

Geometry of Interfaces

Primosten (Croatia) 3-7 October 2011



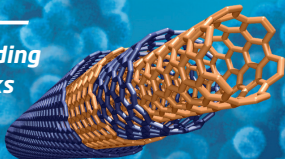
ENGINEERING
OF ADVANCED
MATERIALS

Cluster of Excellence: Engineering of Advanced Materials

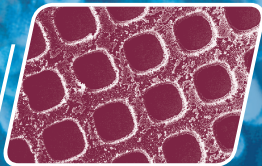
Advanced materials with properties tailored on the nano- and mesoscale are expected to stimulate revolutionary breakthroughs in key growth fields technologies such as information technology, catalysis, energy and transportation.

The Cluster of Excellence “Engineering of Advanced Materials – Hierarchical Structure Formation for Functional Devices” is the only interdisciplinary research collaboration of its type in Germany to focus on the investigation of functional materials and their processing at all length scales.

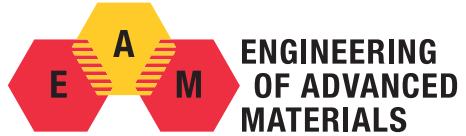
**Building
blocks**



**Super
structures**



**Functional
devices**



ENGINEERING OF ADVANCED MATERIALS

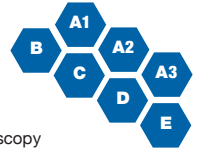
VISION

The vision of the Cluster is to bridge the gap between fundamental research and real-world applications of modern high-performance materials in key scientific and engineering areas. Linking materials design at the molecular level to macroscopic properties (“from molecules to materials to functions”) requires a new form of interdisciplinary cooperation.

At the Cluster 200 researchers from 8 disciplines collaborate in more than 70 projects, from basic research in physics and chemistry as well as many areas of applications such as chemical and electrical engineering and materials science.

RESEARCH AREAS

Cross-sectional topics are explored in three interdisciplinary centers:



- **A1** Functional Particle Systems
- **A2** Nanoanalysis and Electron Microscopy
- **A3** Multiscale Modeling and Simulation

EAM focuses on four fields of application which are organized in value chains that represent hierarchical material classes with increasing complexity:

- **B** Engineering of nanoelectronic materials
- **C** Engineering of photonic and optical materials
- **D** Engineering of catalytic materials
- **E** Engineering of lightweight materials

PROMOTION OF YOUNG RESEARCHERS

- Outstanding support for young researchers across all levels
- Integrated Graduate School “Advanced Materials and Processes”, an interdisciplinary and international program for doctoral students
- Talented young scientists are encouraged to join our dynamic research environment

TECHNOLOGY TRANSFER PROGRAM

- Consultation/evaluation of potential industrial partners
- Bilateral cooperation for specific research questions
- Strategic interdisciplinary alliances to tackle fundamental scientific challenges
- Dynamic research environment
- Talented young scientists are encouraged to apply

CONTACT Friedrich-Alexander University of Erlangen-Nuremberg
Cluster of Excellence Engineering of Advanced Materials

Nägelsbachstraße 49 b | 91052 Erlangen | Germany

Phone: +49.9131.85.20846 | Fax: +49.9131.85.20848

Email: administration@eam.uni-erlangen.de | www.eam.uni-erlangen.de

Program and Abstracts for the EAM conference

Geometry of Interfaces

Primosten, Croatia 2-7 October 2011

An interdisciplinary exploration of genesis and function
of topologically complex patterns in physical and biological materials,
in vivo, in silico and in vitro.



Australian
National
University



Dear Colleagues,

Welcome to Primošten and thank you for joining “Geometry of Interfaces”!

Our vision for “Geometry of Interfaces“ is to be a truly interdisciplinary exploration of physical and biological genesis and function of topologically complex patterns *in vivo*, *in silico* and *in vitro*. The variety of presentations in the program – ranging from biology, physics, chemistry, material science to mathematics – is a promising sign that that vision could be realised. We now hope that the conference will contribute to a better understanding of the unifying concepts and profound links between these different disciplines. We hope that you will in particular benefit from the presentations not directly in your area of expertise. Please bear this hope in mind during your own presentation, and please do not shy away from asking questions when out of your depth.

The name of this conference consciously borrows from the conference “Geometry and Interfaces”, held in Aussois (France) in 1990. In hindsight, it is now clear that that meeting, organised by Elisabeth Dubois-Violette and Brigitte Pansu, marked the coming-of-age of serious exploration of topologically complex patterns in (largely) soft matter, with a particular emphasis on the role of curvature and minimal surfaces in structure of condensed materials. It also united biologists, physicists, chemists and mathematicians in a spirit of common purpose. (Conference papers, published in *Colloque de Physique Colloque C-7*, supplément au no. 23, 1990, remain worth reading!) Twenty years on, we hope that spirit will pervade this meeting. We have consciously sought contributions that touch on the links between geometry, topology, condensed matter and biological materials. At the same time, we have attempted to balance that with studies of synthetic materials. For those reasons the contributions selected for oral presentations are an attempt to survey the current scientific landscape. Other contributions are equally crucial to the success of this meeting, from posters to after-talk discussions.

We hope you will all contribute to discussions, and attempt to bridge the divides between your specialised fields and the bigger questions of self-assembly and pattern formation.

This conference is co-organised with the “Engineering of Advanced Materials” (EAM) cluster of excellence at the Friedrich-Alexander Universität Erlangen-Nürnberg. We gratefully acknowledge the support of EAM and kindly ask you to take note of the information on the front inside cover.

Enjoy your week in Primošten!

Gerd Schröder-Turk and Stephen Hyde



General Information

Meal times

Except for the conference dinner on Thursday, meals are served in buffet-style with the buffet shared with other guests of the hotel. Buffet times are as follows

Breakfast	7:00 am to 10 am
Lunch	12:30 pm to 2 pm
Dinner	6:30 pm to 9 pm

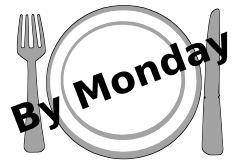
If you have any dietary requirements or food allergies, please discuss these directly with the hotel staff.

Please wear your badge during meal times

The hotel management kindly asks you to wear your name tag also during meal times, or produce it when requested. This allows the waiting staff to identify you as a conference participant, as there are also hotel guests that do not belong to the conference.

Conference dinner Thursday 8pm in the Piano Bar

You are cordially invited to a conference dinner on Thursday 8pm in the Piano Bar of Hotel Zora, to celebrate a hopefully useful and fun conference. Dinner and drinks will be served free of charge.



You will have a choice of two main courses, see the conference notice board. Please tick your preferred choice next to your name on the list near the conference noticeboard by Monday 6 pm, or indicate if you prefer vegetarian food. For serious food allergies and other dietary requirements, please also notify the hotel staff directly.

Wireless Internet Access

Wireless internet access is provided within the conference facilities free of charge by the hotel. A voucher is provided to you on registration. Please see the conference organisers if you need an additional voucher.

Session format and talk style

Talk lengths

For the sake of lively discussion, please strictly respect the following maximal talk times allocated for your presentations

Invited lectures: 45 minutes talk time

Contributed talks: 15 minutes talk time

Flexible session timing and questions

Times allocated for the sessions are generous to allow for in-depth questions and extended discussion. Further, to encourage discussions, start times for individual talks are not fixed; only the duration of a session is. Please feel free to ask lots of questions, even if they require involved answers.

The chair persons will (attempt to) prevent descent to unscheduled chaos and ensure that at least the allocated 20 minutes per contributed talk, including discussion, are left for each speaker.

Poster session

Posters can be displayed for the duration of the conference and there will be a dedicated poster session on Tuesday from 4 to 5:30 pm. Please ensure that you remove your poster by Friday noon. Abstracts for posters can be found on page 71 of this program booklet.

Contributed papers for Interface Focus

Some attendees have agreed to contribute papers to a special conference issue of *Journal of the Royal Society Interface (Focus)*. Due to tight deadlines, we urge those to be submitted latest on arrival at the meeting via the *Interface* web submission portal. Please see Stephen Hyde for clarification if necessary.

Monday

Session 1: 09:00 – 10:55

Chair: Karsten Grosse-Brauckmann

Opening words

Alan Schoen *IL* Reminiscences

Elisabetta Matsumoto *CT* Riemann's Minimal Surface and Sums of Helicoids

Christophe Oguey *CT* 3-colourings of space & 3-arm copolymer self-assembly

10:55 – 11:15 Coffee break

Session 2: 11:15 – 13:00

Chair: Robert Corkery

Doekele Stavenga *IL* Photonic Structures On The Wings Of Birds And Butterflies

Caroline Pouya *CT* Mm-scale replicas of the butterfly gyroid & microwaves

Xia Wu *CT* D-surface photonic crystals in weevil *Entimus imperialis*

13:00 – 15:30 Lunch break

Session 3: 15:30 – 16:55

Chair: Sascha Hilgenfeldt

Klaus Mecke *IL* Morphometric analysis of complex interfaces

Rafael Lopez *CT* Abrupt transitions in striped patterns: bifurcating cylinders

16:55 – 17:20 Coffee break

Session 4: 17:20 – 18:30

Chair: Osamu Terasaki

Toen Castle *CT* Surfactant self-assembly in mesoporous silica

Anan Yaghmur *CT* In-situ observation of bupivacaine-loaded lipid systems

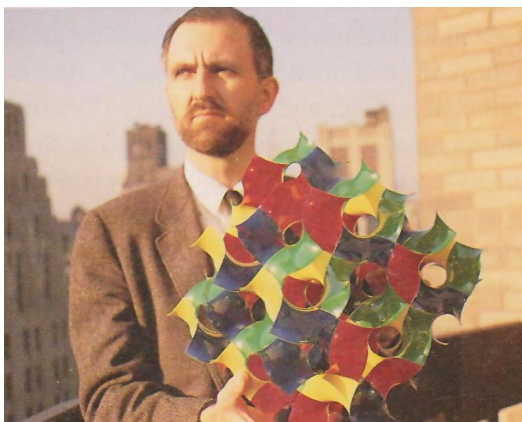
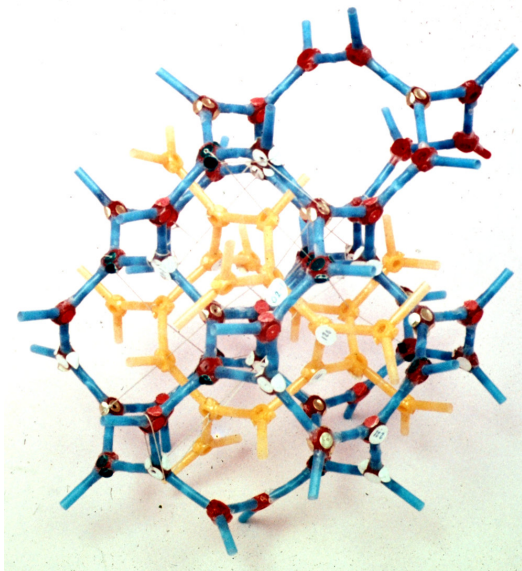
Tatyana Zykova-Timan *CT* Capillary waves of alkali halide solid-liquid interfaces

Reminiscences

Alan H. Schoen

Electrical Engineering, Southern Illinois University/Carbondale (retired), USA

I describe a few details of my search for new examples of TPMS, beginning in 1966, long before I had heard the terms soft matter, mesoscopic, block copolymer, MCM-48, etc. A fuller account can be found at my website <http://www.schoengeometry.com>.



The Taming of the Screw: Riemann’s Minimal Surface and Sums of Helicoids

Elisabetta A. Matsumoto,^{1,2} Christian D. Santangelo,³ and Randall D. Kamien²

¹Princeton Center for Theoretical Science, Princeton University, Princeton NJ 08544, U.S.A.

²Department of Physics & Astronomy, University of Pennsylvania, Philadelphia PA 19104, U.S.A.

³Department of Physics, University of Massachusetts, Amherst, MA 01003, U.S.A.

Minimal surfaces are often the natural starting point when considering the geometry of interfaces and layered structures, such as smectic liquid crystals. The topology of the desired surface may be used to specify a classical minimal surface from which to begin analysis. For instance, an infinite “sum” of screw dislocations, identified as Scherk’s first surface, has been used to model a single twist-grain boundary phase of smectic liquid crystals [1], and Schnerk’s first surface, a continuous map from the Schwarz D surface, describes the smectic layers in the $\frac{\pi}{2}$ twist-grain boundary phase [2]. Similarly, Riemann’s minimal surface, shown in FIG. 1, composed of two oppositely handed helicoids, may be used as a model for a system of layers connected by a series of pores [3].

Upon integration and manipulation of the minimal surface equation $H = 0$, we obtain a closed form expression for Riemann’s minimal surface

$$\Phi = z + \frac{1}{2K(m)} F \left[\tan^{-1} \left(\frac{y - \zeta(2K(m)z, m)}{x - \eta(2K(m)z, m)} \right) - \tan^{-1} \left(\frac{y - \zeta(2K(m)z, m)}{x + \eta(2K(m)z, m)} \right), m \right] = 0,$$

where $F(z, m)$ and $K(m)$ are the incomplete and complete elliptic integrals of the first kind, respectively, $m \in [0, 1]$ is the square of the elliptic modulus, and we define the functions $\zeta(z, m) := \frac{z(1-m) - E(\text{am}(z, m), m)}{2K(m)\sqrt{m(1-m)}}$, where $E(z, m)$ is the incomplete elliptic integral of the second kind and $\text{am}(z, m)$ is the Jacobi elliptic amplitude, and $\eta(z, m) := \frac{dn(z, m)}{2K(m)\sqrt{m(1-m)}}$, where $dn(z, m)$ is a Jacobi elliptic function.

This representation demonstrates clearly that Riemann’s minimal surface may be decomposed into a sum of two oppositely handed helicoids whose cores lie at $\{x, y\} = \{\pm \eta(z, m), \zeta(z, m)\}$, shown in black. At $m = 0$, the cores of the helicoids are straight and infinitely far apart. As m increases, the cores develop undulations, until at $m = 1$ they form circles of infinite radius which approach one another between layers. Likewise, we may trace the evolution of the pores from infinitely large and vertically stacked at $m = 0$ to infinitely separated pores of infinitesimal radius at $m = 1$, seen in FIG. 2. We use this surface to study both the sum of screw dislocations in a smectic liquid crystal and the interface between a bicontinuous system, such as diblock copolymers, connected by pores.

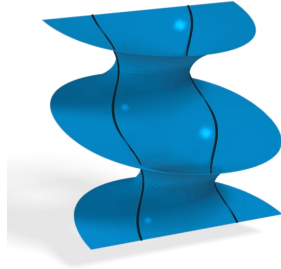


FIG. 1. Riemann’s minimal surface, shown here with elliptic modulus $m=0.5$, is composed of two helicoids whose cores (shown in black) are linear with a superimposed periodic modulation.

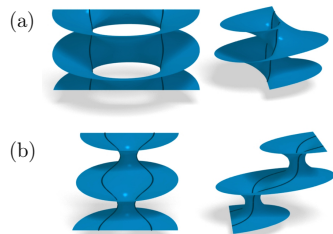


FIG. 2. Two cases of Riemann’s minimal surface are shown here for parameter values (a) $m = 0.1$ and (b) $m = 0.9$.

[1] R. D. Kamien, Appl. Math. Lett., pp. 797–800 (2001).
 [2] C. D. Santangelo and R. D. Kamien, Phys. Rev. Lett., art. 137801 (2006).
 [3] E. A. Matsumoto, dissertation (2011).

3-colourings of space as models of 3-arm mikto copolymer self-assembly

C. Oguey¹ and S.T. Hyde²

¹LPTM, CNRS UMR 8089, Université de Cergy-Pontoise, 95302 Cergy-Pontoise, France

²Applied Mathematics, RSPS, Australian National University, Canberra, Australia

Strongly segregated copolymers can form a rich variety of mesostructures, depending on energy-entropy balance and on the addition of solvent. In the strong segregation limit, where distinct blocks are completely immiscible, the morphology can be described in terms of two-dimensional surfaces — the junction between blocks in linear diblock copolymers.

The analogous situation is more complex for copolymers of star architecture with immiscible arms, also known as “mikto-arm” copolymers [1]. Unusual micro-domain morphologies have been reported [2, 3]. Here we discuss possible morphologies of aggregated star-shaped molecules in its most general setting. A few general laws can be inferred from mathematics and from the basic physics of liquid molecular assemblies.



FIG. 1. 3-star molecules with immiscible ends.

a. The core of star molecules aggregate along lines Under the assumption of complete immiscibility between distinct blocks, the mesostructure of 3-miktoarm star molecules consists in micro-domains separated by branched domain walls. The 3D structure then is a three-colourable partition of space, each colour A, B or C representing one block. The walls are of three types: AB, BC, AC , meeting along lines which are three-fold junctions. On average at the mesoscopic scale, the molecular cores must lie along these edges. In principle, one could also find other junction lines not involving molecular cores, but these will cost additional surface tension energy; so the lowest energy configurations will contain only interfaces imposed by the structure of the molecules.

b. Vertices never appear in a defect free structure In the vicinity of an isolated vertex, the domains consist of conical sectors radiating from the vertex. Since there are only three distinct phases, A, B or C , any vertex figure with four or more cones contains two cones of identical colour. Now this is unstable because the cones of the same colour will either merge or split, yielding a relaxed pattern with vertices of lower connectivity. By induction, the resulting stable pattern is *vertex-free*.

c. At least one domain extends to infinity As the pattern contains only domains, faces and three-fold lines, any point is common to at most three domains. Then Lebesgue’s Covering Theorem [4] implies that at least one of the domains must extend throughout the full width of the pattern. In other words, there is no (periodic) three-colourable cellular partition of space, where all the cells would be bounded domains.

d. 3-coloured partitions induced in sections Any 2D section by a continuous, smooth surface transverse to domain walls and lines, inherits an analogous 3-coloured subdivision. All vertices in the surface are three-coordinated, as traces of three-fold lines. There are classical results on 3-coloured 3-coordinated maps in 2D. In any section, all the bounded connected components of the boundaries of the domains contain a number of sides which is either one or even. From there, one can build a list of sphere patterns: admissible 3-coloured 3-coordinated tilings of the sphere.

Generating stable 3-arm morphologies It would be desirable to have a complete classification of possible morphologies for these 3-arm molecules. This goal has not been achieved yet, but we have a growing collection of examples, and of methods to design new models. We will present a few specimens focusing on high symmetry and comparable volume concentrations.

Support from the French FAST and Australian ARC programs are acknowledged.

[1] Hadjichristidis N. J Polymer Sc Part A-Polymer Chemistry, **37(7)**, (1999), pp. 857-871.

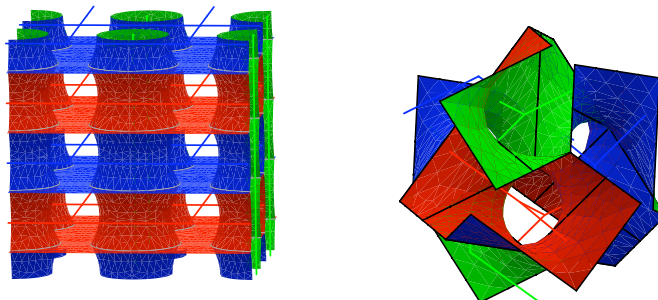


FIG. 2. Left: a simple partition where the triple lines form stacks of circles.
Right: Translation fundamental domain of Elser's partition [5], with congruent *srs* domains.

Support from the French FAST and Australian ARC programs are acknowledged.

- [1] Hadjichristidis N. J Polymer Sc Part A-Polymer Chemistry, **37(7)**, (1999), pp. 857-871.
- [2] S. Okamoto *et al*, Polymer **338** (1997) 5275.
- [3] Sioula S. Hadjichristidis N. Thomas EL., Macromolecules, **31(23)**, (1998), pp. 8429-8432.
- [4] W. Hurewicz and H. Wallman, *Dimension Theory*, Princeton U P, Princeton (1948).
- [5] V. Elser, Phil Trans Roy Soc Lond (A) 354, 2071 (1996)

Photonic Structures On The Wings Of Birds And Butterflies

D.G. Stavenga, J. Tinbergen, and B.D. Wilts

Computational Physics, University of Groningen, Groningen, the Netherlands

The wings of many birds and butterflies are strikingly patterned by colorful feathers and scales. Structural coloration occurs through the application of thin films, multilayers, or 3D-photonics crystals, sometimes in complex combinations and together with pigments. We study animal coloration with various physical methods: (micro)spectrophotometry (MSP), angle-dependent reflectance measurements (ARMs), scanning and transmission electron microscopy (SEM and TEM), imaging scatterometry (ISM) [1], and computational modeling.

Thin films are combined with pigmented multilayers in the breast feathers of the bird of paradise Lawes' parotia (*Parotia lawesii*), allowing sudden changes from blue to green to golden colors [1]. The silvery color of the nape feathers is due to regularly arranged melanin rodlets that create a reflective multilayer peaking in the near-infrared (NIR). The cortex of the feather barbs of the Common Kingfisher (*Alcedo atthis*) also acts as a thin film. In the orange breast feather barbs, the cortex envelopes pigmented cells, but in the blue back feathers and the cyan tail feathers the cortex envelopes sponge cells with quasi-ordered 3D systems.

The glass scales at the wing underside of the Common Bluebottle butterfly (*Graphium sarpedon*) behave as virtually perfect thin films; anatomical studies have shown that the upper and lower lamina of the glass scales are fused. Reflectance spectra measured as a function of angle of light incidence and polarization demonstrate that the wings act as strong reflective polarizers [3]. The wing scales of many blue and/or green lycaenids contain multilayers or gyroid structures, e.g. *Callophrys rubi*, resulting in very directional reflections with spectra that can be quantitatively explained [4, 5].

