses cause both repulsive and attractive colloidal glasses to flow, the observation of structural arrest by DLS indicates that both must be solid when unstressed. Recently Edinburgh has started to study, by various means, the mechanical properties and yielding and flow of these soft solids [8,9]. Fig. 4 shows the results of oscillatory shear measurements on a repulsive glass similar to sample A (above) and an attractive glass similar to sample H. Storage G' and loss G" moduli were measured at frequency $1/2\pi$ s^{-1} as a function of strain amplitude γ_0. At small strains, both glasses are solid with G' » G", and the strongly bonded attractive glass is significantly stronger, larger G', than the repulsive glass. For the repulsive glass, G' starts to decrease as γ_0 is increased, crossing G" at γ_0 ~ 10% where G" also shows a broad peak.

Figure 4



Oscillatory shear at frequency $1/2\pi$ s^{-1}

This is interpreted as yielding and the onset of flow associated with the breaking, or topological rearrangement, of neighbour cages [8]. By contrast, the attractive glass shows a more complex behaviour; G" shows two peaks, at strain amplitudes that span that shown by the repulsive glass. Tentatively the first peak is described to the breaking of the interparticle bonds and the second to the topological rearrangement of neighbours. Further work should shed more light on these interesting findings.

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Acknowledgement

All experiments were performed by Khoa Pham.
I gratefully acknowledge the contributions of other colleagues in Edinburgh, especially of Wilson Poon and Stefan Egelhaaf.

newsletter

Non-equilibrium Phase Behaviour and Vorticity Shear Banding of Rod-like Colloids in Shear Flow

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Abstract

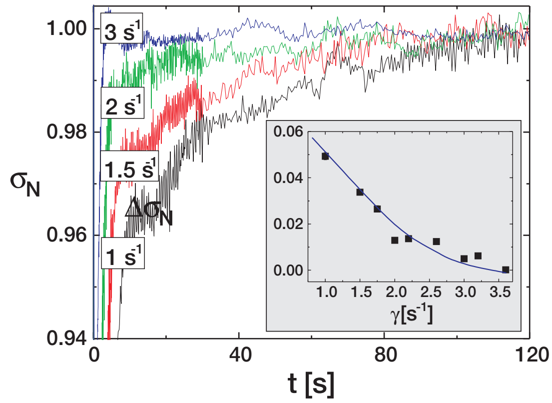
Since simple shear flow tends to align rod-like colloids, the location of the isotropic-nematic (I-N) binodal and spinodals of suspensions of rods all affected by flow. We discuss the experimental determination of the location of the binodal in the shear-rate versus rod-concentration plane for suspensions of long and thin colloidal rods. Vorticity banding is observed within the two-phase region, that is, the region enclosed by the binodal. Here, bands of differing orientational order are regularly stacked in the vorticity direction. The region where such banded structures are found is determined experimentally and the kinetics of band formation is addressed.

As a model system for colloidal rods, we use suspensions of fd virus (880 nm long, 7 nm thick, and 2.2 micron persistence length). The salt concentration is high, such that the Debye screening length is less than 1 nm. Some dextran (radius of gyration is 16 nm) is added to induce depletion attractions between the rods. This leads to a widening of the I-N biphasic gapwidth [1] and accelerates both phase-separation and vorticity-banding kinetics to reasonable experimental time scales.

1. The Non-equilibrium Phase Diagram

The paranematic-nematic binodal is measured by time resolved stress measuements after shear-quench from a high shear rate, where the homogeneous state is stable (a paranematic state is a shear-aligned state which would be isotropic in the absence of flow). The stress will increase in time after a quench below the binodal due to the formation of inhomogeneities and of the more viscous, less ordered phase (see **Fig. 1**), leading eventually to phase separation. The amplitude of the stress response decreases on approach of the binodal and is zero above the binodal. At the binodal, the amplitude of the stress response is zero, which is used to determine the location of the binodal as shown in **Fig. 2** [2].