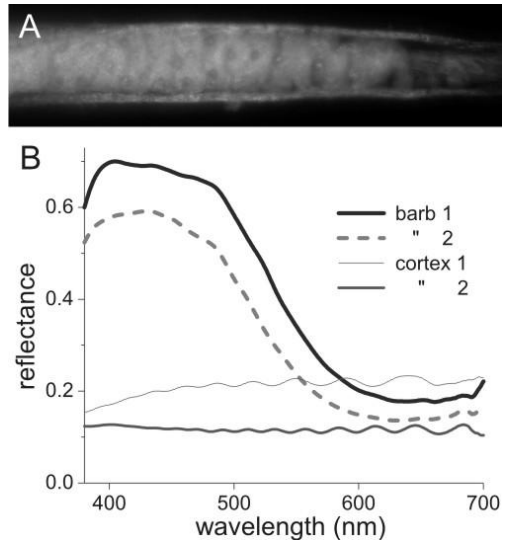


FIG. 1. (A) A very obliquely sectioned barb of a kingfisher tail feather, showing loosened cells enveloped by the barb cortex. Bar: 50 μm . (B) Reflectance spectra measured with a microspectrophotometer from a small area ($5 \times 5 \mu\text{m}^2$) of an undamaged barb (barb 1 and barb 2) and of the cortex, i.e. where the sponge cells were absent (cortex 1 and cortex 2).

- [1] D.G. Stavenga et al., *Opt. Express* 17, 193-202 (2009)
- [2] D.G. Stavenga et al., *Proc. R. Soc. B* 278, 2098-2104 (2011)
- [3] D.G. Stavenga et al., *J. Exp. Biol.* 213, 1731-1739 (2010)
- [4] B.D. Wilts et al., *J. R. Soc. Interface* 6, Suppl 2:S193-202 (2009)
- [5] K. Michielsen et al., *J. R. Soc. Interface* 7, 765-771 (2010)

Electromagnetic characterisation of millimeter scale replicas of the gyroid photonic crystal found in the butterfly *Parides sesostris* in the microwave regime

Caroline Pouya and Pete Vukusic

School of Physics, University of Exeter, EX4 4QL, UK

We present an in-depth electromagnetic characterisation of a gyroid photonic crystal (PC). This is a 3D periodic minimal-surface structure that is responsible for the coloured appearances of some animals, such as several species of butterflies including *Parides sesostris* [1] [2].

We used 3D stereolithography manufacturing methods to fabricate a gyroid PC structure suitable for direct characterisation in the microwave regime (FIG. 1). We chose a filling fraction of 40%: this mimics the gyroid PC structure previously identified in the butterfly *P. sesostris* [2]. We experimentally measured, and theoretically modelled, the detailed polarisation-dependent electromagnetic response of this gyroid PC at gigahertz frequencies, at two azimuthal angles, over a broad range of polar angles (a sample set of this data is presented in FIG. 2). We found excellent agreement between theory and experiment and have identified the source of the complete set of strongly resonant features measured both experimentally and theoretically for the gyroid PC structure.

Through more extensive theoretical modelling using varying filling fractions of material (chitin) and air, we discovered that a gyroid with material volume fraction of 40% is the one that perfectly optimises electromagnetic reflection. This value of 40% is exactly the material volume fraction associated with the naturally occurring PC in the wing-scales of *P. sesostris* [2] and which produces the structurally coloured appearance of the bright green region of its wings [3].

The strong analogy between our microwave model investigation and the optics of *P. sesostris*' colour offers a more complete understanding of this animal's photonic crystal properties. It further adds fundamental insight into the polarisation-dependent and angle-dependent photonic properties of gyroid PCs. This will provide valuable physics-based understanding for the future fabrication and use of PCs in technology.

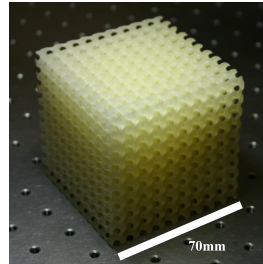


FIG. 1. An example of a gyroid PC structure with material volume fraction of 40%, suitable for probing in the microwave regime.

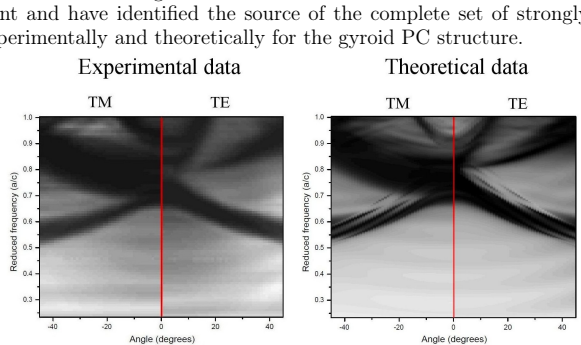


FIG. 2. Experimental and theoretical plots of the electromagnetic transmission response of a gyroid PC structure. The gyroid structure had a lattice constant of 7mm and was arranged in a $15 \times 15 \times 4$ unit cell array. Each plot shows both TM and TE responses for an azimuthal angle of 0° . The experimental and theoretical plots show strong agreement.

- [1] V. Saranathan et al., PNAS, 107, pp. 11676-11681 (2010)
- [2] K. Michielsen and D. G. Stavenga, J. R. Soc., 5, pp. 85-94 (2008)
- [3] P. Vukusic and J. R. Sambles, Nature, 424, pp. 852-855 (2003)

The three-dimensional photonic crystal in scales of the weevil *Entimus imperialis*: a natural D-surface bicontinuous structure

Xia Wu, Andreas Erbe, Helge Fabritius, and Dierk Raabe

Max-Planck Institute für Eisenforschung GmbH, Düsseldorf, Germany

The iridescent scales of the weevil *Entimus imperialis* are subdivided into domains showing nearly all colors from blue to red. By removing the shell of the scales using focused ion beam, we exposed the three-dimensional photonic crystal in differently colored domains (FIG. 1a) and identified it as diamond structure. The structural parameters of the cuticular material were quantitatively determined using scanning electron microscopy (SEM) (FIG. 1b,c) and used as input for a D-surface structure model [1] which recreates the shape and volume fractions of the two phases of the natural structure exactly (inserts in FIG. 1b,c). Using the model, we determined the orientation of the photonic crystal in differently colored domains with respect to the scale surface. Simulations of the photonic band structure (MIT Photonic-Bands (MPB) package, [2]) of corresponding model configurations are in good agreement with the colors observed in different domains. The results show that the construction principle of the photonic crystal in the scales of *E. imperialis* corresponds to the D-surface structure. Therefore, our model can be used to accurately describe the photonic properties of the structure in weevil scales, making it a powerful tool to predict photonic phenomena that can later be used to generate tailored artificial photonic crystals.

We acknowledge financial support through the Max Planck Society.

- [1] Michielsen, K. and Stavenga, D.G., J. R. Soc. Interface 5, pp. 85–94 (2008)
- [2] Johnson, S.G. and Joannopoulos, J.D., Opt. Exp. 8, pp. 173–190 (2001)

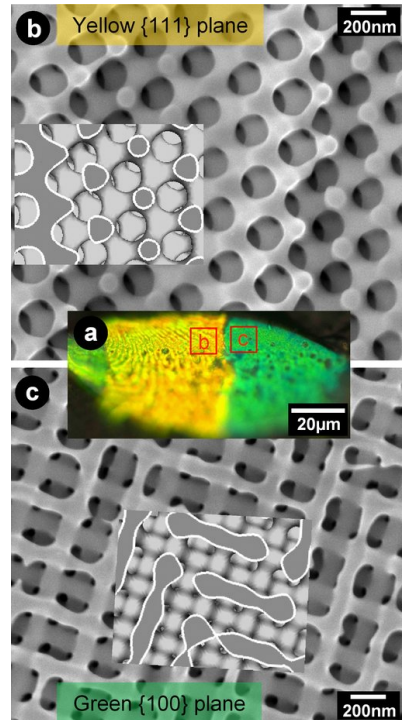


FIG. 1. (a) Light micrograph of an isolated scale with differently colored domains. (b, c) High resolution SEM micrographs showing the yellow (b) and green (c) domains of the scale exposed by focused ion beam (FIB) milling with correspondingly oriented visualizations of the D-surface structure model (inserts).

Morphometric Analysis of complex interfaces

Sebastian Kapfer, Walter Mickel, Gerd Schröder-Turk, and Klaus Mecke

Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

The ‘shape’ of interfaces imbedded in space is a remarkably unprecise defined concept which mainly depends on applications in mind. One systematic approach is provided by integral geometry which furnishes a suitable family of morphological descriptors, so-called tensorial Minkowski functionals. They are related geometrically to curvature integrals and physically to thermodynamic properties of structured materials, what makes them most suitable to derive structure-property relations for condensed matter bounded by complex interfaces.

This analysis is applied to biopolymer networks, to granular bead packs and to triply-periodic minimal surfaces which are often used as structural models for self-assembled amphiphilic phases.

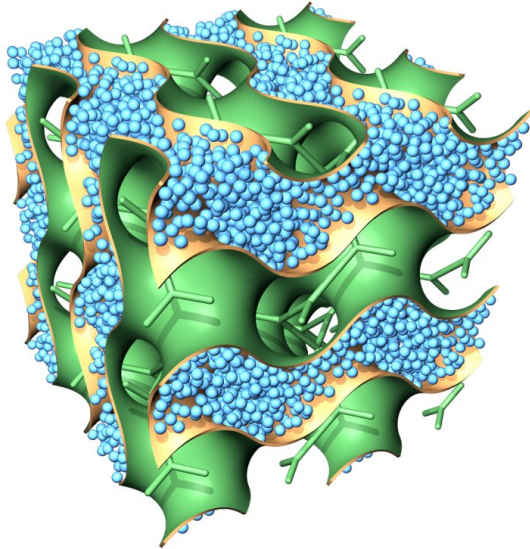


FIG. 1. Hard sphere fluid confined in a gyroid

- [1] K. R. Mecke, *Integral Geometry and Statistical Physics*, International Journal of Modern Physics B **12**, 861-899 (1998).
- [2] K. R. Mecke, *Morphological Thermodynamics of Composite Media*, Fluid Phase Equilibria, **150/151**, 591-598 (1998)
- [3] K. Mecke, *The shapes of parallel surfaces: porous media, fluctuating interfaces and complex fluids*, Physica A **314**, 655-662 (2002).
- [4] C. H. Arns, M. A. Knackstedt, and K. Mecke, *Reconstructing complex materials via effective grain shapes*, Physical Review Letters **91**, 215506 (2003).
- [5] P.-M. König, R. Roth, and K. Mecke, *Morphological thermodynamics of fluids: shape dependence of free energies*, Physical Review Letters **93**, 160601 (2004).
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An abrupt transition on interfacial phenomena in striped patterns: bifurcating cylinders

Rafael López

Departamento de Geometría y Topología. Universidad de Granada. Granada, Spain

In the field of microfluidics, a fundamental question is the study of the wetting morphologies of a liquid when is deposited in a substrate made by surface domains that differ in chemical composition and wettability. The shape of the liquid in mechanical equilibrium depends on the surface tension and the liquid-air phase is modeled by a surface with constant mean curvature. Our interest focuses when we consider a planar surface striped by microchannels formed alternatively by hydrophilic and hydrophobic substrates. In a microscopic scale and in absence of gravity, we place a small amount of liquid in the hydrophilic strips. As we add more liquid, the liquid spreads and remains confined along these channels.

In the initial stages, the liquid inherits the symmetries of the strip and thus it adopts cylindrical shapes. Starting from these cylinders and adding more liquid, experiments show that once reached a certain stage, the shape of liquid changes drastically in an abrupt manner and the liquid exhibits bulges. This has been performed in the Max Planck Institute of Colloids and Interfaces (MPIKG), at Potsdam ([1–3]): see Figure.

This drastic transition between (pieces of) cylinders and new non-rotational morphologies motivates to think in some type of non uniqueness results about the existence of constant mean curvature surfaces emanating from cylinders.

Studying the stability of such cylinders, the talk provides a mathematical proof of the existence of these new interfaces obtained in experiments [4]. We prove that the initial pieces of cylinders bounded by two parallel straight-lines bifurcate in a family of periodic non-rotational surfaces with constant mean curvature and with the same boundary conditions. The analysis is based on the theory of bifurcation by simple eigenvalues of Crandall-Rabinowitz.

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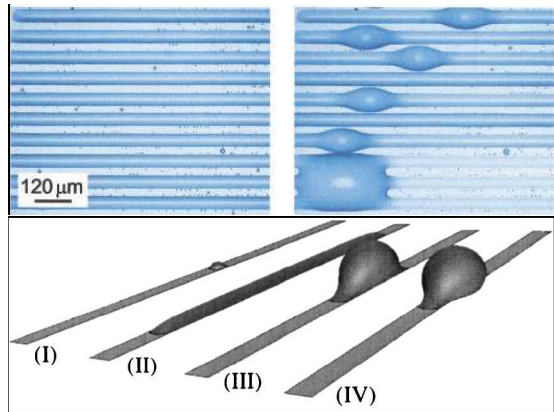


FIG. 1. The different shapes that can be observed when a liquid spreads on an array of hydrophilic and hydrophobic channels (Courtesy of MPIKG).

Geometric influences on surfactant self-assembly in mesoporous silica

Toen Castle,^{1,2} Changhong Xiao,¹ Alfonso Garcia-Bennett,³ and Osamu Terasaki^{1,4}¹MMK, Stockholm Univ., Sweden²Dept. Applied Mathematics, ANU, Australia³Nanotech. & Functional Mat. Dept. of Engin. Sci., Uppsala Univ., Sweden⁴Grad. School of EEWS, KAIST, Republic of Korea

Our group (and collaborators) have solved the structure of various crystalline mesoporous silica phases, including the bicontinuous $Ia\bar{3}d$, $Pn\bar{3}m$ and tricontinuous $P6_3/mcm$ via electron crystallography. This allows the detailed reconstruction of the location of silica walls and surfactant channels within the unit cells. This information allows the analysis of the interface curvatures and the required geometries of the surfactant molecules to form various structures.

Furthermore, our group has synthesised materials containing adjacent domains of different phases ($Ia\bar{3}d$ and $Pn\bar{3}m$, among others) [1], indicating comparable formation energies of these structures under these specific synthesis conditions. This allows the comparison of the different energetic contributions of different interface configurations and more general geometric properties.

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Chemistry - A European Journal,
Accepted, (2011)

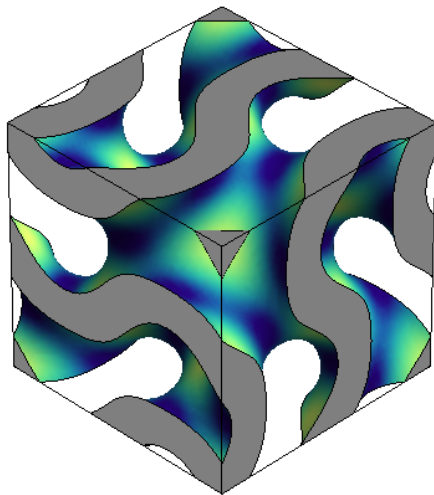


FIG. 1. The mean curvature of the surface of the silica wall within a sample of $Ia\bar{3}d$ mesoporous silica.

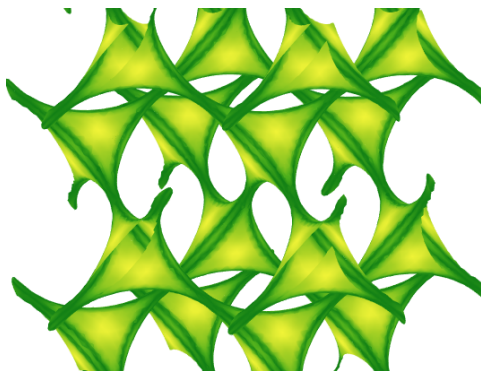


FIG. 2. The shape parameter and channel thickness of the silica wall within a sample of $Pn\bar{3}m$ mesoporous silica. In this graphic the channels are eroded a constant distance to emphasise the channel shape, while the colours show the shape factor at the actual interface.

In-Situ Investigation of Lipidic Bupivacaine-Loaded Formulations

A. Yaghmur,¹ S. W. Larsen,¹ M. Schmitt,^{2,3} J. Østergaard,¹ C. Larsen,¹ H. Jensen,¹ A. Urtti,² and M. Rappolt⁴

¹Department of Pharmaceutics and Analytical Chemistry, Faculty of Pharmaceutical Sciences, University of Copenhagen, Universitetsparken 2, DK-2100 Copenhagen, Denmark

²Centre for Drug Research University of Helsinki, P.O. Box 56, 00014 University of Helsinki, Finland

³Division of Biopharmacy and Pharmacokinetics, University of Helsinki, P.O. Box 56, 00014 University of Helsinki, Finland

⁴Institute of Biophysics and Nanosystems Research (IBN), Austrian Academy of Sciences, Graz, Austria

The dynamical behaviour of local anaesthetic bupivacaine (BUP)-loaded L₂ and H₂ phase precursors (preformulations of BUP), which are attractive as efficient injectable nanocarriers for the sustained release of drugs, was investigated upon rapid exposure to phosphate buffer under simulated body fluid environmental conditions at 37 °C [2]. To determine such structural events *in situ*, a combination of SAXS with remote controlled addition of buffer was used. This study attempted a

detailed structural analysis of the role of the dynamical hydration under physiological conditions during the formation of nanoscaled BUP-loaded non-lamellar structures. The structural mechanism and the possible transition pathways to approach the full hydration and equilibrium conditions were highlighted for three different precursors of inverted type micellar solution (L₂) and an isotropic H₂ phase. It is interesting to note that the obtained results reveal a relatively fast rearrangement of the lipid and solubilized BUP molecules in excess PBS 7.4 since the H₂ structure formed upon the hydration of the L₂ phase approaches within about 1000 sec that of the corresponding equilibrated full hydrated system. In literature, previous studies have demonstrated slower increase in the solubilized water concentration in different non-lamellar liquid crystalline phases based on monoglycerides. It was reported on the need for keeping the samples at least 24 hours to approach the equilibrium conditions. Most strikingly, none of the observed H₂ phase transitions from the self-assembled preformulations are explainable by a simple one-step mechanism, but always an intermediate Pn3m phase forms (Fig. 1). This means that the initial lipid hydration step in these preformulations proceeds at least to some extent the re-distribution of BUP molecules between the polar interface and the hydrophobic regions (the lipid tails and the interstitial areas), i.e. BUP-poor Pn3m phase domains coexist with BUP-rich H₂ phase domains. Interestingly, these Janus-faced – hydrophilic and hydrophobic – rearrangements proceed the fastest utilizing the L₂-phase precursors as they lead to the formation of viscous depots suitable for sustaining drug release.

In this contribution, we discuss also the effects of variations in the lipid composition and/or BUP concentration on the drug release *in vitro* profiles and the structure of the inverted type liquid crystalline phases and microemulsions, which were investigated in the presence of the distilled glycerol monooleate Myverol[®] 18-99K (GMO) and medium-chain triglycerides (MCT).

- [1] A. yaghmur, S. W. Larsen, M. Schmitt, J. Østergaard, C. Larsen, H. Jensen, A. Urtti and M. Rappolt; *In situ* characterization of lipidic bupivacaine-loaded formulations. *Soft Matter* (In press).
- [2] A. yaghmur, M. Rappolt, J. Østergaard, C. Larsen, and S. W. Larsen (manuscript in preparation).

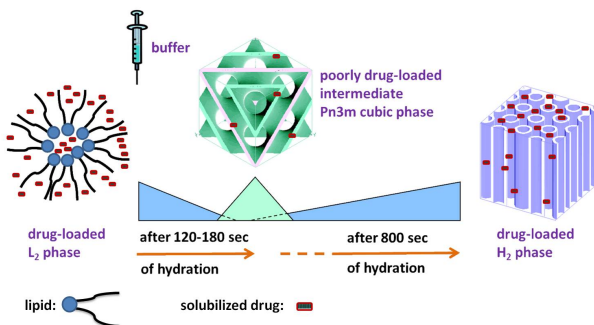


FIG. 1. *In situ* characterization of lipidic bupivacaine-loaded formulations

The capillary wave analysis of alkali halide solid-liquid interfaces

Tatyana Zykova-Timan

Chemistry Department, Cambridge University

E. Tosatti and D. Frenkel

The importance of the interfacial free energy for the equilibrium morphology of crystals is well known. Less quantitative attention has been paid to the so-called “interfacial stiffness” that determines surface fluctuations, especially of solid-melt boundaries. We report extensive molecular dynamics simulations of capillary waves fluctuations of the NaCl(100) solid-liquid interface and of adjacent vicinal planes using classical Born-Mayer-Huggins-Fumi-Tosi potentials. Through a fit of capillary wave spectra we obtain the increasing interfacial stiffness for a class of vicinals in this ionic system at solid-liquid coexistence. From that we also estimate the NaCl(100) solid-liquid interfacial free energy, and comparing the result of $60 \pm 5 \text{ mJ/m}^2$ with those ranging from 36 to $84 \pm 5 \text{ mJ/m}^2$ obtained for the same potentials by other simulation methods we comment on the origin of differences.

Session 1: 09:00 – 10:50

Chair: John Seddon

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|------------------------------|-----------|---|
| Yuru Deng | <i>IL</i> | A “Look” through the Folded Cubic Cell Membrane |
| Krisztian Kertesz | <i>CT</i> | Polyommatine butterfly nanostructures & gas sensing |
| Vinodkumar Saranathan | <i>CT</i> | Diversity of Insect Scale Photonic Nanostructures |
-

10:50 – 11:15 Coffee break

Session 2: 11:15 – 13:00

Chair: Doekele Stavenga

- | | | |
|----------------------------|-----------|--|
| Siewert-Jan Marrink | <i>IL</i> | Cubic phases arising from the interplay of lipids and peptides |
| Matthias Saba | <i>CT</i> | Circular Dichroism in Cubic Chiral Nets |
| Martin Müller | <i>CT</i> | Self-contacts & anisotropic growth of biological tissues |
-

13:00 – 14:30 Lunch break

Session 3: 14:30 – 16:00

Chair: Alan Schoen

- | | | |
|-----------------------------|-----------|---|
| Karsten G-Brauckmann | <i>IL</i> | Mathematics of Minimal Surfaces |
| Birgit Kaufmann | <i>CT</i> | Double Gyroid wire network: Quantum and Classical |
-

Session 4: 16:00 – 17:30

- | | |
|-----------------------|---------------------------------|
| Poster Session | See poster abstracts on Page 71 |
|-----------------------|---------------------------------|

(with coffee, wine and snacks)

A “Look” through the Folded Cubic Cell Membrane

Yuru Deng,¹ Zakaria Almsherqi,¹ and Felix Margadant²

¹*Dept. of Physiology, Yong Loo Lin School of Medicine, National University of Singapore*

²*MechanoBiology Institute, National University of Singapore*

Far from being simple flat sheets, cell membranes may fold into 3-dimensional nano-periodic cubic structures in biological systems. Similar geometries are well studied in other disciplines such as mathematics, physics and polymer chemistry. The fundamental function of cubic membranes in biological system has not been uncovered yet, however, their appearance in specialized cell types indicates roles as structural templates or perhaps direct physical entities with specialized biophysical/optical properties. For instance, intracellular membranes with cubic symmetry are required to produce captivating structural colors of many butterfly wing scales. These photonic nanostructures initially develop within scale cells as a core-shell double gyroid nanostructure that is subsequently transformed into a single gyroid network through the deposition of chitin in the extracellular space followed by the degeneration of the rest of the cell. This control over the expression and evolution of photonic scale structures may thus be not entirely genetic and rather involves self-assembly processes as well.

Likewise, the mitochondria located at the inner segment of the retinal cone cells of the tree shrew (*Tupaia belangeri*) contain unique patterns of concentric cristae with a highly ordered membrane organization similar to the photonic nanostructures observed in butterfly wing cells that produce chitin scales. Using a direct template matching method we have identified the inner mitochondrial membrane organization to consist of 12-layers of parallel and closely packed gyroid-based cubic membrane arrangements in these cone cells. Computer simulation of the light transmission through these cubic membranes in photoreceptors revealed that cubic membranes should act similar to a material of an average elevated refractive index when it comes to refraction while adding interference filter properties. Our simulations suggest that a simplified assembly of such membranes bears the potential to reduce UV transmission by as much as 50% and features sufficiently steep transitions in order not to block the visible light from reaching the neurons. Cubic membrane arrangements in these photoreceptors can also function as dichroic lenses with multiple focal points, depending on the wavelength of the incident light. The membrane contribution to the differences in optical properties between cubic phases and cubic membranes with the same geometry will be addressed.

The folded membrane in the cubic arrangement between the two compartments adds greatly to the complexity of the computer simulation. Neither can a scattering approach be used – as the membrane does contribute to the interference process – nor did wave-optical approaches prove to be successful, as the high complexity of the interface provides no satisfying convergence criteria. We present a ray-based simulator approach, which jettisons the accurate description of the diffraction properties in favor of runtime efficiency and an acceptable description of the interference properties.

These observations highlight for the first time the significance of highly ordered multi-layer cubic membranes organizations to achieve near- or quasi-photonic crystal properties through a simple and reversible biological process of membrane folding.

Polyommatine butterfly wing nanostructures applied for gas sensing

Krisztián Kertész,¹ Gábor Piszter,^{1,2} Zofia Vértesy,¹ Zsolt Bálint,³ and László Péter Biró¹

¹Research Institute for Technical Physics and Materials Science, Konkoly-Thege út 29-33, H-1121 Budapest, Hungary

²Budapest University of Technology and Economics, Műegyetem rkp. 3-9, H-1111 Budapest, Hungary

³Hungarian Natural History Museum, Baross utca 13, H-1088 Budapest, Hungary

Photonic crystals are periodic dielectric nanocomposites which have photonic band gaps that forbid the propagation of light within certain frequency ranges. This property enables one to manipulate light with amazing facility and produce effects that are impossible with conventional optics.

Various animals possess photonic band gap structures in their body. This structural colour completes the chemical colouration (pigment) adding new effects like iridescence. A particularly rich variety of structural colours are found in the wings of butterflies and in the cuticle of beetles. These colouring nanostructures are built from chitin and air voids.

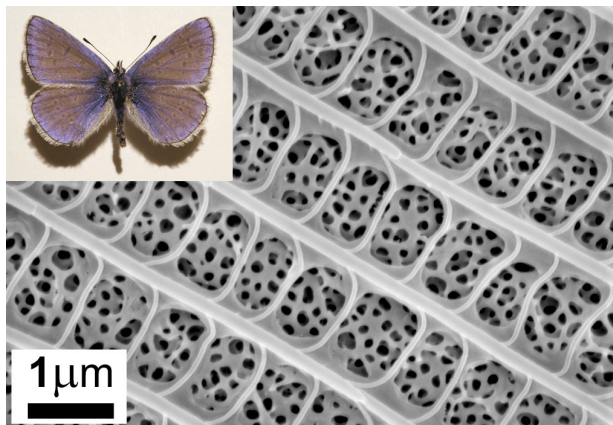


FIG. 1. One of the nine investigated species. Photograph of male *Polyommatus icarus* and scanning electron microscope image of a dorsal wing scale.

The optical response on chemical changes in the environment was first measured on *Morpho* butterflies [1]. The spectral change of the reflected light depends on the composition of the ambient atmosphere and also on the wing nanostructure [2]. In this work we will show the results of recent measurements on nine Polyommatine species. Their wing scales contain a “pepper-pot” type nanoarchitecture (Fig. 1).

Earlier we showed that the variation of the nanostructure results in different blue reflectance, characteristic for each of the nine investigated species [3]. Changing the ambient atmosphere from air to an air/gas (vapour) mixture will result in reflectance alteration. The characteristic differences between the response of the closely related species will be discussed. The effects of analyte concentration and measurement reproducibility will be investigated.

This work was supported by the Hungarian OTKA PD 83483. KK acknowledge financial support by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences.

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- [3] Piszter G., Kertész K., Vértesy Z., Bálint Zs., Biró L. P., *Analytical Methods* 3, pp. 78-83 (2011)

Diversity of Self-assembled Insect Scale Photonic Nanostructures

Vinodkumar Saranathan

Edward Grey Institute, Department of Zoology, University of Oxford, South Parks Road, Oxford, OX1 3PS, United Kingdom

Organismal structural colours are produced by the scattering of light by biological integumentary nanostructures with *meso-scale* (150-350 nm) material (refractive index) variations [1]. These biophotonic nanostructures can vary in nanostructure in either 1, 2, or 3 dimensions, by analogy to engineered photonic crystals [2]. However, they may also vary in whether they have long-range, crystalline periodicity, or only short-range, nearest neighbour order (amorphous or quasi-ordered). Structural colours with millions of years of evolutionary history in invertebrates, form an important aspect of the phenotype of many insects [1] and are frequently used in social and intersexual signalling, aposematic (warning) communication, *etc.* While most insect structural colours are well characterised, being produced by diffraction gratings, lamellar thin-film and multi-layer reflectors [1], the precise nanoscale organisation and development of certain complex three-dimensional nanostructures are more difficult to understand using current techniques. However, a precise mechanistic characterisation of the diversity of biophotonic nanostructures in a comparative framework is essential to understand how such biological signals evolve, and function in the lives of animals.

By applying synchrotron small angle X-ray scattering (SAXS) as a high-throughput, precision tool to structurally characterise the biophotonic nanostructures in an unprecedentedly large number of species from major lineages of insects with structurally coloured scales, we identify a broad diversity of 3D chitin and air nanostructures within these scales. Like in butterflies [3], the SAXS structural data has led to the insight that major lineages of insects have independently evolved to develop these nanostructures by co-opting the curvature-driven self-assembling physical dynamics of biological lipid-bilayer membranes, a property innate to essentially all membrane-bound cellular organelles [4]. However, unlike conventional soft matter systems, these structures are assembled at much larger optical length scales [3]. Thus the self-assembled insect photonic nanostructures may offer a convenient biomimetic route for accessing a variety of designer, optically tunable mesophases [5].

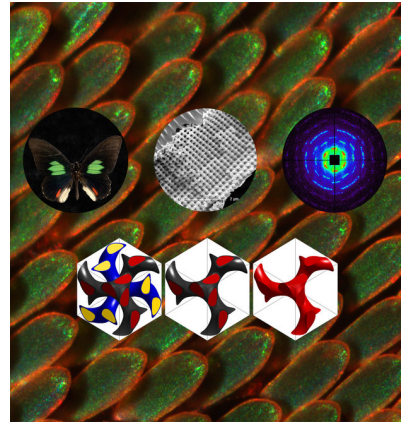


FIG. 1. Self-assembly of single gyroid photonic crystal in iridescent green Papilionid butterfly wing scales via membrane-folding, a process reminiscent of contemporary engineering approaches to synthesizing a single gyroid ($I_{41}32$) network from a core-shell double gyroid ($Ia3d$) precursor.

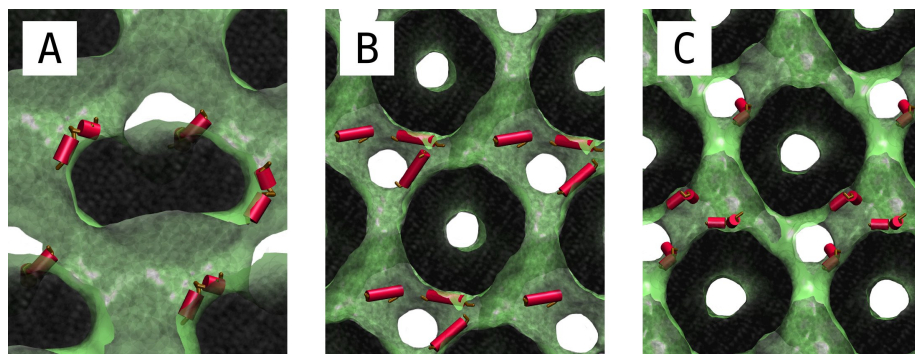
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Cubic phases arising from the interplay of lipids and peptides

Siewert J. Marrink

University of Groningen, The Netherlands

Lipids and other amphiphiles have the unique ability to form lyotropic phases when mixed with water. Peptides are known to modify this phase behavior, altering the phase diagram and facilitating transitions between phases. This modulating effect is of great importance for many membrane related processes *in vivo*, such as fusion and fission, protein segregation, and transport. To understand the physicochemical basis of lipid/peptide interplay, computer simulation studies are becoming increasingly useful. In this talk, I discuss recent results [1, 2] from molecular dynamics simulations to study the phase behavior of lipids in the presence of a particular peptide, the Influenza HA fusion peptide. This fusion peptide forms the N-terminal part of the hemagglutinin protein and is inserted in the target membrane during viral infection. I will show that this peptide induces the formation of a single bicontinuous cubic phase in model membranes. This phase, which is characterized by a periodically replicated peptide-stabilized stalk/pore complex (Figure), has not been observed before and provides insight into the possible biological function of this fusion peptide.



- [1] M. Fuhrmans, V. Knecht, S.J. Marrink. A single bicontinuous cubic phase induced by fusion peptides. *JACS*, 131:9166-9167, 2009
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Circular Dichroism in Biological Photonic Crystals and Cubic Chiral Nets

M. Saba,¹ G.E. Schröder-Turk,¹ K. Mecke,¹ M. Thiel,² M.D. Turner,³ M. Gu,³ D.N. Neshev,⁴ and K. Grosse-Brauckmann⁵

¹Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

²Angewandte Physik & Center for Functional Nanostructures, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

³Centre for Micro-Photonics & CUDOS, Swinburne University of Technology, VIC 3122, Australia

⁴Nonlinear Physics Centre, Research School of Physics and Engineering, Australian National University, Canberra, Australia

⁵Fachbereich Mathematik, Technische Universität Darmstadt, 64289 Darmstadt, Germany

We introduce a chirality index that measures the circular dichroism of chiral photonic crystals by quantifying the degree of circular polarisation of the photonic band structure eigenmodes [1]. This measure is used to analyse photonic crystals based on networks of different symmetry and topology to shed some light on the poorly understood relationship between geometry and photonic response. Nature provides a variety of examples for structural color, for example in bird feathers, beetle shells and butterfly wings. It is widely accepted that the green color of *callophrys Rubi*, a common butterfly in Europe and Asia, is caused by the network-like structure of the chitin wing-scales. The structure is modelled by the gyroid minimal surface and acts as a photonic crystal [2, 3]. Our method backed up by an alternative numerical transmission calculation based on a scattering matrix approach [4] reveals a strong circular dichroism response of the chiral gyroid photonic crystal in the near UV. This response is a remarkable finding for a photonic crystal made of air and chitin with a low dielectric contrast.

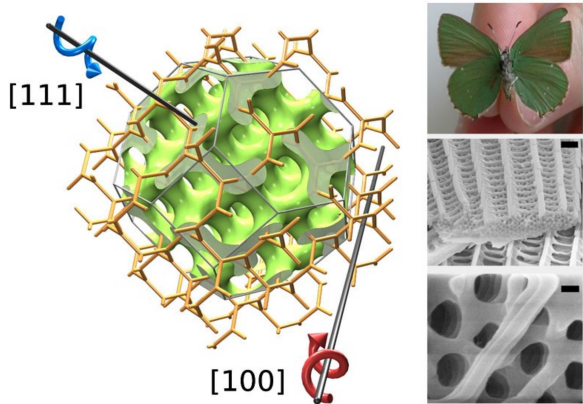


FIG. 1. Gyroid structure. (Left) 1srs networks and gyroid surface with volume fraction $\Phi = 0.18$ clipped to truncated octahedron (the shape of the Brillouin Zone for a body centered cubic geometry). The chitin domain has a left handed three-screw along $[111]$ and a right handed four-screw along $[100]$, perpendicular to the truncated octahedron's faces. (Right) *callophrys Rubi* and SEM images of its wing scale. The scale bars are 1 μm (middle) and 100 nm (bottom).

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- [3] G.E. Schröder-Turk, S. Wickham, H. Averdunk, F. Brink, J.D. Fitz Gerald, L. Poladian, M.C.J. Large and S.T. Hyde, J. Struct. Biol. 174(2), 290 (2011)
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Modeling self-contacts in the anisotropic growth of thin biological tissues

Martin Michael Müller

Equipe BioPhysStat, Université Paul Verlaine-Metz, France

During their growth soft biological tissues are often subjected to forces that affect their shape. In particular, beyond a critical growth factor they will start to make self-contacts. For simple cases such as a thin growing elastic disc a combination of finite element simulations and analytical methods can be used to determine the resulting geometries and stresses. These methods are not restricted to elastic membranes but can be applied to other interfaces as well.

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IL

Karsten Grosse-Brauckmann

Session: 14³⁰ – 16⁰⁰

Mathematics of Minimal Surfaces

Karsten Grosse-Brauckmann

Fachbereich Mathematik, TU Darmstadt, Schlossgartenstr. 7, 64289 Darmstadt, Germany

I will discuss mathematical aspects of minimal and constant mean curvature surfaces. Questions I will address include the following:

- Do minimal surfaces have minimal area?
- How many triply periodic minimal surfaces with a given space group are there and how can we classify them?
- Can each triply periodic minimal surface be deformed to constant mean curvature?
- What is the genus and how do I read it off a triply periodic minimal surface?

Moreover, I want to indicate what kind of existence results rigorous mathematical methods can yield.

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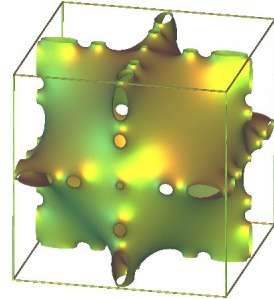
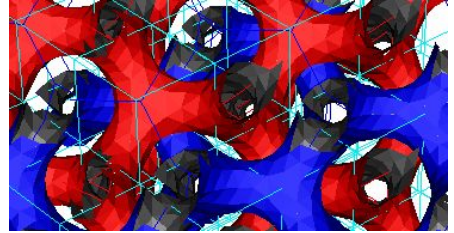


FIG. 1. A constant mean curvature double gyroid (top) and a $Pm\bar{3}m$ -symmetric minimal surface of genus 27 (bottom)

CT

Birgit Kaufmann

Session: 14³⁰ – 16⁰⁰

The geometry of the Double Gyroid wire network: Quantum and Classical

R. Kaufmann, S. Khlebnikov, and B. Wehefritz-Kaufmann

Purdue University, Mathematics and Physics, West Lafayette, IN, USA

We discuss a novel nano material structure of a Double Gyroid (DG) wire network. We start by introducing the geometrical structure of the DG and its fabrication as background. We then use methods of commutative and non-commutative geometry to describe this quantum wire network. Its non-commutative geometry is closely related to non-commutative 3-tori as we discuss in detail.

Session 1: 09:00 – 10:55

Chair: Stephen Hyde

- | | | |
|----------------------------|-----------|---|
| Jean-François Sadoc | <i>IL</i> | <i>The Yves Bouligand Lecture:
Analyzing the collagen structure</i> |
| Kell Mortensen | <i>CT</i> | Real time SANS of Hexagonal to Gyroid transition |
| Tomonari Dotera | <i>CT</i> | Hard Spheres on the Gyroid Surface |
-

10:55 – 11:15 Coffee break

Session 2: 11:15 – 13:00

Chair: Vinod Saranathan

- | | | |
|---------------------------|-----------|---|
| John Seddon | <i>IL</i> | Discontinuous and Bicontinuous Inverse Phases of Lipids |
| Halim Kusumaatmaja | <i>CT</i> | Wetting on membranes: Vesicles in aqueous phases |
| Maria Barbi | <i>CT</i> | On the topology of chromatin fibers |
-

13:00 – 15:30 Lunch break

Session 3: 15:30 – 16:55

Chair: Marianne Impéror

- | | | |
|--------------------------------|-----------|---|
| Peter Vukusic (S. Luke) | <i>IL</i> | Evolutionary Photonics |
| Osamu Terasaki | <i>CT</i> | The role of curvature in silica mesoporous crystals |
-

16:55 – 17:20 Coffee break

Session 4: 17:20 – 18:30

Chair: Tomonari Dotera

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| Robert Magerle | <i>CT</i> | Imaging the Dynamics of Block Copolymer Microdomains |
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| Filipa Alves | <i>CT</i> | Evolution of butterfly pigmentation patterns |

Yves Bouligand

died January 21, 2011 (aged 75 years)

We honour today Yves Bouligand, whose scientific researches are impressive testimony to the importance of looking beyond our own specific field to explain the natural world.

A feature of many scientific questions under discussion at this meeting is their inherent breadth. For example, it is difficult to explain the growth and stability of cubic membranes *in vivo* without exploration of the physics of liquid crystals, as well as the biochemical composition that steers the membranes towards apparent translational order. Further complexity emerges when considering the formation of wing-scales in butterflies, or insect carapaces, where soft matter (lipids, proteins, etc.) “templates” the hard chitin matrix; a feature seen also in mesoporous materials that today occupy the interests of so many card-carrying materials scientists. Nor can we ignore the relevance of hyperbolic geometry and periodic minimal surfaces to the structures of these materials. Similar stories can be told for the more complex patterns in froths and multi-component polyphiles.



The recognition of the importance of traversing the often high walls that separate the various disciplines – between mathematics and biology, between physics and materials science and so on – has an illustrious, if intermittent history. D’Arcy Wentworth Thompson, the Scottish biologist (and classical scholar) was an early disciple of this credo, applying the theory of geometric transformations to explain related morphologies of various fish species and soap films to model the patterns found in the then newly-discovered *Radiolaria* (see “*On Growth and Form*”).

Yves Bouligand was an outstanding successor to Thompson, both in his life-long interest in biological form and in his awareness of the relevance of physics, chemistry and geometry to biology. Indeed, he made frequent reference to Thompson’s work. Already as a biology student at the Ecole Normale Supérieure in Paris, Yves wondered how Thompson’s theory of geometric transformations could be applied to various polyhedral forms of Haeckel’s radiolaria (described in detail in an anecdotal account of meeting the celebrated French protistologist Fauré-Frémiet [1]). His interest in Thompson’s ideas remained throughout his life; given his own spectacular observations de-

scribed below, he could not fail to notice Thompson’s brief description of liquid crystals as possible components of living forms.

While he remained a biologist, Yves' perspective on his own field was coloured by his awareness of the formidable advances being made in Paris (Orsay) on liquid crystals by condensed-matter physicists (led by Friedel and de Gennes). Thus, he recognised the striking “morphological convergence” of textures seen in the chitin-rich shells of crabs and the packing of molecules in cholesteric liquid crystals. Similar parallels were also found in the textures of hard tissues, plant cell walls and chromosomes. This convergence was later shown to be more than coincidental, when his colleagues at his own workplace in Ivry and elsewhere showed that many biopolymers (chitin, collagen, cellulose, indeed DNA) can self-assemble to form cholesteric liquid crystalline phases. His insight into biological form thus led to a new class of liquid crystalline polymeric materials *in vitro*. His contributions to zoology, physics and materials science go deeper and we urge you to explore his own writings [2]

He was in fact equally imaginative in exploring the physics of liquid crystals as he was in the biological domain. He published a number of important papers in defects in liquid crystals (often in *Journal de Physique*) that reveal a profound understanding of geometry, physics and chemistry (see for example his abstract in [3]). (Undoubtedly, Yves' polymath universe was influenced by his father, a professor of mathematics at the Sorbonne, and occasional co-author with his son). As a friend Jean Thiery has noted in a charming “dernier hommage” to Yves [4], one of his most remarkable papers is co-authored with four others: three top-ranking condensed matter physicists and and a geometric topologist [5]!