Figure 1



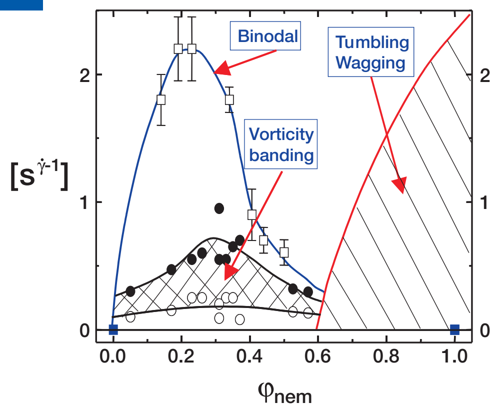
The determination of the paranematic-nematic binodal line for a mixture of fd-virus and dextran with time resolved rheology, where the stress is measured as a function of time after a shear-rate quench. The amplitude of the stress response decreases as the shear-rate increases and vanishes on the binodal, as shown in the inset.

Here, φ_{nem} is a scaled concentration of fd virus at a fixed chemical potential of dextran, such that φ_{nem} = 0 and = 1 corresponds to the lower and upper isotropic-nematic binodal concentration without flow, respectively. As can be seen from this figure, it is not possible to induce a phase transition by applying shear flow, since the slope of the binodal is positive at low concentrations and negative at higher concentrations. This might be different for semi-flexible repulsive rods, where the shear-induced displacement of spinodals is found to be much more pronounced [3]. In the phase diagram in Fig. 2, is the region where tumbling and wagging of rods occurs is indicated [4]. At these higher concentrations, no vorticity banding could be detected and no binodal could be measured (except in the absence of flow).

2. Vorticity Shear Banding

Within the doubly shaded region indicated in **Fig. 2**, bands are formed along the vorticity direction, which can be made visible by observing an optical couette cell between crossed polarizers, as depicted in **Fig. 3a**. Apparently, the overall orientational order within the two types of bands differs.

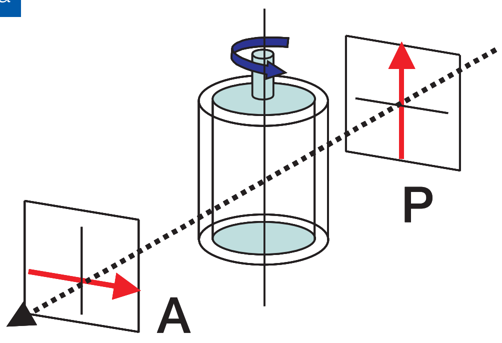
Figure 2



Non-equilibrium phase diagram in the shear-rate versus rod-concentration plane, where the binodal line and the region where vorticity banding occurs are indicated. The doubly shaded area marks the region where vorticity banding occurs, while the singly shaded area at higher concentration roughly indicates the region where tumbling and wagging occurs.

Banded structures are given in Fig. 3b for a few shear rates. Note that vorticity banding occurs only within the two-phase region (defined here as the region bounded by the paranematic-nematic binodal). By means of spatial Fourier mode analysis of intensity profiles in the vorticity direction, we are able to distinguish the *upper* and *lower* border shear-rates of the banding region for a given rod-concentration. At these border shear rates, the amplitude and regularity of the intensity profiles change in a discontinuous fashion: the image on the far right in Fig. 3 is just above the upper border shear rate. Here, only shear-stretched inhomogeneities are observed with little contrast differences along the vorticity direction.

Figure 3a



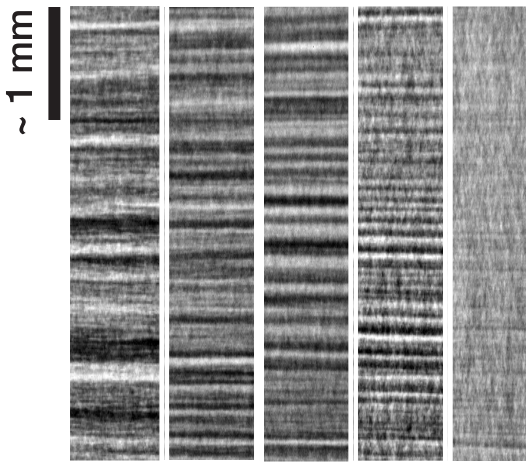
The experimental set-up for the observation of vorticity banding.