Yves Bouligand's achievements offer all of us interested in structural complexity a stirring role model. It is a great pleasure to honour his remarkable career with an invited lecture by Yves' friend and colleague from Orsay, Jean-François Sadoc.

[1] <http://www.univ-bpclermont.fr/ASSOC/gplf/GPLF%20info%20.htm>

[2] a collection of his papers and essays has been deposited at
http://people.physics.anu.edu.au/~sth110/bouligand_papers.html

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Analyzing the collagen structure

Jean-François Sadoc and Jean Charvolin

Laboratoire de Physique des Solide, Université de Paris-Sud, Orsay, France

Yves Bouligand was very intrigued by the structure of collagen. He have done a lot of fine observations of collagen in different situations and he has inspired a lot of works among his collaborators and colleagues [1–3]. With Yves, Jean Charvolin [4], Nicolas Rivier [5], Jean-François Sadoc, we spent time in stimulating discussion about collagen: a fascinating problem where some points are well understood, some others are not clear... and some are said to be resolved which indeed are not. Really, Yves was very good to see hidden details making difficult to accept some established propositions. In this talk dedicated to Yves Bouligand we shall present a few questions about collagen.

First is the question of fibrils organization and how is it related to the hierarchy of structures from the polypeptide chain to the fibre? Collagen fibrils, cable-like assemblies of long biological molecules, are dominant components of connective tissues. Their determinant morphological and functional roles motivated a large number of studies concerning their formation and structure. However, these two points are still open questions and, particularly, that of their organization which is certainly dense but not strictly that of a crystal. A model based on phyllotaxis help to understand the structure as a finite dense structure frustrated by a cylindrical surface bordering it finite structure. It is clear that a dense packing of parallel rods is hexagonal, but this is true if the packing is infinite, or large. If the packing is small, with a cylindrical border the phyllotaxis provides another solution. It is the interface between the inside and outside of the fiber which create a frustration, solved as usual by metric distortions and topological defect.

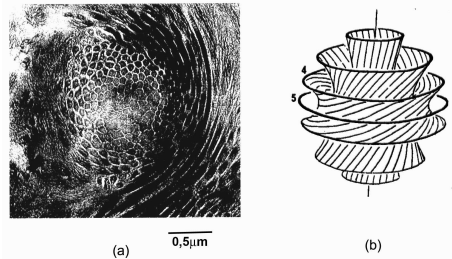


FIG. 1. Electron micrograph of a precipitated collagen fibrils extract from calfskin, the fibrils are seen in cross section in the central part then more and more oblique towards its periphery revealing the existence of a double twist in a area of limited extension (a) and schematic drawing (b). According to [2].

Yves was worry about the question of double twist in collagen, as suggested by figure 1 or by behavior of collagen in liquid crystal states [3]. In fact it is very difficult to conciliate double twist and crystalline structure. He propose a nice idea which is to relate twist with screw dislocation walls : this remain as one of his last projects of publication still not perfectly coined, but which has to be deeply investigated. We propose to give the main terms of this description applied to a crystalline structure mixing squares and triangles.

It is fascinating to see on the figure 1 how collagen in calfskin appears like a Hopf fibration which is the theoretical template to understand double twist, nevertheless in an abstract spherical geometry. But here again the fact that the structure is finite is certainly important as a local part of a Hopf fibration can be described without difficulties in the usual Euclidean geometry. These double twist recall that of blue phases, but the scale is quite different: for blue phase it is at the nanoscopic scale, here it is at microscopic scale. It is a clear example where we are far from definitive answer, even if double twist is clear at the molecular scale, within triple helices, and at the fiber scale, what happen at intermediate scales is not understood (see on figure 2 the different scales for collagen).

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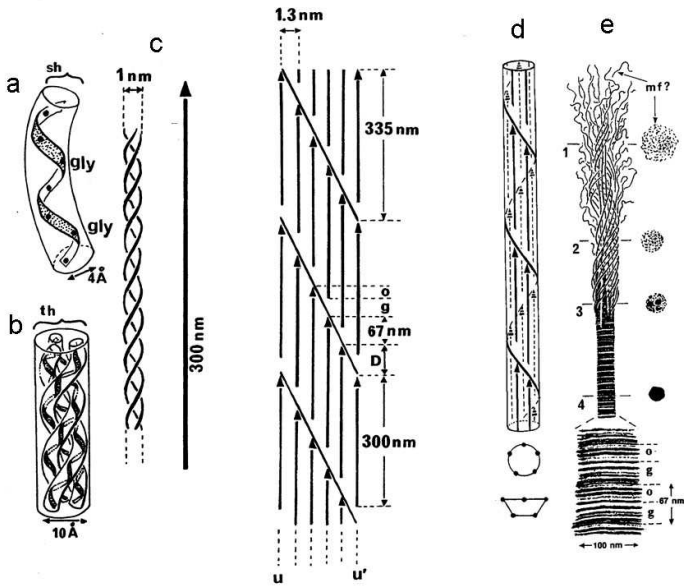


FIG. 2. A figure done by Yves Bouligand in order to explain different levels in the structure of collagen fibers from the peptide chain to the fiber. (a) Polypeptide chain with a periodicity of three for "Gly", (b) triple helix molecule formed with three chains, (c) sizes of this molecule, (d) organization of molecules leading to "overlap" and "gap" regions, (e) a schematic view of the organization of five molecules and (f) a fibre with fibrils inside. The schematic view (e) has to be considered carefully, it is just an indication that in overlaps there are five molecules for four in gap, but how molecular structure respects this ratio is not clearly confirmed.

Real time SANS Studies on the Transformation from Hexagonal Cylinder Phase to bi-Continuous Gyroid Structure

Kell Mortensen¹ and Martin Vigild²

¹ University of Copenhagen, Frederiksberg, Denmark

² Technical University of Denmark, Lyngby, Denmark

Combined applications of small-angle neutron scattering and oscillatory shear instrumentation are effective tools for studying structure and real-time dynamics of soft matter materials. Applying well-controlled large-amplitude oscillatory shear can be used to effectively control the texture of soft materials in the ordered states [1-3]. As an example, we present results on block copolymer systems with shear-induced texture in form of single-domain crystals, twin-domain crystals and two-dimensional powders, as revealed in respectively cylinder and spherical micellar-like systems and bi-continuous membrane-line systems. We show further how a given textures of soft matter materials can be controlled in detail with the application of specific shear-rate and shear-amplitude [1]. Shear may also affect the thermodynamic ground state, causing shear induced ordering and disordering (melting), and shear-induced order-order transitions. We will present data showing that the gyroid state of diblock copolymer melts is unstable when exposed to large-amplitude and high-frequency shear, transforming into the hexagonal cylinder phase, as shown in Fig. 1. The transformation is completely reversibly, and with the relative slow kinetics in the transformation back from hexagonal to gyroid, it is possibly in detail to follow the complex materials transformation from one-dimensional cylinders to the complex three-dimensional bi-continuous networks expressed in the cubic gyroid phase of block copolymers.

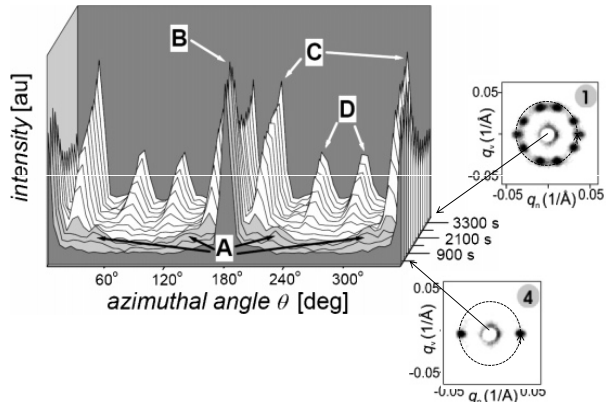


FIG. 1. Time resolved small-angle neutron scattering results of PS-PI block copolymer after being exposed to shear. In the relaxed state, the block copolymer reveal bicontinuous gyroid structure; when exposed to large-amplitude/high-frequency shear, the structure transforms to hexagonal cylinder-structure.

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Hard Spheres on the Gyroid Surface

Tomonari Dotera,¹ Masakiyo Kimoto,¹ and Junichi Matsuzawa²

¹Department of Physics, Kinki University, Higashi-Osaka 577-8502, Japan

²Department of Mathematics, Nara Women's University, Nara 630-8506, Japan

What is regular arrangement when a surface is curved? On a flat surface, the hexagonal arrangement is ubiquitous from atoms, to molecules, liquid crystals, polymers, and colloidal particles with spherical shape. The arrangement stems from the densest packing of hard spheres, space division, or interactions between particles, for instance, the excluded-volume effect of hard spheres that plays a fundamental role in soft materials. Since triply periodic saddle-shaped surfaces such as gyroid (G), diamond, and primitive surfaces are realized in many soft materials like biological lipids, surfactants, and block copolymers, it is worth studying regular arrangement on these surfaces.[1–4]

Here, we consider regular arrangement of hard spheres on the G surface.[5] We propose three regular arrangements: a triangular tiling ($3^6:3^8$), an Archimedean tiling ($3^3.4.3.4$), and a tiling ($3^6; 3^2.4.3^2.4$) consisting of 40, 48, and 64 vertices per unit cell on the G surface, respectively. The set of integers (n_1, n_2, n_3, \dots) denotes a tiling of a vertex-type in the way that n_1 -gon, n_2 -gon, and n_3 -gon, \dots , meet consecutively on each vertex, and superscripts are employed to abbreviate when possible. Two of them are made up of two types of vertices. We presume that these tilings are hyperbolic extensions of the flat plane tessellation (3^6). For ($3^3.4.3.4$), the space group is $I43d$ (No.220), which is one of the cubic subgroups of $Ia\bar{3}d$ (No.230). We mention that these arrangements can be viewed as hyperbolic tiling on the Poincaré disk; The arrangement ($3^3.4.3.4$) is equivalent to that of angels or devils in Escher's Circle Limit IV.

Using Monte Carlo simulation, we found that 48/64 hard spheres per unit cell on the G surface were selforganized. Fig. 1A displays self-organized 864 (48/per unit cell) hard spheres whose centers were confined on the G surface. It exhibited an entropy-driven liquid-solid transition, when the radius of spheres was greater than about 0.118 in the unit of the lattice constant. Fig.1B plots the movable probability (acceptance ratio) of trial moves as a function of radius. For the regular configuration, we observed higher probability ensuring entropic stability of the ordered state. In the green region spheres were fixed on regular sites that acted as a solid interface. Without the solid region, we found random configurations, which ended up with glassy states.

Recently, a regular arrangement on the G surface has been found in an ABC star block copolymer melt.[6] This result suggests that regulated membranes in soft materials can be scaffolds to self-assemble more complex but controlled arrangement.

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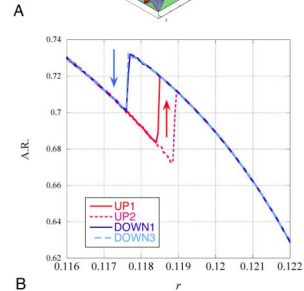
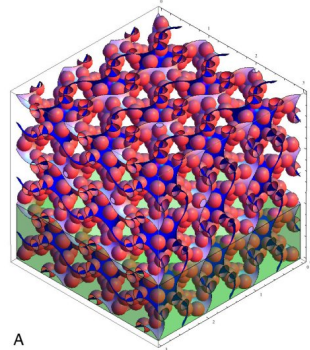


FIG. 1. A. Self-organized spheres on the G surface. B. Plot of acceptance ratios as a function of sphere radius.

Discontinuous and Bicontinuous Inverse Phases of Lipids

J. M. Seddon, N. J. Brooks, G. C. Shearman, A. I. I. Tyler, T.-Y. Tang, C. V. Kulkarni, A. M. Seddon, O. Ces, R. H. Templer, and R. V. Law

Chemistry Department and Institute of Chemical Biology, Imperial College London, London SW7 2AZ. U.K

Various amphiphile / water mixtures will self-assemble into complex three-dimensional lyotropic liquid crystal inverse phases. These nanostructured fluids fall into two main families: the sponge-like bicontinuous cubic phases, and discontinuous structures based upon ordered packings of inverse micelles [1]. Both types of phase have great potential in nanotechnology and medicine, for encapsulating and delivering drugs and other molecules to cells.

We have discovered a novel lyotropic liquid crystal phase of space group $P6_3/mmc$, whose structure is based upon a hexagonal close packing of identical quasi-spherical inverse micelles [2]. The system consists of a hydrated mixture of dioleoylphosphatidylcholine, dioleoylglycerol, and cholesterol. This novel phase has a number of unique features which may render it useful for a wide range of applications. Firstly, it is the only known self-assembled lyotropic phase whose structure consists of a periodic close packing of *identical* inverse micelles. Secondly, it is stable in excess aqueous solution, which is very important for potential biological or biomedical applications.

We have recently elucidated the role of chain splay in controlling the structure and stability of bicontinuous cubic phases formed by monoacylglycerols [3], a biocompatible lipid which is widely investigated as an encapsulating system.

We have previously shown that by addition of weakly-polar amphiphiles such as diacylglycerols to phospholipids, one can tune the preferred interfacial curvature to be strongly inverse, leading to the formation of a discontinuous cubic phase of spacegroup $Fd\bar{3}m$, with a structure based upon a complex close packing of two types of inverse micelle of different diameters. We have recently investigated the effect of hydrostatic pressure on the structure and stability of this phase, and have discovered a number of novel effects [4].

We have recently discovered a novel inverse ribbon phase in the branched-chain polyoxyethylene surfactant system tetradecyloctadecyl-tetraoxyethylene ether ($C_{14}C_{16}EO_4$) in excess water [5]. This phase is stabilised by the application of hydrostatic pressure. The lattice parameters of the inverse ribbon phase were found to vary with pressure, with the structure becoming increasingly distorted away from 2-D hexagonal symmetry ($b/a = \sqrt{3}$) with increasing pressure.

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Wetting on membranes: Vesicles in contact with multiple aqueous phases

Halim Kusumaatmaja, Rumiana Dimova, and Reinhard Lipowsky

Theory & Biosystems, Max Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany

Recently novel soft matter systems consisting of lipid vesicles and phase separating polymer solutions have been introduced [1]. They provide a model system for studying wetting behaviors on flexible membranes. Here we first describe how the usual (Canham-Helfrich) free energy model for bending of a thin membrane can be extended to account for the wetting energy contributions. Our theoretical analysis reveals the existence of an intrinsic contact angle [2] between the membranes and the aqueous phases, and an explicit relation is derived by which the intrinsic angle can be determined from the effective contact angles as measured by optical microscopy. Comparison between theory and experiment provides strong evidence that the intrinsic contact angle represents a material parameter, independent of extensive variables such as the volume and area of the vesicles. The theory is then used to describe a novel budding transition [3], where one of the aqueous phases protrudes from the vesicle body to minimize the interfacial energy between the aqueous phases. Finally, if time permits, we will describe the observation of membrane nanotubes in these systems [4], and how our theory may explain the competition between budding and tube formation, as the systems spend the excess membrane area created during the deflation of the vesicles.

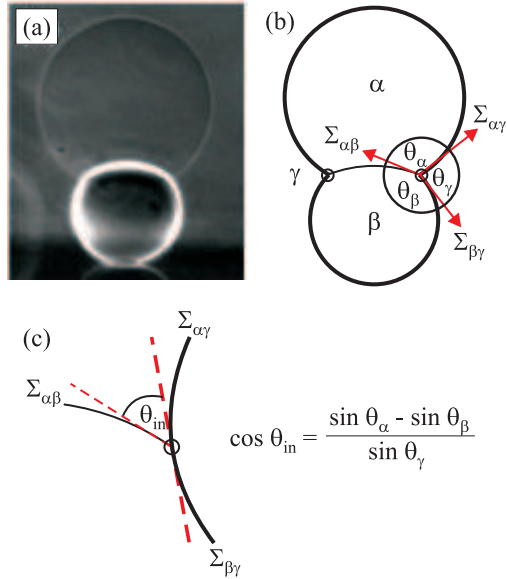


FIG. 1. (a) Side-view phase contrast image of a vesicle containing two aqueous phases suspended in an exterior solution. (b) A schematic diagram of panel (a). The shape of the vesicle can be characterized by three effective angles θ_α , θ_β , and θ_γ . (c) Enlarged view close to the contact line: Intrinsic contact angle θ_{in} between the two planes that are tangential to the $\alpha\beta$ interface and to the smoothly curved vesicle membrane, respectively. The intrinsic contact angle can be determined from the effective angles.

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On the topology of chromatin fibers

Maria Barbi, Julien Mozziconacci, and Jean-Marc Victor

Laboratoire de Physique Théorique des la Matière Condensée (LPTMC), Université Pierre et Marie Curie, Paris, France

The eukaryotic cell's ability to hold, use and duplicate the DNA remains one of the most fascinating questions in biology. Meters of DNA are compacted into the nucleus through the action of protein structural act as spools on which DNA can be wrapped and folded, leading to a complex structure called the chromatin. The assembly must be compact enough, but at the same time it must allow access to different regions of the genome according to the needs of the cell.

In trying to understand the organization and dynamics of chromatin can be useful to consider the physical and topological constraints acting on it. Using a simple geometric model, we propose a general method for computing the topological properties (twist, writhe and linking number) of the DNA embedded in chromatin fibers. The relevance of the method is reviewed through the single molecule experiments that have been performed *in vitro* with magnetic tweezers.

We compute the linking number of the DNA in the manifold conformational space of the nucleosome which have been evidenced in these experiments. Moreover we discuss the mechanical behavior of single chromatin fibers submitted to torques in the light of these multiple states.

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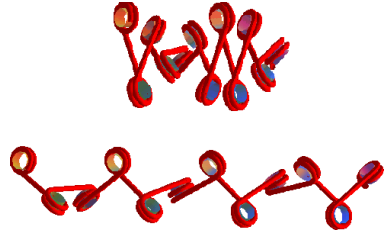


FIG. 1. The basic structure of the chromatin assembly is the chromatin fiber, formed by a chain of protein spools on which the DNA is wrapped for about 2 turns, called the nucleosome. Nucleosomes are typically spaced in a regular manner and separated by a stretch of DNA called linker DNA. Different compactions of the fiber can be obtained by changing its local geometry.

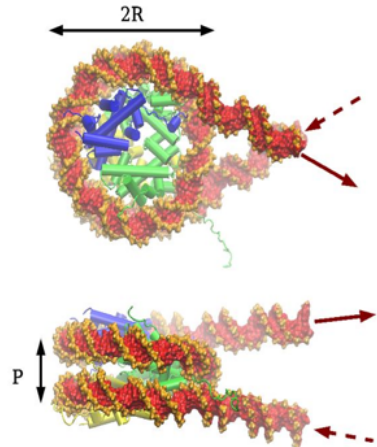


FIG. 2. A detailed view of the nucleosome in its chiral conformation.

Evolutionary Photonics: natural designs for manipulating the flow of light and colour

Peter Vukusic and Stephen Luke

School of Physics, University of Exeter, UK

The study of structural colour in brightly coloured animals is an exciting interdisciplinary area of research. Complex photonic bandgap (PBG) structures (which prevent the propagation of a band of wavelengths through them – causing strong coloured reflections) in insects like beetles and butterflies suggest broad innovation in nature's use of materials and its manipulation of light. In specific butterflies for instance, ultra-long-range visibility of up to one half-mile is attributed to photonic nanostructures that are formed by discrete multilayers of cuticle and air. This contrasts, in other butterfly species, to photonic structures designed more for crypsis and which not only produce strong polarisation effects but can also create additive colour mixing using highly adapted geometries. Biological systems also exist that employ remarkable 2D and 3D photonic crystals of protein-based material to produce partial PBGs, with the effect that bright colour is reflected or inhibited, over specific angle ranges. From the perspective of modern optical technology, these structures indicate a significant evolutionary step, since in principle, these 2D and 3D periodicities are potentially able to manipulate the flow of light in all directions.

This talk will present an overview of this emerging field of study, as well as several of the exciting recent discoveries that reflect nature's optical design ingenuity, and the technological applications to which they are currently being applied.

The role of curvature in silica mesoporous crystals

Keiichi Miyasaka,¹ Lu Han,² Changhong Xiao,³ Alfonso Garcia-Bennett,⁴ Han Yu,⁵ Toen Castle,³ Yasuhiro Sakamoto,⁶ Nobuhisa Fujita,⁷ Shunai Che,² and Osamu Terasaki^{1,3}

¹*Grad. School of EEWS, KAIST, Republic of Korea*

²*School of Chem. Chem. Tech., Shanghai Jiao Tong Univ., P.R. China*

³*MMK, Stockholm Univ., Sweden*

⁴*Nanotech. & Functional Mat. Dept. of Engin. Sci., Uppsala Univ., Sweden*

⁵*KAUST, Saudi Arabia*

⁶*Osaka Prefecture Univ., Japan*

⁷*IMRAM, Tohoku Univ., Japan*

We have solved structures of various silica mesoporous crystals including cage type ($Fm-3m$, $P6_3/mmc$, $Pm-3n$, $Fd-3m$, $P4_2/mnm$ etc), rod type ($p6mm$), bi-continuous ($Ia-3d$ & $Pn-3m$) and tri-continuous ($P6_3/mcm$) crystals based on transmission electron microscopy observations.

The organic/inorganic interface curvature or the packing parameter may control formation energies of the crystals and change their structures depending on gel compositions.

The role of interface curvature in stabilising silica mesoporous crystals will be discussed based on our observations.

Imaging the Dynamics of Block Copolymer Microdomains: Kinks, Lattice Defects, and Structural Phase Transitions

Robert Magerle

Chemische Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

With tapping mode atomic force microscopy (AFM) we have imaged the microdomain dynamics at the surface of thin films of block copolymer melts and concentrated solutions in real time and with 10 nm spatial resolution. Our sequences of AFM images (movies) provide insight in the fundamental processes of structure formation of block copolymer microdomain structures in their fluid state. Computer simulations based on density functional theory and a Langevin equation reproduce the structure formation processes in stunning detail. In my presentation, I will present an overview of our work and report on new discoveries.

We succeeded in observing the elementary processes during a sequence of structural phase transitions in a thin, fluid film of a cylinder-forming block copolymer forming a concentrated solution in chloroform [1]. As the film thickness is changing we observed the cylinders transforming to a hexagonal perforated lamella. From the kinetics of this phase transition we estimated the interfacial tension between the cylinder and the perforated lamella phase. Its very small value of 2.5 $\mu\text{N/m}$ shows that lattice defects cost very little energy. Thus, defects and shape fluctuations are intrinsic features of fluid block copolymer microdomain structures. In another experiment we studied the micro-domain dynamics in a thin film of a block copolymer melt and observed repetitive transitions between distinct defect configurations on a time scale of tens of seconds [2]. The velocity of these transitions suggests a cooperative movement of clusters of polymer chains. Further observations are shape fluctuations of cylinders [2–5] and lamellae [4] and the annihilation of defects via the formation of transient phases [3].

Recent work focuses on analyzing the dynamics of shape fluctuations of cylinders [2–5]. Small-angle kinks are omnipresent defects in cylinder-forming and (more general) two-dimensional (2D) stripe-forming systems. At finite temperature, small-angle kinks are also found in perfectly ordered systems without topological defects. In AFM movies [2–5] as well as in 2D computer simulations of a stripe-forming system [6], we observe fluctuations of the position of kinks. A detailed analysis of the temporal correlations of the local orientation of stripes and their local curvature reveals aging behaviour and a glassy dynamics of kinks within perfectly ordered stripes [6].

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Confinement of semi-flexible polymers within closed surfaces

Jemal Guven and Pablo Vázquez-Montejo

Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México, Apdo. Postal 70-543, 04510 México, DF, MEXICO

A variational framework is developed to describe the equilibrium states of a semi-flexible polymer that is constrained to lie on a fixed surface. This framework is applied to examine the confinement of a polymer loop of fixed length $2\pi R$ within a sphere of radius $R_0 \leq R$.

It will be shown that there is an infinite number of distinct completely attached states, labeled by a pair of integers. Small loops oscillate about a geodesic circle with an n -fold symmetry, $n = 1, 2, \dots$. The two-fold is the stable ground state. For finite values of R , all higher n -folds exhibit instabilities.

The bending energy E of the ground state as well as the total force F that gets transmitted to the surface is determined as a function of R . The energy decomposes into a sum of two terms, one associated with deviations from geodesic behavior, the other associated with the constant normal curvature inherited from the sphere and proportional to R . For large values of R , the latter dominates, independent of the value of n : the ground state becomes infinitely degenerate.

Whenever $R = mR_0$, $m = 3, 5, \dots$, the ground state undergoes a transition from orbital to oscillatory behavior as the loop passes through an m -fold covering of a geodesic circle. Discontinuities are exhibited in F vs. R at these values of R reflecting the existence of an Euler buckling instability. Whereas F is always positive, the local force may be negative in places. Both E and F exhibit approximately periodic maxima at intermediate values of R associated with the increase in geodesic curvature when R is incommensurate with an odd multiple of R_0 . Asymptotically, F , like the energy, grows linearly with R .

When $R \geq 2R_0$ a new set of states appears beginning with a loop that assumes the form of a doubly covered geodesic circle. While these states possess a lower energy than the two-fold ground state in a set of finite bands of values of R , the latter continues to be stable classically within these bands.

Extensions to other confining geometries as well as the constraints on the polymer geometry at the boundary of the contact region will be briefly described.

Modeling the development and evolution of pigmentation patterns in butterflies

Filipa Alves

Instituto Gulbenkian de Ciéncia, Rua da Quinta Grande 6, 2780-156 Oeiras, Portugal

We are interested in understanding the biophysical and genetic bases of pattern formation and morphogenesis, both from the developmental and the evolutionary points of view. Our research is focused on the interplay between the biophysical mechanisms underlying cell and tissue morphogenesis and the different functional levels of regulatory networks (e.g. genetic, metabolic, and ionic). We are especially interested in how this interplay both generates and constrains the phenotypic variation observed in patterns and shapes within and among species.

Here, I will present an ongoing study on the formation of pigmentation patterns in butterfly wings, exploring how the generation of phenotypic variation may depend on the underlying gene network topology and respective biophysical and regulatory parameters.

We address these questions by using a multilevel modeling approach developed in close relation with the experimental data. We are modeling the genetic regulatory networks using partial differential equations and representing the spatial gene expression patterns in 2D using finite differences methods. Furthermore, we are developing image analysis algorithms to quantify the experimental images, and implementing optimization methods to estimate the models' parameter values.

Our results provide some testable hypotheses for how the observed variation on the pigmentation patterns may depend on subtle changes on specific biological parameters, opening interesting perspectives to understand the evolution of these mechanisms.

Session 1: 09:00 – 10:55

Chair: Yuru Deng

- | | | |
|--------------------------|-----------|---|
| Marianne Impérator-Clerc | <i>IL</i> | 3D-periodic complex structures in soft matter |
| Nicolas Rivier | <i>CT</i> | Generalised foams, disorder and entropy |
| Stuart Ramsden | <i>CT</i> | EPINET: Euclidean Patterns in Non-Euclidean Tilings |
-

10:55 – 11:15 Coffee break

Session 2: 11:15 – 13:00

Chair: Klaus Mecke

- | | | |
|----------------------------|-----------|--|
| Randall Kamien | <i>IL</i> | Layered Liquid Crystals |
| Sascha Hilgenfeldt | <i>CT</i> | Packings and Tilings: Size-Topology Correlations |
| Michael O’Keeffe (unconf.) | <i>CT</i> | 3-periodic minimal nets and minimal minimal surfaces |
-

13:00 – 14:30 Lunch break

Session 3: 14:30 – 16:20

Chair: Kell Mortensen

- | | | |
|--------------|-----------|--|
| Kåre Larsson | <i>IL</i> | Structure and function of the lipid bilayer
– with a historical perspective |
| Shunai Che | <i>CT</i> | Hierarchical Architectures in DNA & Silica Mineralization |
| David Siegel | <i>CT</i> | Lamellar-to-bicontinuous transition in phospholipids |
-

16:20 – 16:45 Coffee break

Session 4: 16:45 – 18:00

Chair: Robert Magerle

- | | | |
|--------------------|-----------|--|
| Robert Corkery | <i>CT</i> | Inorganic replicas of butterfly wing scales |
| Jacob Kirkensgaard | <i>CT</i> | Self-Assembly of multi-component miktoarm copolymers |
| Carsten Tschierske | <i>CT</i> | Complex tiling patterns in liquid crystals |
-

20:00 Conference Dinner

IL

Marianne Imp  rator-Clerc

Session: 9⁰⁰ – 10⁵⁵

3D-periodic complex structures in soft matter

Marianne Imp  rator-Clerc

Laboratoire de Physique des Solides, Bat 510, Universit   Paris-Sud, Orsay, France

Several 3D-periodic complex structures are encountered in many various soft matter systems such as liquid crystals, bloc-copolymer phases and related nano-structured materials. They exhibit well-defined topologies: 2D-hexagonal phase, 3D-packing of spheres, tetrahedral close packing (tcp), bi-continuous and tri-continuous cubic phases. We will summarize how small angle X-ray scattering experiments can elucidate these different structures and give an overview of the available structural models.

CT

Nicolas Rivier

Session: 9⁰⁰ – 10⁵⁵

Generalised Foams, Disorder and Entropy

Christophe Oguey¹ and Nicolas Rivier²

¹*LPTM, Universit   de Cergy-Pontoise, France*

²*IPCMS, Universit   de Strasbourg, France*

A foam is a cellular complex, a tessellation of \mathbb{R}^3 into cells bounded by interfaces that are irreducible circuits of edges. It is therefore a graded set of topological elements, vertices, edges, interfaces and cells related by incidence and boundary relations, with a corresponding dual network.

The structure of diamond is a foam, with 6-edge ‘‘chairs’’ as irreducible circuits. This foam is described either as: (i) a self-dual tiling by ‘‘saddle solids’’ $s\{3,3\}$, or as (ii) an Archimedean tiling 1:1 of tetrahedra (around the vertices) and truncated tetrahedra (cells), with vertices at the middle of the edges of the original diamond structure.[1] Morse critical points can be associated to its topological elements.

This foam can be disordered by repeated elementary topological transformations (*wwwflip*[2]), into the tetravalent structure *sillium*, a model for amorphous silicon an dits corresponding dual network.[3] The structure remains a foam at all stages, but the irreducible circuits are modified; there appear notably *twisted boats* and *overlapping* 7- circuits (on which three cells are incident). On the latter, three Morse critical points merge into a cubic critical point of the monkey-saddle type. The dual network (the Rnetwork dual to odd irreducible circuits) yields the entropy of the foam as the sum of two, combinatorial and configurational contributions. We can check that the final structure has maximal entropy.[4]

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[4] Rivier, N and Wooten, F, MATCH (Comm. Math. Comput. Chem.) 48 (2003) 145-153

EPINET: Euclidean Patterns in Non-Euclidean Tilings - Extending the Structure Zoo

Stuart Ramsden,^{1,2} Prof. Stephen Hyde,² and Dr. Vanessa Robins²

¹ANU Supercomputer Facility, ANU

²Department of Applied Mathematics, Research School of Physics and Engineering, ANU

We present the latest work in an ongoing investigation into the links between 2D Non-Euclidean Hyperbolic Tilings and Nets in 3D Euclidean space. The algorithm for enumerating a simple subset these structures has been outlined in [1] and our most recent results generalises the approach to a large family of related examples. The procedure uses recent advances in Computational Group Theory, the theory of Automatic Groups as realised in the KBMAG project [2], as well as Combinatorial Tiling Theory utilising the 2D Orbifold symmetry symbols of Thurston and Conway and the D-Tiling symbols of Dress, Huson and Delgado-Friedrichs [3]. The essential ingredient of these methods are definitions of discrete symbols for both 2D and 3D structures, whose isomorphism can be checked computationally and in some cases, enumerated for given symmetry and complexity constraints.

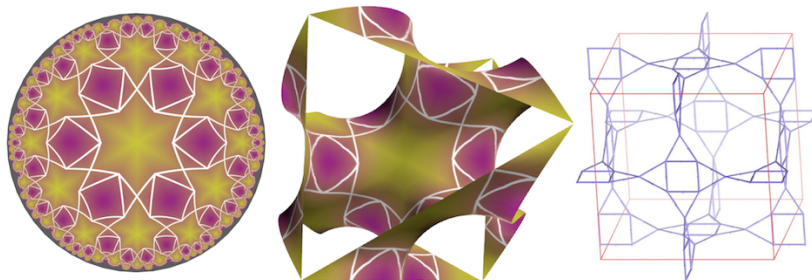


FIG. 1. The unit cell of the triply-periodic "P" minimal surface, shown above middle, is the link between the geometry of 2D Hyperbolic space (its intrinsic surface geometry, as shown on the left) and the extrinsic embedding space of regular Euclidean 3D space, where surface tilings are transformed to 3D nets.

Triply Periodic Minimal Surfaces (TPMS), the simplest of these being the P Primitive cubic (the example in the figure), the D Diamond or the G Gyroid Surface, are the link between the geometry of 2D Hyperbolic space (their intrinsic surface geometry) and their extrinsic embedding space of regular Euclidean 3D space. Depending on the direction of this process, we can derive periodic nets from surface tilings or show how a 3D net can be unwrapped into 2D Hyperbolic space. Importantly, the TPMSs provide constraints on the allowed symmetries, and these can be both enumerated and their supported tiling structures catalogued, up to a given complexity. We have built a database backed website to store and serve these structures, with sophisticated data mining tools for structure analysis, and comprehensive hyperlinks between related structures in both 2D and 3D available online at <http://epinet.anu.edu.au>

This work is supported by the ANU Supercomputer Facility, and the Australian Research Council

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- [2] D. Holt KBMAG v2.4, University of Warwick, Coventry, UK.
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Layered Liquid Crystals

Randall D. Kamien

Department of Physics and Astronomy, University of Pennsylvania, 209 S. 33rd St, Philadelphia, PA 19104-6396, USA

The homotopy theory of topological defects in ordered media fails to completely characterize systems with broken translational symmetry [1]. We argue that the problem can be understood in terms of the lack of rotational Goldstone modes in such systems and provide an alternate approach that correctly accounts for the interaction between translations and rotations. Dislocations are associated, as usual, with branch points in a phase field, whereas disclinations arise as critical points and singularities in the phase field [2]. We introduce a three-dimensional model for two-dimensional smectics that clarifies the topology of disclinations and geometrically captures known results without the need to add compatibility conditions. We will also discuss new constructions to generate equally-spaced, smectic ground states [3, 4].

This work was supported in part by NSF Grants DMR05-47230 and DMR05-20020.

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- [3] G.P. Alexander, B.G. Chen, E.A. Matsumoto, R.D. Kamien, *Phys. Rev. Lett.* **104**, 257802 (2010).
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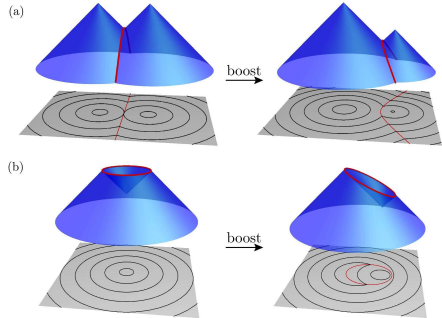


FIG. 1. Boundaries for (a) a pair of space-like and (b) time-like separated events, both in their rest frames (left) and in a general frame (right). The corresponding smectic textures are shown below each surface, with focal lines indicated in red. From [3].

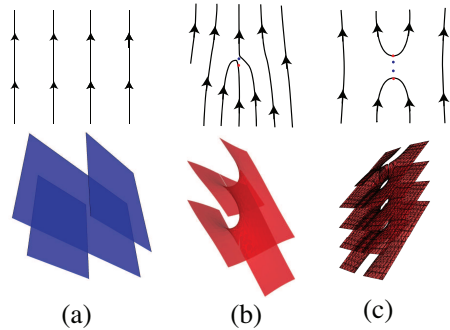


FIG. 2. Directed lines in the plane. The top row shows the layers derived from slicing the surface shown in the bottom row at integer values of the height, *i.e.* taking level sets. Red dots indicate the positions of branch points and blue dots indicate the positions of -1 index critical points (saddle point). (a) ground state (b) dislocation / helicoid, (c) two dislocations, note the cylindrical "hole" puncturing the planes, reminiscent of Riemann's minimal surface. From [2].

Statistics of Packings and Tilings: Size-Topology Correlations

 Sascha Hilgenfeldt¹ and Matthew P. Miklius²
¹*Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA*
²*Engineering Sciences and Applied Mathematics, Northwestern University, Evanston, IL 60208*

A polygonal tiling of the plane is a system with surprisingly complex statistics, as well as a model representing a variety of important physical and biological surface structures, from foams to domain materials and many epithelial or endothelial tissues. Both proliferating and remodeling tissues show distinctive statistical signatures in the distribution functions of areas and number of neighbors, but the two are also closely correlated, in a way not fundamentally understood.

Using a strictly local mean-field formalism (a generalization of the granocentric model [2] with no free parameters), we provide the first analytical insight into this correlation, which has been empirically seen in a large variety of living and inanimate systems, and show that it is compatible with both the quasistatic process of tissue remodeling and the dynamics of cell proliferation.

The model distinguishes (at least) two classes of systems: those where the minimization of an energy functional leads to compact shapes of the domains (these are well-described by the hard-disc theory), and those where such an energy functional is absent (mainly random Poisson-Voronoi tilings or related tilings where random cells are constructed under hard-disc exclusion processes). The latter systems display a significantly higher topological disorder when prepared at a given size disorder than the former systems, which tends to be the ones realized in physical systems like foam and tissue. When a random Voronoi cell system is assigned a perimeter energy functional (e.g. by importing it as a foam structure into surface evolver), the topological disorder decreases through topological changes in the cellular structure and settles at or near the value predicted by the granocentric model.

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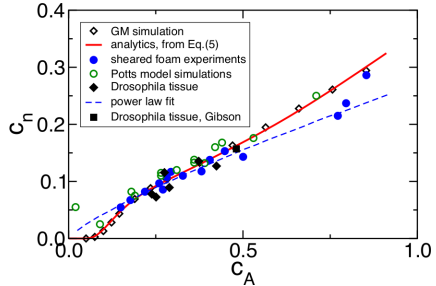


FIG. 1. Correlation between the coefficient of variation of area distribution c_A and coefficient of variation of neighbor distribution c_n for a variety of experimental systems (filled symbols), numerical simulations (open symbols), and the present analytical theory (solid line). The near-monodisperse regime for $c_A < 0.106$ displays crystallization of hard disks (almost perfect hexagonal coordination). For higher c_A , both polydisperse disc and polydisperse cellular systems closely follow the predicted correlation as long as the systems exhibit some minimization of interfacial energy. GM=granocentric model [2, 3].

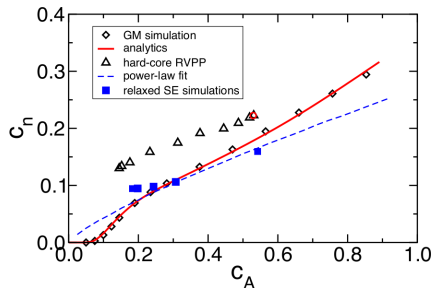


FIG. 2. Unminimized systems of random Voronoi polyhedra (RVP) with and without hard cores are not in agreement with theory. Simulations with the Surface Evolver [1] remodel these systems by energy minimization and move them towards the universal theory. GM=granocentric model [2, 3].

settles at or near the value predicted by the granocentric

Three-periodic minimal nets and minimal minimal surfaces

Michael O’Keeffe

Department of Chemistry, Arizona State University

In collaboration with Olaf Delgado-Friedrichs and Stephen T. Hyde (Australian National University)

The term *minimal* is used in two senses. Applied to d -periodic structures (graphs, surfaces) it means genus d per primitive cell. Applied to surfaces it means zero mean curvature. A *net* is a special kind of periodic graph; one that is simple and connected.

Associated with a net may be a *natural* tiling embedded in d -dimensional Euclidean space and which has a dual which carries a dual net. And associated with this pair of nets is a periodic surface which lies between the two nets so that each net is completely on the opposite side of the net from the other. The nets are the labyrinth graphs of the surface.

A minimal net has a finite quotient graph (graph with the translations factored out) with cyclomatic number d and it has long been known from work of Beukemann and Klee that there exactly 15 such nets for $d = 3$.

The 15 nets fall into two classes. 8 of them admit tilings and have associated surfaces. However some of these surfaces are topologically equivalent and only the five known minimal minimal surfaces appear as distinct surfaces. Thus the relation of nets to surfaces is seen to be many to one.

The remaining 7 minimal nets do not admit tilings (a precise definition of the meaning of this statement is so far lacking). They have the interesting property that in their maximum symmetry embeddings, some edges are of zero length and the pattern of the non-zero edges is exactly that of one of the labyrinth graphs of the known minimal minimal surfaces.

Thus we reconcile the apparent paradox that there are 15 minimal nets but only 5 minimal minimal surfaces.

Examples of higher genus nets and surfaces will also be given.

Structure and function of the lipid bilayer – with a historic perspective

Kåre Larsson

Camurus Lipid Research Foundation, Lund university, S-221 00 Lund, Sweden

Cell membranes form interfaces of fundamental importance in all living organisms. The knowledge of lipid bilayer structure and functionality during the 1950s were usually based on single crystal structure determinations and surface balance measurements of simple lipids. The evolution of our understanding of the lipid bilayer will be reviewed from that period and forward. The most important milestone was the structure determinations of the liquid-crystalline phases in soap-water systems, reported by Vittorio Luzzati and coworkers in 1960. The same types of structures were later observed also in aqueous systems of lipids, including cell membrane components, and in amphiphilic polymers.

Starting with some general features of hydrocarbon acyl chain packing in the solid state and the gel-state of lipids, the phases segregation induced by cholesterol will be discussed. Fatty acid monoglyceride phase diagrams and the structures of their liquid-crystalline phases will be shown with special regard to their cubic phases. In 1967 Luzzati and Spegd determined an $Ia\bar{3}d$ rod network structure of anhydrous sodium myristate. The knowledge on the aqueous cubic phases remained limited, although the demonstration of a bicontinuous character of the cubic glycerolmonooleate-water phase was a step forward. But then the introduction of the concepts introduced in Alan Schoen's report "Infinite periodic minimal surfaces without self-intersections" opened this field. The monoglyceride-water cubic structures were proven through the observed Bonnet relations between the dimensions of co-existing cubic phases (Hyde et al. 1984). Current work will be summarized, involving the incorporation of proteins into these cubic phases and their dispersions into nanoparticles.

The lipid bilayer organization at the alveolar lining of the lungs will then be considered. The first studies by cryo-transmission electron microscopy demonstrated the existence of a uniform liquid-crystalline surface phase by direct deposition of the alveolar surface film on the microscopy grid. Aggregates termed tubular myelin of this phase had earlier been studied and assumed to consist of intersecting bilayers forming a square cross-section pattern. The observed flow properties and interfacial orientation, however, indicated a continuous bilayer structure. Two minimal surface structure models of this phase are proposed. One is a CLP surface with space group $P4/mcc$, whereas the other is a tP surface with space group $I4/mmm$, both modified due to the scaffolding effects of the surfactant proteins. Depending upon the association of the surfactant protein A at its N-terminal, both bilayer alternatives may even coexist *in vivo*. Furthermore recent studies of lung surfactant present in the amniotic fluid indicate that a lamellar liquid-crystalline surface phase is formed at the first breath, induced by exposure towards an air surface.