The mechanism leading to vorticity banding is not known (see, however, ref.[5], where the condition for the occurrence of vorticity banding is identified with a shear stress that is multi-valued as a function of shear rate, which indeed happens only within the two-phase region). There are strong indications that pressure gradients along the gradient direction of the flow are at the origin of the vorticity banding transition, similar to the elastic instability that leads to the rod-climbing or Weissenberg effect: tracking a seed particle within a band indicates that there is a rolling flow within the bands.

The inhomogeneities formed after a shear-rate quench are essential for the banding transition, where probably the inhomogeneous stretching along the gradient direction and/or bending elasticity of the inhomogeneities are at the origin of the pressure gradient along the gradient direction of the flow.

Just above the region in Fig. 2 where vorticity banding occurs, there is a relatively small interval of shear rates where bands *nucleate* heterogeneously. Here, after some time, bands appear only in a small part of the couette cell.

Figure 3b



Vorticity banding morphology in the stationary state for shear rates equal to 0.45, 0.55, 0.65, 0.75, and 0.84 /sec from left to right. The figure on the far right is just above the upper border shear rate, where no banding occurs anymore and only shear-elongated inhomogeneities are seen.

References

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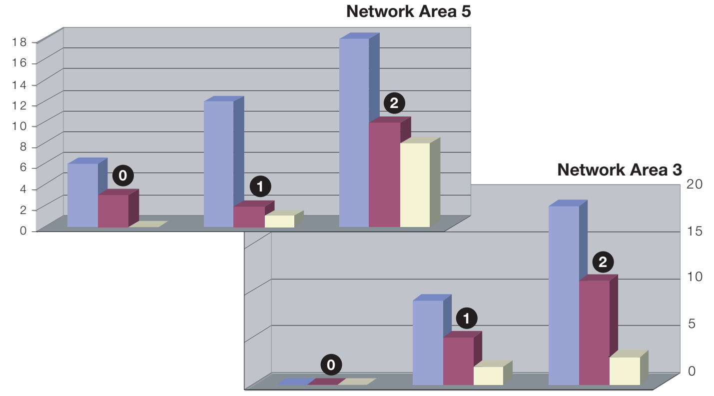
Coordinator's Column

Soft matter research in Europe is well established and is competitive worldwide. In order to foster integration of the community, the SoftComp Network of Excellence initiates and supports efforts to make this integration possible, durable and efficient. European scientists came together in the SoftComp project in order to share their expertise, to build a common infrastructure, and to create joint research in the field of soft matter composites.

The integration process within the SoftComp Network of Excellence is now well under way. This is manifested in a strong increase in the joint publications between different partners – 54 in the second year – and, in particular, in the evolution of collaborations within SoftComp. As an example, Figure 1 displays the evolution of collaborations within Network Area 3 *"Complex Membranes"* and 5 *"Gels and Glasses from Simple and Composite Soft Materials"*.
Network Area 3 started with very little interaction between participating groups and now counts more than 30 specific collaborations. In Network Area 5, again a very strong evolution is observed, showing the cohesive effect of SoftComp. Furthermore, the strong overlaps between work in Network Area 1 *"Colloidal Composites"* and Network Area 5 induced a merger of the two areas.

Figure 1



Evolution of collaborations in Network Areas 3 and 5.
Columns: blue (experiment), red (theory), yellow (synthesis).

In order to strengthen and increase cross-border activities between different Network Areas over the coming years, convergence will be stimulated by investigating scientific topics across network areas. For this purpose, SoftComp will have a number of topical discussion meetings bringing together scientists from different Network Areas. The first will take place in December 2006 in San Sebastian, where the topic *"Confinement"* will bring together scientists from all different Network Areas. In January 2007, there will be a second discussion meeting in Paris on *"Bio-inspired Materials and Biomimetics"*, which will unite scientists from Network Areas 2 and 3. Finally, a third discussion meeting on *"Molecular Engineering of Rheology"* will unite scientists from Network Areas 1, 2 and 4.