The classical electrophysiological mechanism of nerve signal conduction has recently been challenged by the soliton theory proposed by Heimburg & Jackson (2005). According to the new theory, a phase transition wave involving crystallization of the nerve membrane bilayer, can explain the signal propagation. A clustering mechanism of lipid rafts, as described by Kai Simons, may play a significant role in the phase behavior. The conduction of the nerve signal is discussed here as an illustrative example of a lipid bilayer function, which involves robustness combined with high precision.

Formation of Hierarchical Architectures by DNA Self-Assembly and Silica Mineralization

Ben Liu, Lu Han, and Shunai Che

School of Chemistry and Chemical Engineering, State Key Laboratory of Metal Matrix Composites, Shanghai Jiao Tong University, 800 Dongchuan Road, Shanghai, P. R. China

Study of biomineralization has inspired various organic/inorganic hybrid materials with different shape, structure and superior properties. In vivo, meters of DNA are naturally packed into compact structures by a variety of methods that are optimized for specific requirements. Here, we report the synthesis of a DNA-silica complex with two-dimensional $p6mm$ and a rare two-dimensional $p4mm$ structure, together with the structural analysis using transmission electron microscopy. Based on the cooperative effects of quaternary ammonium silane, both acting as a DNA condensing agent through the positively charged quaternary ammonium group and stabilizing silica mineralization by co-condensing silane with the silica source. The small interaxial separation of DNAs formed upon quaternary ammonium-phosphate electrostatic “zipping” along the DNA-DNA contacts and the silica wall formed between the DNAs in the diagonal position were considered to be optimal for the formation of the $p4mm$ structure.[1, 2] Furthermore, alkaline earth metal ions were found to induce DNA chiral packing of two-dimensional square $p4mm$ mesostructures to give impeller-like helical DNA-silica complexes (IHDSCs). Antipodal IHDSCs were formed by tuning temperature, pH value and quaternary ammonium:DNA molar ratio due to the antipodal DNA layer-by-layer chiral packing. It has been suggested that the alkaline earth metal ions favor the stabilization of right-handed DNA helical stacking, while the chirality can be readily reversed by increasing the interaction between DNA and quaternary ammonium groups.

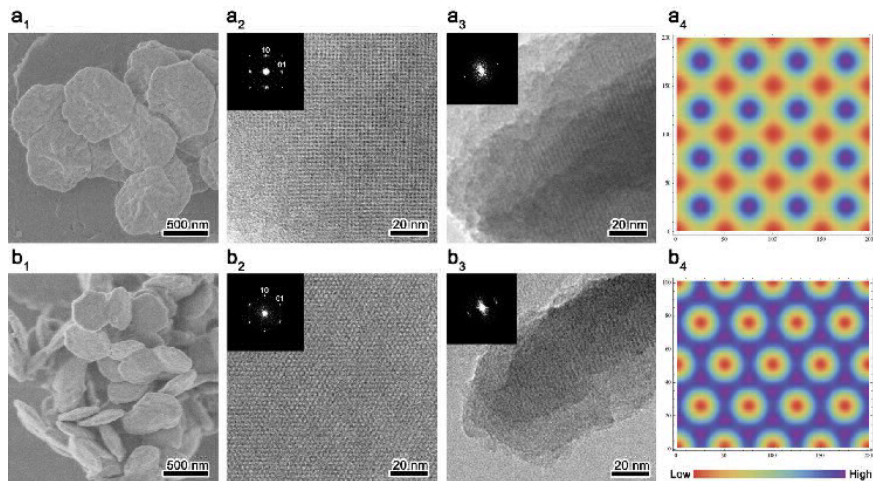


FIG. 1. Morphologies and structures of DSCs with the $p4mm$ (a) and $p6mm$ symmetry (b).

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The lamellar-to-bicontinuous inverted cubic ($L_\alpha \rightarrow Q_{II}$) phase transition is a frustrated second order phase transition: experimental evidence from a phospholipid system.

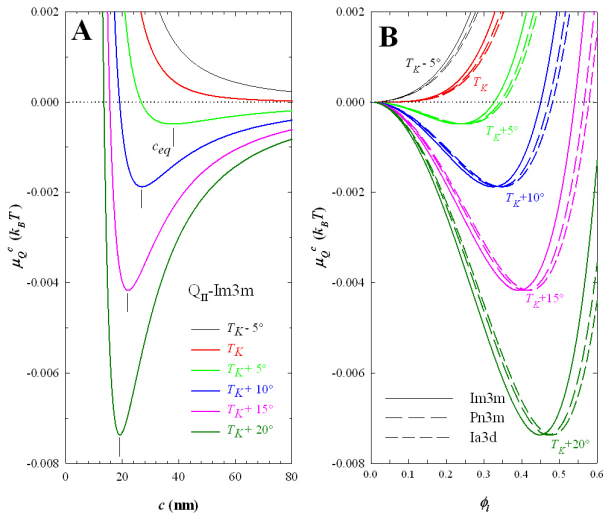
D.P. Siegel

Givaudan Inc., 1199 Edison Drive, Cincinnati, OH 45216, U.S.A.

It is important to understand the stability of the Q_{II} phase vs. the L_α phase, and the mechanism of the $L_\alpha \rightarrow Q_{II}$ phase transition, in order to understand the mechanism of biomembrane fusion. The susceptibility of a lipid composition to fusion is a function of its proximity to the L_α/Q_{II} phase boundary[1]. Membrane fusion is an obligatory step in the phase transition. In addition, peptides representing function-critical portions of one membrane fusion-mediating protein have been found to stabilize Q_{II} phases, while sequences representing fusionincapable mutants of this protein are much less effective [2]. This may be due to effects of amphipathic peptides on the curvature elastic constants of the lipid/peptide monolayers which stabilize fusion intermediates [3].

A recent analysis [4] of the phase transition in Nmethylated dioleoliphosphatidylethanolamine[5] shows that there is an equilibrium value of the cell constant for each Q_{II} phase in excess water, c_{eq} ; and that the dependence of c_{eq} on temperature is as predicted by a fourth order model of the curvature elastic energy (i.e., including a term for the square of the Gaussian curvature). As pointed out by Helfrich and Renschuh[6], this curvature energy model results in a second-order phase transition with order parameter c_{eq}^{-1} . However, the finite water content of real samples frustrates this transition, making it quasi-first order, with a temperature range of L_α/Q_{II} phase coexistence and an enthalpy of transition that depend on the water content of the sample. The concentration effects are predictable and are consistent with observations. The dependence of the difference in curvature energy between the L_α and Q_{II} phases ($\Delta\mu_Q^0$) on c_{eq} and on lipid concentration in a sample, ϕ , at different temperatures relative to the second order phase transition temperature T_K , is shown in the Figure. $\Delta\mu_Q^0$ is in terms of $k_B T$ per lipid molecule, at a reference T of 22°C (k_B is the Boltzmann constant).

$\Delta\mu_Q^0$ is very small over a wide temperature range. Small non-curvature energy contributions to the total energy difference between the two phases, which have negligible effects on other liquid crystalline phase transitions, strongly perturb the phase behavior as predicted solely on the basis of curvature energy. The most important such contribution identified so far is the unbinding energy in the L_α phase, which shifts the L_α/Q_{II} transition to higher temperatures[7]. In the case of phosphatidylethanolamines, attractive inter-bilayer forces are strong enough to destabilize the Q_{II} phase with respect to the H_{II} phase: no Q_{II} phase is observed in heating experiments. This model does not consider the elastic energy due to putative variations in lipid bilayer thickness. Its success so far suggests that such energies do not play a leading role in determining Q_{II} phase stability. The three Q_{II} phases have the same energy in excess water



role in determining Q_{II} phase stability. The three Q_{II} phases have the same energy in excess water at equilibrium. The relative predominance of them is postulated to be due to kinetic factors, perhaps due to differences in curvature energy of intermediates in transformations between them [8] at different degrees of swelling and temperature.

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CT

Robert Corkery

Session: 16⁴⁵ – 17⁴⁵

Inorganic replicas of butterfly wing scales

Christian Mille, Eric Tyrode, and Robert W. Corkery

YKI, Institute for Surface Chemistry, Stockholm, Sweden

Chitin wing scales of the butterfly *Callophrys rubi* (Green Hairstreak) contain gyroid structured, 3D, optically active photonic crystals. These provide a nicely preformed structure for studying natural and synthetic ordered 3D bicontinuous structures and their photonic properties. We test various methods of replicating the wing scale fine structure using relatively stable inorganic materials as fillers and several different synthetic approaches. We collect reflectance spectra using a CCD detector, diffraction grating and microscope with several objectives of high and low power and numerical apertures from dozens of replicated scales made under different conditions. The absolute reflectivity of the replicas and original scales are determined using silver and dielectric mirror standards with several light sources and linear and circular polarizations. Spectra and optical activity of the replicated scales will be discussed in relation to their proposed I₄32 gyroid structure, microscopic and mesoscopic order, dielectric properties, volume fractions and unit cell sizes.

Complex self-assembly morphologies of multicomponent miktoarm star copolymer melts

Jacob Judas Kain Kirkensgaard

Dept. Basic Sciences and Environment, LIFE, University of Copenhagen, Denmark

I will present an overview of simulations and experiments investigating the self-assembly morphologies of various complex architecture miktoarm star copolymers consisting of more than two components (see figure for examples). The star topology of such molecules allow a wealth of new structures to be controllably realized as a function of composition, interaction parameters and molecular architecture [1, 2].

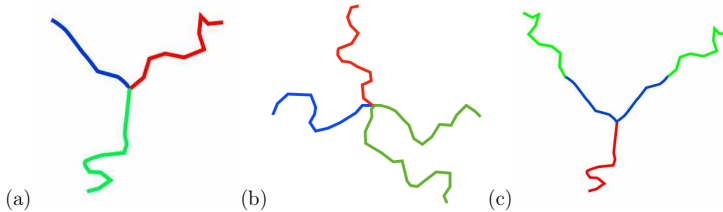


FIG. 1. Examples of block copolymer molecular designs with varying structural complexity. (a) Star-shaped ABC 3-miktoarm terpolymer (b) Star-shaped ABC₂ 4-miktoarm terpolymer (c) Star-shaped A(BC)₂ 3-miktoarm terpolymer.

JJKK acknowledge financial support from the Lundbeck foundation.

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Complex Tiling Patterns in Liquid Crystals

C. Tschierske,¹ C. Nürnberger,¹ H. Ebert,¹ B. Glettner,¹ M. Prehm,¹ F. Liu,² X.-B. Zeng,² and G. Ungar²

¹*Institute of Chemistry, Organic Chemistry, Martin-Luther University Halle-Wittenberg, Kurt-Mothes Str. 2, 06120 Halle/Saale, Germany*

²*Department of Engineering Materials and Centre for Molecular Materials, University of Sheffield, Mappin Street, Sheffield S1 3JD, UK*

Specifically designed polyphilic molecules can self-assemble into a series of fluid (liquid crystalline) honeycomb structures based on polygons with cross sectional shapes ranging from triangles via squares and pentagons to hexagons and beyond. [1] These honeycombs can be regarded as tilings of a plane which are extended in the third dimension. Most of them represent Archimedial tilings, but also their topological duals, the Laves tilings, have been obtained.

By further increase of the number of incompatible units combined in these polyphiles fluid self assembled honeycomb structures were obtained where the cells have distinct compositions, i.e. these LC phases can be described as multicolour tilings of a plane extended in the third dimension. Finetuning of geometric frustration and miscibility frustration allows formation of structures with a number of distinct compartments exceeding the number of incompatible units actually combined in the molecular tectons. In this way new tiling patterns with unique complexity have been obtained by slight variation of the molecular structure, leading multicolour tilings composed of very different tiles, as for example (triangles + hexagons = Kagome), (squares + pentagons), (squares + hexagons), (triangles + squares + pentagons), and numerous patterns combining squares rhombs and triangles in distinct ratios, leading to huge lattice parameters and tiling patterns composed of even 5 distinct tiles having different color and distinct shape [2].

[1] C. Tschierske, Chem. Soc. Rev. 2007, 36, 1930.

[2] X. Zeng, R. Kieffer, B. Glettner, C. Nürnberger, F. Liu, K. Pelz, M. Prehm, U. Baumeister, H. Hahn, H. Lang, G. A. Geringer, C. H. M. Weber, J. K. Hobbs, C. Tschierske, G. Ungar, Science 2011, 311, 1302.

Session 1: 09:00 – 10:20

Chair: Randall Kamien

- | | |
|-------------------------|---|
| Douglas Cleaver | <i>CT</i> Hierarchical Chiral Fibers from Achiral Particles |
| Tommy Nylander | <i>CT</i> Lipase Action on Lipid Liquid crystalline Nanoparticles |
| Oksana Manyuhina | <i>CT</i> (De)formation of spherical vesicles in magnetic fields |
-

10:20 – 10:50 Coffee break

Session 2: 10:50 – 12:00

Chair: Gerd Schröder-Turk

- | | |
|------------------------|---|
| Bodo Wilts | <i>CT</i> Brillouin zone imaging of biological photonic crystals |
| Björn Stuhmann | <i>CT</i> Cellular Self-Organization by Actin-Filled Liposomes |
| Debby Chang | <i>CT</i> Interfacial behavior of Lipid LC Nanoparticle on Surfaces |
| Closing Remarks | |
-

CT

Douglas Cleaver

Session: 9⁰⁰ – 10²⁰

Hierarchical Self-Assembly of Chiral Fibers from Achiral Particles

Doug Cleaver,¹ Pavel Prybytak,¹ and Bill Frith²

¹Materials and Engineering Research Institute, Sheffield Hallam University, Howard Street, Sheffield, S1 1WB, United Kingdom

²Unilever Discover, Colworth Laboratories, Bedfordshire, United Kingdom

We show, using particle-based simulation, that chiral fibers can freely self assemble from achiral disks. The chirality results from frustration between the hexagonal packing and interdigitation of neighboring threads in nucleating clusters, the pitch being set by particle shape. Defect-free fibres are found to grow via an identifiable hierarchy of structures and processes, the growth being controlled by self-assembly kinetics rather than thermodynamics. We also investigate whether chiral fibres have a limiting radius.

P. P. acknowledge financial support from Unilever and Sheffield Hallam University.

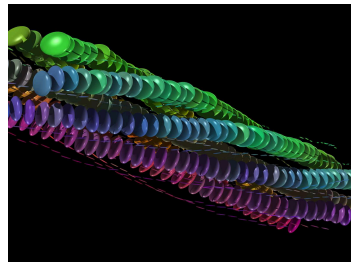


FIG. 1. Central thread and second layer threads from a self-assembled chiral fibre.

CT

Tommy Nylander

Session: 9⁰⁰ – 10²⁰

Lipase Action on Self-Assembled Lipid Liquid Crystalline Nanoparticles

Justas Barauskas,¹ Daniel Anderberg,¹ Allan Svendsen,² and Tommy Nylander¹

¹Physical Chemistry 1, Center for Chemistry and Chemical Engineering, Lund University, P.O. Box 124, SE-221 00 Lund, Sweden

²Novozymes A/S, Smørumsevej 25, DK-2880, Bagsvaerd, Denmark

Natural lipase substrates are supramolecular assemblies, either emulsion droplets or liquid crystalline aggregates. Most of the lipolysis takes place at interfaces and is dependent on the structure and organization of the lipid/water boundary as well as internal structure of the aggregate. The internal structure controls both the access of the substrate as well as the ability to take care of the product. During the course of the reaction, hydrolysis products interact with lipid substrate, continuously change the interface curvature, charge and hydrophobicity as well as other aggregate characteristics. Most of the studies so far have been focused on the changes of that take place at the lipid aqueous interface without taken into account the change in curvature and self-assembly structure. We have used non-lamellar self-assembled lipid nanoparticles as well defined and biomimicking substrate in order to gain fundamental knowledge on lipase (*Thermomyces lanuginosus lipase*) catalyzed processes in terms of the changes in morphology and internal structure of the lipid aggregate (substrate). The results from two types of substrate structures will be presented, namely glycerol monooleate-based cubic and reversed hexagonal liquid crystalline nano-particles. These types nano-particles are likely to occur during the lipolysis process and also have potential use as drug delivery vehicles. The changes in lipid aggregate morphology and internal structure as a function of a lipase action have been investigated by means pH-stat titration, cryogenic transmission electron microscopy (cryo-TEM) and synchrotron X-ray diffraction techniques. In the cryo-TEM study we also used lipase conjugated to gold nanoparticles, enzymatically active hybrid nanoparticles, to simultaneously visualize the location of the enzyme and the effects of enzymatic digestion of lipid aggregates. Our results clearly show that the enzyme action is strongly influenced by the self-assembled structure and the lipid composition providing the possibility to control lipase activity.

(De)formation of spherical vesicles in high magnetic fieldsOksana Manyuhina,¹ Annalisa Fasolino,² and Mikhail Katsnelson²¹*Nordic Institute for Theoretical Physics, Roslagstullsbacken 23, 10691 Stockholm, Sweden*²*Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands*

Magnetic forces tend to align diamagnetic molecules, which leads to deformation of self-assembled spherical vesicles towards superspheroids [1]. In order to explain experimental data and to extract the values of elastic constants, we compare the predictions of two phenomenological models. We find that at low magnetic fields (up to 3 T) the deformations are described by the Helfrich model. At high magnetic fields (up to 20 T) the fourth order Landau–Ginsburg free energy accounts for the anharmonic behaviour and allows to discuss the overall stability of vesicles. This model predicts spherical as well as non-spherical shapes with dimples, bumps and ridges to be the energy minimizers. Our results suggest that the buckling and faceting transitions, usually associated with crystalline matter, can also be an intrinsic property of non-crystalline membranes [2].

Because of the vanishingly small surface tension vesicles can easily adjust their shape in presence of magnetic field, temperature or other external influences. However, one cannot exclude the possibility of the change of topology. As an example, we consider topological transformations between spherical vesicles and double bubble [3], a shape composed of two spherical caps separated by a flat membrane. A simple geometric approach allows to take into account the details of microscopic interactions into phenomenological models, by introducing topological defects. These defects result from the stacking of flat aromatic molecules on a curved surface. In presence of two defects on spheroid the equilibrium shape of vesicles turns out to be elongated [4]. The interaction of the defects with magnetic field may result in new phenomena.

- [1] O. V. Manyuhina, I. O. Shklyarevskiy, P. Jonkheijm, P. C. M. Christianen, A. Fasolino, M. I. Katsnelson, A. P. H. J. Schenning, E. W. Meijer, O. Henze, A. F. M. Kilbinger, W. J. Feast, and J. C. Maan, *Phys. Rev. Lett.* 98, 146101 (2007)
- [2] O. V. Manyuhina, J. J. Hetzel, M. I. Katsnelson, and A. Fasolino, *Eur. Phys. J. E* 32, 223 (2010) [Cover]
- [3] O. V. Manyuhina, A. Fasolino, P. C. M. Christianen, and M. I. Katsnelson, *Phys. Rev. E* 80, R010403 (2009)
- [4] O. V. Manyuhina, A. Fasolino, and M. I. Katsnelson, *J. Phys. Chem. B* 113, 10549 (2009)

Direct Brillouin zone imaging of biological photonic crystals

Bodo Wilts,¹ Kristel Michielsen,² Hans De Raedt,¹ and Doekele Stavenga¹

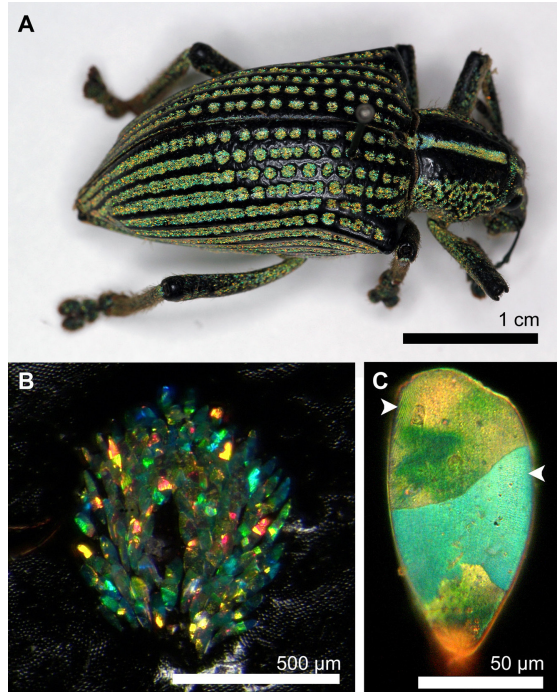
¹Computational Physics, Zernike Institute for Advanced Materials, University of Groningen, NL-9717 AG Groningen, The Netherlands

²Institute for Advanced Simulation, Jülich Supercomputing Centre, Research Centre Jülich, D-52425 Jülich, Germany

The brilliant body colours of many animals, specifically butterflies, beetles and birds, are created by the presence of three-dimensional biological photonic crystals. The refractive index distribution in the photonic crystals is usually topologically arranged in one of three minimal energy surfaces and tuned to reflect light in a restricted, visible wavelength range.