The creation of a common infrastructure for soft matter research is one of the driving forces behind integration within SoftComp. The scientific infrastructure has been organized in three research platforms: (i) synthesis, (ii) experimental techniques and (iii) theory and simulation. In the second year of SoftComp, three specific Memoranda of Understanding were agreed upon, which regulate the access to the resources within these platforms. In the second year, these platforms were widely used by SoftComp members. Last year, both the synthesis and exchange of samples, as well as the visits to the experimental platform, increased by about a factor of 3 as compared to the first year.

The dissemination and education programme of SoftComp was very well received and had a strong impact on the outside world. We had about 50 joint publications, about 300 SoftComp related publications, and have organized 11 summer schools and workshops. SoftComp members contributed allmost 400 posters and talks of at various conferences, of which more than a third were invited presentations.

The main objective for the next years is the creation of a durable structure for SoftComp collaborations. With the second Memorandum of Understanding on the research platforms, the SoftComp partners have already committed themselves to maintaining the SoftComp infrastructures beyond the EU's funding period. Within the next half year, the SoftComp partners will have to decide on the direction they want the Network to take and how they will further strengthen their cooperation and integration. Over the next few months, a first version of a research road map will be drafted, which will show medium and long term scientific goals. This will be connected to an organisational road map, which will display the elements of durability and financing. This should lead to a mutual agreement before the end of the third SoftComp year.

About SoftComp

SoftComp is a Network of Excellence – a tool developed under the 6th Framework Programme of the European Commission dealing with the integration of European research, with the intention to strengthen scientific and technological excellence. In particular, SoftComp aims to establish a knowledge base for an intelligent design of functional and nanoscale soft matter composites. It will do so by overcoming the present fragmentation of this important field for the development of new materials at the interface of non-living and living matter, where the delicate principles of self-organisation in polymeric, surfactant and colloidal matter are ubiquitous. This Network of Excellence created an integrated team able to activate the European potential in soft matter composite materials and thus to disseminate excellence through extensive training and knowledge transfer schemes.
Presently 240 SoftComp members have registered to SoftComp's web portal.
For registration, please contact: f.h.bohn@fz-juelich.de

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SoftComp Communication Manager: f.h.bohn@fz-juelich.de
SoftComp Web Portal: www.eu-softcomp.net

Vacancies

Postdoc or PhD position...

...available in the field of mesoscale hydrodynamics simulations of polymers in flow, in the theory group at the Institute of Solid State Research (IFF) in Jülich.
www.fz-juelich.de/iff/e_th2
Contact: G. Gompper or R.G. Winkler
Email: g.gompper@fz-juelich.de
r.winkler@fz-juelich.de

Two years postdoc position available at Research Centre Jülich...

...molecular rheology of branched polymers using small angle neutron scattering
Starting date: as soon as possible
Contact: D. Richter
Institute for Solid State Research
Research Centre Jülich
D-52425 Jülich Germany
Email: d.richter@fz-juelich.de

Post-doctoral position in the adhesion group at CRPP, Pessac, France...

...for details see:
www.eu-softcomp.net/news/jobs
Contact: P. Fabre
Email: fabre@crpp-bordeaux.cnrs.fr

Postdoctoral position in soft matter and biomaterials theory...

... www.weizmann.ac.il/fluids/SafranGroup
Email: sam.safran@weizmann.ac.il
Postdoctoral fellows benefit from interaction with the wide variety of research conducted at the interface between physics and biology and physics and materials science in other groups at Weizmann, as well as the opportunity to travel to conferences in Europe and the US.
www.weizmann.ac.il/feinberg/postdoc_fell/

Student (MSc, PhD) & post-doc position available in experimental biological physics...