A very intriguing animal is the Diamond Weevil, *Entimus imperialis*. By electron microscopy, we found that the weevil's body colours are created by diamond-type photonic crystals, which are found inside scales covering the elytron (see below). We, for the first time, were able to directly visualize the Brillouin zones of the photonic crystal, having fcc-symmetry, by using imaging scatterometry. The symmetries of the underlying structural minimal symmetry representation were directly discernible. With the scatterometer technique, we were able to measure the spectral response of differently oriented crystals. We confirmed that the reflected colour space is restricted to that of the ideal crystal structure. Our approach also allowed the precise measurement of the photonic bandgap diagram of the crystal in arbitrary directions and the determination of the crystal orientation in the scales.

The unique possibility of direct imaging of the Brillouin zones provides key insights not only for artificial mimicking photonic crystal structures, but also for non-invasive determination of unknown photonic structures encountered in other animals.



Physics of Cellular Self-Organization Studied with Biomimetic Actin-Filled Liposomes

Björn Stuhmann, Feng-Ching Tsai, and Gijsje Koenderink

FOM Institute AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands

Living cells are pervaded by a three-dimensional biopolymer network, the cytoskeleton. This composite active gel dynamically self-organizes into a multitude of structural arrangements which chiefly determine cell shape, mechanics, dynamics, and function. Driven by a complex interplay of enthalpic and entropic effects which occur far from thermodynamic equilibrium, cytoskeletal organization demands for new descriptions which extend classical polymer and statistical physics. The inherent complexity and variability of cells hampers the identification of physical working principles and demands for chemically defined *in vitro* assays for quantitative and systematic investigation. We have built realistic *in vitro* models of living cells by encapsulating cross-linked actin networks together with myosin motors in cell-sized membranous containers (liposomes) (FIG. 1) [1]. Combined contour fluctuation analysis and confocal microscopy allows us the examination of mechanical and 3D structural properties of these biomimetic cells. I will relate observed network architectures to liposome contour fluctuation spectra. I will further

report on a laser microrheology protocol which will permit the extraction of the non-Brownian component of network fluctuations, thereby yielding insights into nano-scale mechanisms of force generation. This model system can guide future quantitative studies of the physical regulation of confined active gels that determine cellular processes such as cell spreading, contraction and blebbing, and myosin-based mechanosensing.

This work was financially supported by The Netherlands Organisation for Scientific Research (NWO) through a VIDI grant (F.-C.T. and G.K.) and by the European Union through a Marie Curie IE Fellowship (B.S.).

[1] F.-C. Tsai, B. Stuhmann, and G. H. Koenderink, *Langmuir*, DOI:10.1021/la201604z (2011)

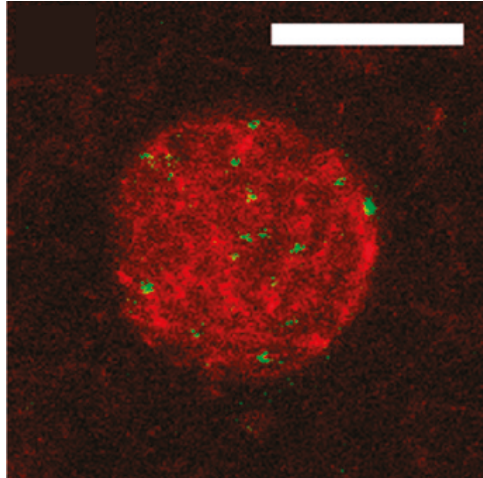


FIG. 1. A biomimetic model of a living cell's confined cytoskeleton comprised of an active gel (actin filaments in red) co-encapsulated with molecular motors (myosin II proteins in green) in a spherical lipid membrane container. Scale bar 10 μm . Taken from [1].

Interfacial behavior of Lipid Liquid Crystalline Nanoparticle on Surfaces

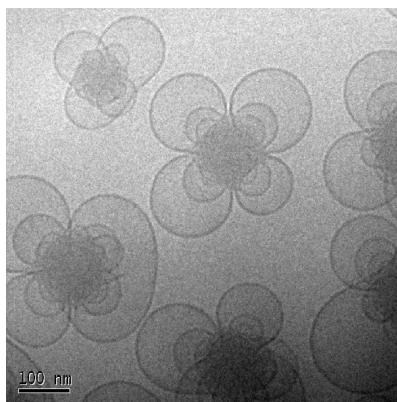
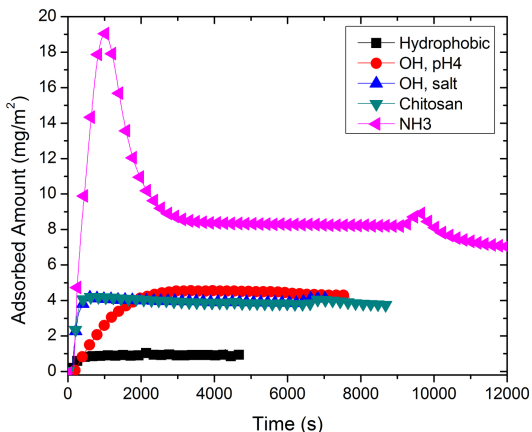
Debby P. Chang,¹ Justas Barauskas,² Fredrik Tiberg,^{3,1} and Tommy Nylander¹

¹Department of Physical Chemistry, Lund University, Lund, Sweden

²Institute of Biochemistry, Vilnius University, Vilnius, Lithuania

³Camurus AB, Ideon Science Park, Lund, Sweden

Investigation of non-lamellar nanoparticles formed by dispersion of self-assembled lipid mesophases is stimulated by their potential uses in science and technology due to encapsulating and space-dividing nature; featuring both hydrophilic and hydrophobic domains forming mono- or bi-continuous networks [1]. The non-lamellar aggregates at physiologically relevant temperatures can form a bicontinuous cubic phase which can be dispersed into non-lamellar nanoparticles in excess aqueous solution [2, 3]. In this study, we monitored the adsorption of lipid liquid crystalline nanoparticle (LCNP) on model surfaces with the use of ellipsometry. The technique allows time-resolved monitoring of layer thickness and adsorbed amount, which provides important insights into the restructuring of the lipid nanoparticle upon adsorption. The effect of solvent condition, electrolyte concentration, particle size, particle concentration and surface chemistry on adsorption was investigated. These LCNP are shown to form thin functional layer of liquid crystal on surface. The adsorption process is strongly dependent on the surface chemistry. On the hydrophobic surface, large hydrophobic attraction results in structural relaxation of LCNP, dissociating the particles and forming monolayer coverage of lipid on surface. In contrast, a thick surface layer of LCNP is formed on hydrophilic surfaces. The layer thickness is dependent on the particle size, where particle reorganization can be observed in real time. Understanding the interfacial behavior of LCNP on surfaces can shed light into the drug release mechanisms and also provide a way to form well-defined nanostructure layers as functional surface coating.



- [1] Barauskas, J., Nylander, T. 2008, In *Delivery and controlled release of bioactives in foods and nutraceuticals*. Ed. N. Garti. Woodhead Publishing Ltd: Cambridge, pp. 107-131.
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- [3] Barauskas, J., Johnsson, M., Joabsson, F., Tiberg F., 2005, *Langmuir*, 21, 2569-2577.

Poster Session

Tuesday, Session 4: 16:00 – 17:30

See poster abstracts on the following pages

Includes coffee break with wine and snacks

Investigation of the formation of silica mesoporous materials prepared in acidic condition

Ling Qin and Michael W. Anderson

Centre for Nanoporous Materials, School of Chemistry, The University of Manchester, Oxford Road, Manchester. M13 9PL, UK

Mesoporous silica materials have attracted great scientific interest since discovered by scientists in Mobil[1]. It is a natural elegance that inorganic siliceous species form minimal surfaces spontaneously while wrapping amphiphilic templates. Recently, a constant-curvature surface (CCS) was proposed with the study in synthetic mechanism of SBA-1[2]. In this work, an electron density map of several as-prepared and calcined mesoporous materials synthesized in acidic condition (SBA-1, SBA-16, AMS-8 and AMS-10) was compared with the corresponding CCS calculated by Surface Evolver. Both experimental and modelling data are refined by pore volume from nitrogen adsorption, giving the exact interface between silica moieties and surfactant micelles. As-prepared SBA-16 powders are treated under the ozone flow, allowing template removal under mild conditions, without enduring any shrinkage of the silica. A t-plot from nitrogen adsorption data shows ozone decomposes the surfactant molecules in the mesopores completely and keeps those in the micropores nearly intact.

According to the comparison figures for SBA-16, it is shown that during the sol-gel process, the nonelectrostatic interaction between hydrophilic ends of tri-block F127 and silica oligomers resists the inorganic species forming the minimal surface, giving a distinct discrepancy between electron density contour and constant-curvature scatter plot (Fig. 1a). Also an excellent fit for the calcined SBA-16 (Fig. 1b) shows the silica moieties start a further minimization in surface area during calcination, when surfactants are burnt out and unable to affect the solid wall.

Ling Qin is sponsored by China Scholarship Council (CSC) and the University of Manchester.

- [1] Beck, J. S. et al, Journal of the American Chemical Society 114, pp. 10834-10843 (1992)
- [2] Anderson, M. W. et al. Studies in Surface Science and Catalysis. 165, pp. 13-16 (Elsevier, 2007)

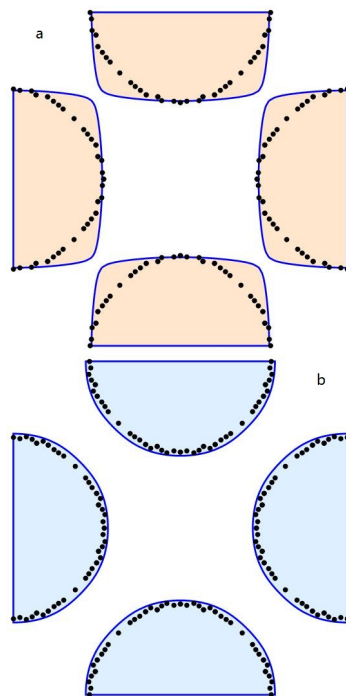


FIG. 1. Comparison between constant-curvature surface (dotted) and electron-density contours of as-synthesized (a) and calcined (b) SBA-16

From three-dimensional weavings to swollen corneocytes

Myfanwy E. Evans¹ and Stephen T. Hyde²

¹*Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen Deutschland*

²*Department of Applied Mathematics, Australian National University, Canberra, Australia*

A novel technique to generate three-dimensional Euclidean weavings, composed of close-packed, periodic arrays of one-dimensional fibres, is described in this talk. These weavings are constructed as decorations of Triply-Periodic Minimal Surfaces. Some of these weavings are shown to dilate by simple shape changes of the constituent fibres (such as fibre straightening).

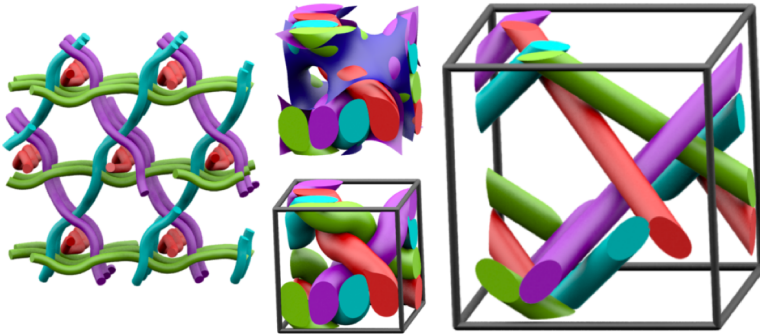


FIG. 1. The ideal G_{129} weaving lies almost completely within one channel of the gyroid, and is finitely dilatant. (Left) The extended ideal G_{129} weaving. (Centre) One unit cell of the ideal weaving, which lies almost completely within one channel of the gyroid. (Right) The swollen configuration of the weaving is the Σ^+ rod packing.

In particular, the free volume within a chiral cubic example of a dilatant weaving, the ideal conformation of the G_{129} weaving related to the Σ^+ rod packing, expands more than five-fold on filament straightening. This remarkable three-dimensional weaving, therefore, allows an unprecedented variation of packing density without loss of structural rigidity and is an attractive design target for materials.

We propose that the G_{129} weaving (ideal Σ^+ weaving) is formed by keratin fibres in the outermost layer of mammalian skin, probably templated by a folded membrane [1].

[1] M.E. Evans and S.T. Hyde, J. R. Soc. Interface, doi:10.1098/rsif.2010.0722 (2011)

The shape of deformed of foam cells

Myfanwy E. Evans,¹ Johannes Zirkelbach,¹ Gerd E. Schröder-Turk,¹ Andrew M. Kraynik,^{1,2} and Klaus Mecke¹

¹*Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*

²*CEAS, University of Manchester, UK*

This poster presents some preliminary results of the analysis of various shape measures of individual cells in random monodisperse foams (as previously considered in [1]). The shape measures considered are the suite of Minkowski tensors [3]. Further, we explore how these quantities change for each cell as the foam undergoes a shear deformation, where cells may either deform elastically or flow (*i.e* change topologically).

The growth rate of foam cells by diffusive coarsening is governed by the mean curvature of the faces of the cells at equilibrium. We examine measures of the shape of deformed isotropic Plateau polyhedral cells [2] to gain insight into how the growth rate of these models changes with deformation. We find that this growth rate may increase or decrease depending on the particular deformation applied. An experimental verification of the deformed cubic Plateau polyhedra is also constructed, as shown in Fig. 1.

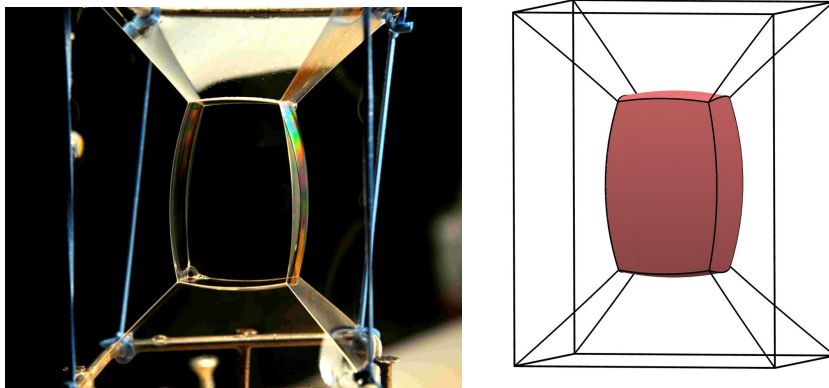


FIG. 1. Experiment and simulation of a cubic, isotropic Plateau polyhedron, deformed by an extension.

We acknowledge support by the DFG through the research group “Geometry and Physics of Spatial Random Systems” under grant SCHR 1148/3-1.

[1] A.M. Kraynik and D.A. Reinelt and F. van Swol, *Phys Rev E*, 67, 031403 (2003)

[2] S. Hilgenfeldt and A.M. Kraynik and D.J. Reinelt and J. Sullivan, *Europhys Lett*, 67, 484–490 (2004)

[3] G. E. Schröder-Turk et al., *Adv. Mater.*, 23, 2535–2553 (2011)

Peter Falkman, Lina Pedersen, and Johan Engblom

Faculty of Health and Society, Malmö University, Malmö, Sweden

The project aims at mapping the lyotropic and thermotropic phase behavior of the DOPS/DOPE/water system, with particular focus on finding and characterizing any potential bicontinuous mesophases.

Diolyl phosphatidyl ethanolamine (DOPE) is known to form mostly an inverted hexagonal structure (H_{II}) in aqueous systems (lamellar liquid crystalline (L_a) at low temperatures and medium hydration)[1–3], but reports also exist of cubic phases at low temperatures.[2–4] To our knowledge, no cubic phases at room temperature have been reported so far. Diolyl phosphatidyl serine (DOPS) is less studied, but is known to form L_a structures upon hydration.

Synchrotron SAXD and optical microscopy have been used to construct a phase diagram, showing a large $L1s$ phase towards the DOPS corner, with a maximum swelling above 80% water, and a smaller H_{II} phase with a maximum swelling at 32% water towards the DOPE corner. Two bicontinuous cubic phases, $Pn3m$ and $Ia3d$, have been identified, the position of which have been calculated from a swelling analysis of the cubic parts of the 2-phase samples.[5] The $Pn3m$ resides close to the DOPE side and at medium hydration, while the $Ia3d$ is closer to DOPS/DOPE 35/65, also at medium hydration. Additionally, a highly swollen $Im3m$ bicontinuous cubic phase has been observed at high water and DOPE content.

- [1] Shalaev E.Y., Steponkus, P.L., *Biochim Biophys Acta* 1419 (1999) 229-47
- [2] Gawrisch K. et al., *Biochemistry* 31 (1992) 2856-64
- [3] Rand R. P., Fuller N.L., *Biophys J* 66 (1994) 2127-38
- [4] Shyamsunder E. et al., *Biochemistry* 27 (1988) 2332-36
- [5] Engblom J., Hyde S.T., *J Phys II (France)* 5 (1995) 171-190

Chemical Reaction Diffusion Systems

Laurent Helden,¹ Christian Scholz,¹ and Clemens Bechinger^{1,2}

¹ *Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart*

² *Max-Planck-Institut für intelligente Systeme, Heisenbergstraße 3, 70569 Stuttgart*

Chemical reaction diffusion systems are versatile realizations of pattern formation. We present first results of a recently build up gel reactor for the CDIMA (chlorine dioxid, iodine, malonic acid) reaction. Various Turing patterns are displayed and compared with the Lengjel-Eppstein model. In addition non stationary turbulent states were observed. Preliminary results of an analysis of these pattern in terms of Minkowski functionals [1] are discussed.

- [1] K. Mecke, Morphological characterization of patterns in reaction-diffusion systems, *Phys. Rev. E* 53, 4794 (1996)

Ryo Nakazawa,¹ Akihiro Kuroda,² Eisuke Nihei,³ Takaaki Ishigure,³ Yuichiro Suzuki,³ and Kouichi Asakura¹

¹Department of Applied Chemistry, Faculty of Science and Technology, Keio University, 3-14-1, Hiyoshi, Kohoku, Yokohama, 223-8522, Japan

²Cosmetecno Co., Ltd, Yokohama Office, 87-6, Nakayama-cho, Midori, Yokohama, 226-0011, Japan

³Department of Applied Physics and Physico-Informatics, Faculty of Science and Technology, Keio University, 3-14-1, Hiyoshi, Kohoku, Yokohama 223-8522, Japan

Micro lens arrays, i.e. multiple lenses formed in a two-dimensional array on a substrate, are important photonic devices[1]. One important their character is a light diffusion property. In general, they have been fabricated by molding. The methods to prepare templates, however, usually include expensive and multistep processes. Development of simple and low-cost methods for the production of micro lens arrays is thus expected.

In this study, attempts were made to apply the phenomenon called directional viscous fingering[2], an example of pattern formation in far-from-equilibrium system, to the technology for fabricating a device that possesses a light diffusion property. Directional viscous fingering is a spatially periodic stripe pattern formation by passing a viscous fluid through a small gap or peeling two pieces of adhesive tape that are stuck to each other. We have reported that the directional viscous fingering could be utilized for fabricating water-repellent surface[3]. Here, we show that the phenomenon can be utilized for fabricating a device that possesses light diffusion property.

A suspension of moisture curing silicone resin in volatile silicone, decamethyl cyclopentasiloxane, was spread on a glass plate by dragging an applicator across the top. A stripe pattern parallel to the direction of dragging was formed, and the surface profile was analyzed as shown in FIG. 1. By changing the weight fraction of silicone resin in samples from 0.40 to 0.85 and dragging

A light diffusion property of the patterned surface was analyzed using a red laser beam (635nm). The laser beam was injected to the sample with the stripe pattern, and then, the far-field image of the laser beam 2 m apart from the sample plate was analyzed. FIG. 2 (a) and (b) are the expanded laser beam images from a grating prepared for a control experiment and a sample plate on which the stripe pattern was formed, respectively. Although the slit width of the grating and the characteristic length of the stripe pattern was almost the same, light diffusion property of the stripe pattern was much larger than the one of the grating. Two-dimensional beam expansion was realized by passing the laser beam to a pair of the sample plate placed to be perpendicular to each other as shown in FIG. 2 (b'). Testing many stripe patterns formed on the glass plate, larger optical diffusion property of the stripe pattern was observed when the characteristic length was relatively large and the gap was relatively small. To analyze the light diffusion property of the patterned surface, we used a laser beam propagation simulation software.

[1] Sazena, K., Jain, V.K., Mehta, D.S., Optical Materials 32, pp. 221-233 (2009)

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[3] Kuroda, A., Ishihara, T., Takeshige, H. and Asakura, K., J. Phys. Chem. B 112, pp. 1163-1169 (2008)

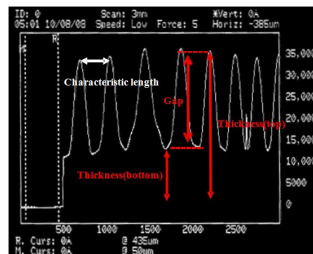


FIG. 1. Surface structure analysis by surface profile measuring system DEKTAK 3030.

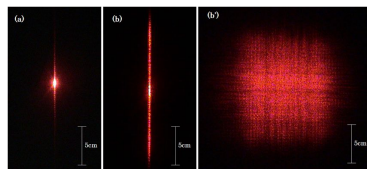


FIG. 2. Expanded laser beam by the spatially periodic pattern. (a) Expanded by a grating having a slit width of 300 μm . (b) Expanded by the stripe pattern having a characteristic length of about 400 μm and a gap of about 7 μm . (b') Expanded by two stripe patterns placed to be perpendicular to each other.

Change in membrane curvature due to drug-headgroup interactions

Drew Parsons, Shannon Notley, and Barry Ninham

Dept. of Applied Mathematics, Research School of Physical Sciences and Engineering, Australian National University

Membrane curvature may be characterised by the ratio of head group volume to tail group volume. It is believed that the pharmacological effect of certain classes of drugs arises due to a change in the membrane curvature induced by the drug. π -cation interactions between aromatic molecules and cationic head groups have been suggested as the mechanism responsible, causing a shift in the area and hence volume per head group. We probe this hypothesis through quantum chemical calculations of isomers of dihydroxybenzene interacting with tertiary ammonium surfactant molecules.