...the Weizmann Institute of Science is looking for students (MSc, PhD) & post-docs to work on a project in experimental biological physics: studying cellular dynamics using single-molecule fluorescence. The project is a collaboration between the experimental group of G. Haran and the theoretical group of N. Gov, in the Chemical Physics Department.
www.weizmann.ac.il/chemphys/gov/
Postdoctoral programme:
www.weizmann.ac.il/feinberg/postdoc_fell/
Contact: nir.gov@weizmann.ac.il

Postdoctoral position in polymer simulations...

...available at the Institut für Theoretische Pysik at the Georg-August Universität in Göttingen, Germany.
www.theorie.physik.uni-goettingen.de/forschung/mm/jobs/
Contact:
mmueller@theorie.physik.uni-goettingen.de

Post Doc position in "Dynamics of Solvent/Polymer Systems"...

...available at the new Rhodia/ CNRS Joint Laboratory in Saint FONS.
Contacts: ludovic.odoni@eu.rhodia.com or
long@lps.u-psud.fr

SoftComp events related to PhD education

Date	Conference/Place	Contact
7-25 Aug 06	**Summer School on Computer Simulation in Polymer Synthesis** Technical University DK Lyngby · Denmark	K. Mortensen
14-26 Aug 06	**Summer School on Physics of Cellular Objects** CNRS · Institut Curie Paris · France	J.F. Joanny
06-15 Sep 06	**Summer School on Advanced Polymer Chemistry** Technical University DK Lyngby · Denmark	S. Hvilsted
19-24 Nov 06	**CNRS School on Dynamics of Interfacial Films: an interdisciplinary approach of the friction** **www.lps.u-psud.fr/Collectif/SlidingDynamics** Valpré (Lyon) · France	P. Richetti
12-23 Mar 07	**Summer School Probing the Nanoworld** Jülich · Germany	K. Urban
Apr 07	**Soft Condensed Matter & Advanced Colloid Systems** Utrecht · The Netherlands	A. van Blaaderen
Sep 07	**European School on Rheology: Rheomoligical Measurements** Katholieke Universiteit Leuven Belgium	P. Molderaers
Fall 2007	**11th JCNS Laboratory Course on Neutron Scattering** Jülich/München · Germany	D. Richter
Fall 2007	**Lab Course on Broadband Dielectric Spectroscopy Methods in Polymers and Related Materials** San Sebastián · Spain	J. Colmenero

Coming up...

SoftComp Conferences & Workshops	Date
4th SoftComp Area Network Meetings	
Netwok Area 4 · San Sebastián · Spain Cross-border meeting "Confinement" Coordinator: J. Colmenero	11-12 Dec 06
Netwok Area 2+3 · Paris · France Cross-border meeting "Biomimetics" Coordinator: G. Gompper · P. Bassereau	15-16 Jan 07
Netwok Area 1 · Leuven · Belgium Coordinator: D. Vlassopoulos	Jan 07
Annual SoftComp Meeting Erice Sicily, Italy	**02-05 May 07**
• **Joint NA-Meetings**	02-03 May 07
• **EU Report Meeting**	04-05 May 07
SFB TR6 Summer School on Soft Matter Institut d' Ètudes Scientifiques de Cargéses Cargèse, Corsica (France) www.iesc.univ-corse.fr	02-13 Oct 06
Colloids and Liquid Crystals; Simulation vs. Experiment Konstanz · Germany Contact: W. Paul	Oct 2006
Jülich Soft Matter Days Bonn · Germany Contact: J.K.G. Dhont	14-17 Nov 06
Mainz Materials Simulation Days 2007 Mainz · Germany Contact: W. Paul	13 Jun - 15 Jun 07
Laponite Workshop Amsterdam · The Netherlands Contact: D. Bonn	Summer 07
Length scales and Heterogeneous Dynamics in Glassy Materials Oxford · UK Contact: L. Cipelletti	Summer 07
International Soft Matter Conference 2007 Eurogress Aachen · Germany Contact: G. Gompper www.soft-matter.net	01-05 Oct 07
***FIT:* French Israeli Trends in soft matter, biophysics and microfluidics. 4th French-Israeli Soft Matter Meeting** Biarritz · France Contact: P. Fabre	04-07 Oct 07

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