We find a shift in the ratio of head group to tail group volumes as expected, implying a change in curvature. However π -cation interactions do not appear to be the driving mechanism. Instead, the aromatic part of the molecule appears to prefer the hydrophobic tail group. Interaction with the head group is dominated by electrostatic attraction between the cationic head group and electronegative hydroxyl groups of the aromatic molecule. Significantly, the change in curvature arises as a consequence of the distribution of the hydroxyl groups around the aromatic ring. In the ortho configuration the hydroxyl groups have a cooperative interaction with head groups, enabling the aromatic ring to sink into the tail group region and thereby increasing the relative volume of the tail group. In the para configuration the hydroxyl groups compete with each other to gain proximity to the head groups, lifting the aromatic ring towards the head groups and thereby increasing the relative volume of the head groups.

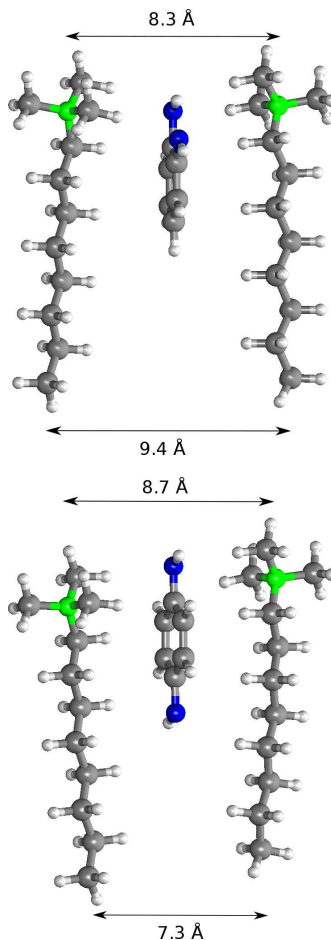


FIG. 1. Optimal packing for catechol (top) and hydroquinone (bottom) between trimethyloctylammonium surfactant molecules.

Preparation of biomorphous photonic structures for high-temperature gas sensor applications

Daniel Van Opdenbosch, Maren Johannes, and Cordt Zollfrank

Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Materialwissenschaften und Werkstofftechnik, Lehrstuhl Glas und Keramik, Martensstraße 5, Deutschland

Photonic materials found in nature can comprise highly complex one- two- or three-dimensional structures that currently cannot be reproduced by artificial structuring techniques [1]. Since photonic responses change with the structures' changing optical thicknesses (i.e. with changing refractive index for constant structural dimensions), photonic materials have recently attained further interest as gas sensors [2, 3]. Our work shows a convenient route to directly replicate natural photonic structures into amorphous inorganic silica, which is capable of withstanding temperatures up to 600 °C. The D-surface structured natural photonic crystal, contained in the scales of the beetle *Entimus imperialis*, was successfully replicated, 1. The processing involved harvesting the scales, infiltrating them with polydivinyl- and polyhydromethylsiloxane mixtures and curing in the presence of platinum complexes by hydrosilylation. An adapted heating cycle removed the organic photonic template and yielded a negative replica of the original structure. We were able to tune the shrinkage from 12 % to 40 % by varying the siloxane precursor molecule chain length. This correspondingly changed the band structure of the replica 2. Therefore, this rapid, two-step process allows one not only to create high-temperature gas sensors but also ones with a photonic response adapted to the subsequent implementation, i.e. the atmosphere to be analyzed.

We thank Xia Wu and Dr. Helge Fabritius from the Max Planck Institut für Eisenforschung in Düsseldorf for the band structure calculations, the sample preparation and the many helpful discussions.

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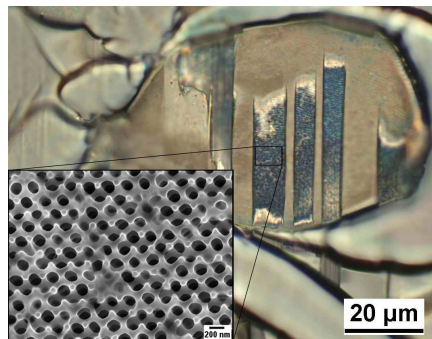


FIG. 1. Light micrograph showing a silica replicate of a scale of *Entimus imperialis*.

Inset: Scanning electron micrograph of the internal structure of the scale illustrating the detailed three-dimensional structural features.

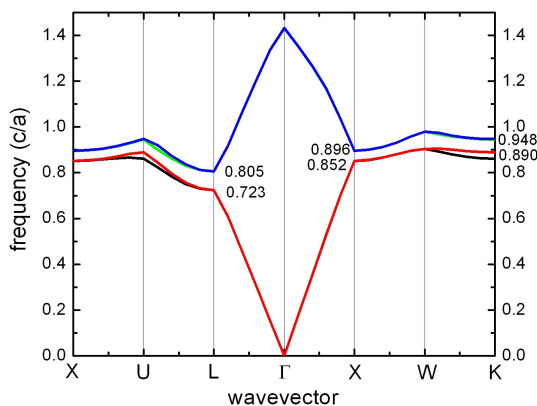


FIG. 2. Calculated photonic response of the scale replica in 1. The band gaps in this case corresponds to wavelengths in the blue to green range (380 nm to 500 nm).

The physical origin of strikingly different colour appearances in four subspecies of *Torynorrhina* beetles

Alfie J. Lethbridge and Peter Vukusic

School of Physics, University of Exeter, EX4 4QL, UK

We present a detailed characterisation of four *Torynorrhina* beetle subspecies (fig. 1). Their optical properties were investigated using spectrophotometry and scatterometry. The geometries of their elytral micro and nano structures were probed using transmission electron microscopy (TEM). We undertook finite element method (FEM) theoretical analysis using the structural information taken from the electron microscopy and from published values of refractive index [1].

Experimentally obtained reflectance spectra reveal maxima in reflection for the blue, green, orange and red beetles to be 477 nm, 540 nm, 606 nm and 690 nm respectively (fig. 2(a)). The relationship between the reflection maxima and the lattice constants for each beetle structure appears non-linear (fig. 2(b)). This is in contrast to the linear relationship expected for conventional multilayering.

The structures of the beetles all exhibit multilayer geometries with a periodicity running perpendicular to the surface of the elytra (fig. 2(c)). The multilayers are intersected orthogonally by an array of straight cuticle-filled channels that exhibit a quasi-ordered spatial arrangement. This combination of multilayering and straight channels produces a hybrid 3D photonic crystal structure. This hybrid structure appears to modify the angle-dependent scattering profile of the beetles' elytral surfaces. Experimental scatterometry data (fig. 3) reveal that even under normally-incident broadband illumination there is minimal coloured specular reflection: instead, strong coloured reflection is observed in a distinct annulus at an angle of 15° around the specular position.

The combination of multilayering and quasi-ordered channelling is unusual in natural systems [2]. While the evolutionary optical benefit that may be ascribed to the presence of the channels in these beetles' systems is uncertain, in a synthetic bio-inspired replica they would enable the introduction of fluid or foreign matter into the core of a multilayer system. This potentially offers the facility for fluid-based tunability of multilayer optics.

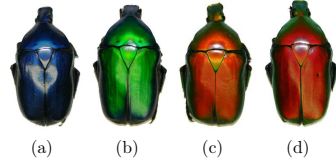


FIG. 1. Photograph showing the four subspecies of *T. flammea* (a) *violets*, (b) *chicheryi*, (c) *flammea* and (d) *red form*.

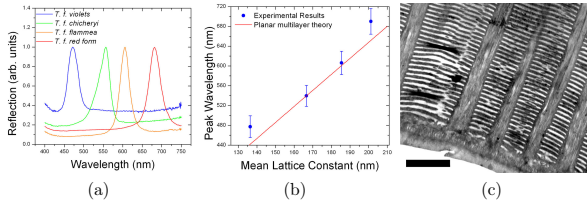


FIG. 2. (a) shows reflection data as a function of wavelength taken using microspectrophotometry for each of the four subspecies. (b) shows the non-linear relationship between the wavelength of the reflection maximum and the lattice constant for the four beetles. Error bars show the standard deviation. The red line shows the theoretical linear relationship of planar multilayers. (c) and (d) TEM images showing the multilayer structure intersected with rods. Scale bar (c) 2 μm .

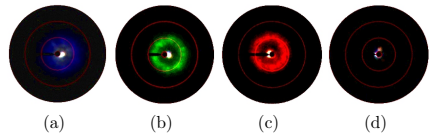


FIG. 3. Scatterometry images showing a 2D projection of the 3D scattered hemisphere for (a) *violets*, (b) *chicheryi*, (c) *flammea* and (d) *red form*. The rings going out from the centre show 5°, 30°, 60° and 90° scattered angle.

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Highly optimised multilayering in the wing membrane of the damselfly *Matronoides cyaneipennis*

M.R. Nixon and P. Vukusic

School of Physics, University of Exeter, EX4 4QL, United Kingdom

Odonata (dragonflies and damselflies) can exhibit a range of bright structural colours in their wing membranes and body [1–4].

We have investigated the appearance of the damselfly *Matronoides cyaneipennis*, whose wings exhibit iridescence that is blue dorsally and green ventrally (FIG. 1). Transmission electron microscopy reveals two near-identical 5-layer distributed Bragg reflectors (DBRs) as the origin of both colours. These are separated in the middle of the wing by a thick absorbing layer (FIG. 2). The key difference between the dorsal and ventral DBRs is the thickness of only one of their corresponding layers; the second layer from each surface. Whereas the thicknesses of all other corresponding layers are nearly identical, the thicknesses of the second layer in each DBR differ by approximately 20%. This creates the significant difference in their reflected spectra and the observed dorsal and ventral wing colours.

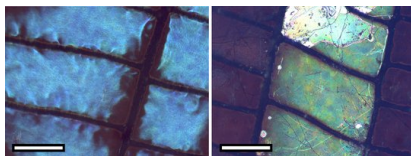


FIG. 1. Optical images showing the blue and green iridescence from the dorsal and ventral sides of *M. cyaneipennis*. [Scale bars 0.2 mm].

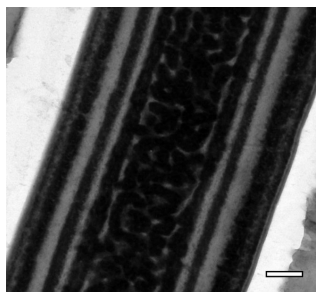


FIG. 2. A TEM image through the *M. cyaneipennis* wing membrane showing its two multilayer structures. [Scale bar 250 nm].

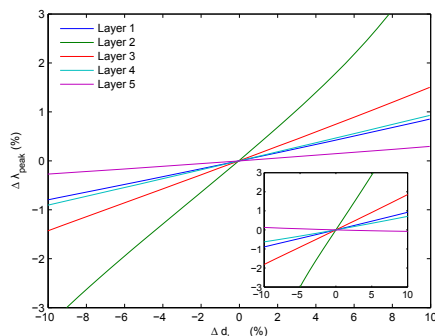


FIG. 3. Graph showing the change in theoretical peak wavelength ($\Delta\lambda_{\text{peak}}$) against change in the thickness of an individual layer (Δd_{layer}) for light incident on the modelled dorsal DBR (insert shows the same for the modelled ventral DBR.)

Interestingly, modelling of these DBR designs, based on measured thicknesses of individual layer, indicates that changes to the thickness of this second layer are most optimally sensitive to the peak reflection wavelength of the DBR as a whole. Namely, a small change in thickness of this layer alone will modify the colour of the wing significantly more than similar changes in any of the other 4 layers in the DBR (FIG. 3). We assert that selection pressures on the development of the coloured wing appearance of *M. cyaneipennis* may have identified the most efficient route for significantly modifying the colour of a simple multilayer.

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Tetrahedrally Close-Packed Structure in Silica-Water-Surfactant System

Y. Sakamoto¹ and O. Terasaki^{2,3}¹Nanoscience and Nanotechnology Research Center, Osaka Prefecture University, Sakai, 599-8570, Japan²Graduate School of EEWS (WCU), KAIST, Korea³Department of Materials and Environmental Chemistry, Stockholm University, Sweden

Since the first silica mesoporous crystals were discovered in the early 1990s, a number of mesoporous materials have been reported, such as bicontinuous, cylindrical and cage-type. Among these silica mesoporous crystals, cage-type mesoporous crystals display rich structural diversity.

Cage-type mesoporous crystals can be classified into two categories. The structure of the first has a single type of cage. Typical examples are $Im-3m$ and $Fm-3m$ structures, which have, respectively, body-centered and face-centered arrangements of cages. The structure of the second category, hereafter called multi-modal cage-type mesoporous crystals, has several types of cage. For example, multi-modal cage-type mesoporous crystals with cubic $Pm-3n$ (SBA-1 and SBA-6), cubic $Fd-3m$ (AMS-8) and tetragonal $P4_2/mnm$ (AMS-9) structures contain two or three types of cage, and all the interstices between cages are exclusively tetrahedrally surrounded. These structures are called tetrahedrally close-packed (*tcp*) structures, and are well known for intermetallic compounds. On the other hand, in the $Fm-3m$ structure, *e.g.* SBA-12, the interstices are not only tetrahedrally but also octahedrally surrounded by the adjacent cages.

Multi-modal cage-type mesoporous crystals can be described in terms of four kinds of polyhedron, as shown in Fig. 1. All the polyhedra have 12 pentagonal faces like a dodecahedron (5^{12} polyhedron), and $5^{12}6^2$, $5^{12}6^3$ and $5^{12}6^4$ polyhedra have two, three and four additional hexagonal faces respectively.

In the polyhedral description, the $Fd-3m$ structure can be described by 5^{12} and $5^{12}6^4$ polyhedra, and these two polyhedra construct two kinds of layer which stack alternately along the $[111]$ direction. One of the layers consists of 5^{12} polyhedra in the Kagomé net arrangement (termed layer A, B or C), and the other consists of 5^{12} and $5^{12}6^4$ polyhedra (termed layer α , β or γ), as shown in Fig. 2. Layer A stacks with ABC sequences along the $[111]$ direction, with layer α (or β or γ) inbetween. The sequence of the $Fd-3m$ structure along the $[111]$ direction can be described as $|A\alpha B\beta C\gamma|$, based on these two kinds of layer.

We have investigated tetrahedrally close-packed structure in silica-water-surfactant system. [1-3]

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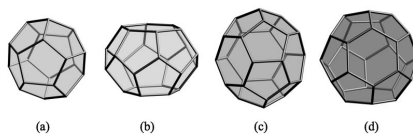


FIG. 1. Schematic drawings of four types of polyhedron. (a) 5^{12} , (b) $5^{12}6^2$, (c) $5^{12}6^3$, and (d) $5^{12}6^4$ polyhedron.

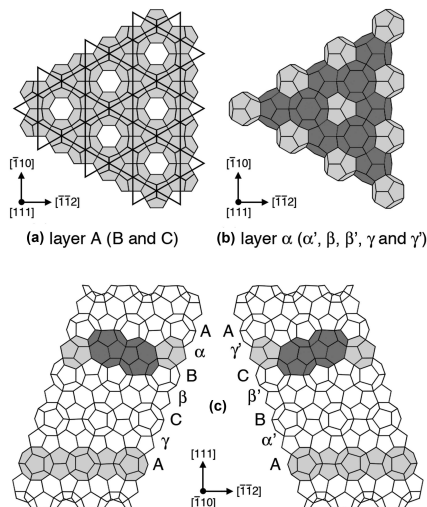


FIG. 2. Schematic drawings of (a) layer A and (b) layer α , and (c) $Fd-3m$ structure.

In Situ Characterization of Lipidic Aqueous Dispersions

Anan Yaghmur,¹ Peter Laggner,² Mats Almgren,³ Barbara Sartori,² Lauri Paasonen,^{4,5} Marjo Yliperttula,⁴ Arto Urtti,⁵ and Michael Rappolt²

¹Department of Pharmaceutics and Analytical Chemistry, Faculty of Pharmaceutical Sciences, University of Copenhagen, Denmark

²Institute of Biophysics and Nanosystems Research (IBN), Austrian Academy of Sciences, Graz, Austria

³Department of Physical Chemistry, Uppsala University, Uppsala, Sweden

⁴Centre for Drug Research, University of Helsinki, Helsinki, Finland

⁵Division of Biopharmacy and Pharmacokinetics, Faculty of Pharmacy, University of Helsinki, Helsinki, Finland

Colloidal nanostructural aqueous dispersions (such as cubosomes, hexosomes, and micellar cubosomes) that display nanostructures closely related to those observed in biological membranes is receiving much attention in pharmaceutical applications [1].

In a recent study, our ultimate goal was as shown in Fig. 1 to experimentally demonstrate the direct transition from vesicles to cubosomes by heating the monoelaidin (ME, a rod-like monoglyceride containing a *trans*-monounsaturated acyl chain)-based dispersions [2]. In the present contribution, we focus also on describing (i) our recent investigations on combining synchrotron SAXS with a UV light source (*in situ* SAXS-UV irradiation) for determining the structure response of gold nanoparticles (NPs)-loaded vesicles [3], (iii) the combination of synchrotron SAXS with a stopped-flow apparatus for monitoring *in situ* the structural transitions induced by rapidly added calcium ions to negatively charged vesicles [4, 5]. The *in situ* investigations of the calcium triggered phase transitions reveal a very fast re-organization of the lipid molecules in the aqueous media to form a variety of nanostructures. Fig. 2 shows a schematic illustration of the various intriguing and fast structural transitions observed in the present study. One of the most striking features in these investigations is the occurrence of disordered-ordered transitions within milliseconds to seconds range.

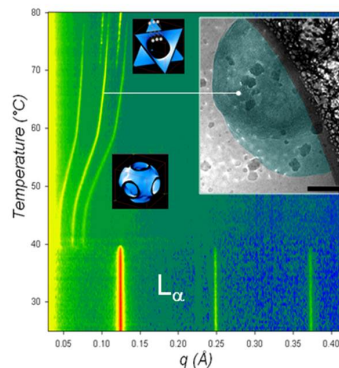


FIG. 1. Heating ME dispersion induces direct transformation of liposomes to cubosomes

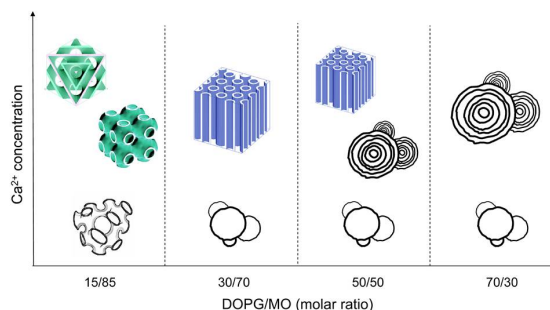


FIG. 2. Schematic illustration of the lipid composition dependence of the rapid calcium-triggered nanostructures in DOPG/MO-based aqueous dispersions.

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Morphology of interstitial space at grain boundaries in metals

Jan Kuriplach

Department of Low Temperature Physics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, CZ-180 00 Prague, Czech Republic

Grain boundaries (GBs) are planar defects frequently encountered in polycrystalline and nanocrystalline materials. GBs break the three dimensional periodicity of otherwise perfect crystal. Therefore, the GB atomic structure and related geometrical characteristics differ from the undisturbed material. Due to this effect, GBs may influence macroscopic materials properties. This is why it is important to study and understand geometry related GB characteristics. The so called excess free volume associated with GBs has been found to be an important GB property [1, 2]. The morphology of interstitial space (IS) is investigated rarely only though it is directly related to the excess free volume of GBs and gives also valuable information about positions and ways of diffusion of interstitial impurities at GBs.

Here we study grain boundaries in face centered cubic (fcc) nickel and body centered cubic (bcc) iron metals. The realistic atomic configurations are obtained using molecular dynamics simulations and *ab initio* calculations. In order to explore the interstitial space for such configurations, we employ a geometrical procedure [3] based on a fine real space mesh covering the atomic configurations examined. For every mesh point the distance to surrounding atoms is calculated. Regions with largest distances to atoms are identified with the IS. An example of the IS determined in this way is shown in Fig. 1 for the $\Sigma 5$ (210) [001] symmetrical tilt GB in fcc Ni. Large interstitial regions also define positions of interstitial segregating atoms at this GB.

In this contribution, we discuss in detail the morphology of the interstitial space for selected GBs in fcc Ni and bcc Fe, including ‘percolation’ effects. Furthermore, the relations of the IS at GBs, the excess free volume, and the GB energy are examined. Finally, the effect of GB imperfections – like impurities and vacancies – on the interstitial space is also investigated.

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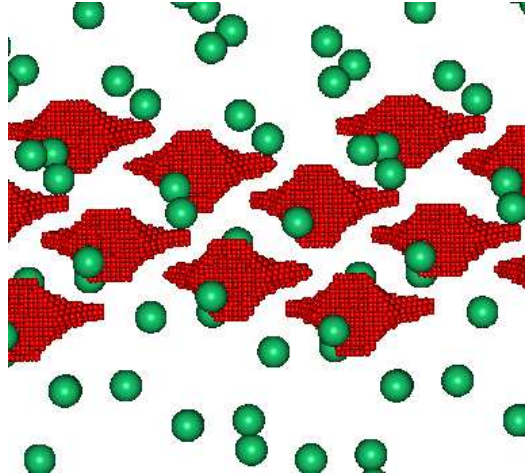


FIG. 1. Visualization of the interstitial space at the $\Sigma 5$ GB in fcc Ni. Ni atoms are shown as green (lighter) spheres. Red (darker) small spheres represent interstitial space.

Instability patterns in thin nematic films: stripes versus squares

Oksana Manyuhina,¹ Anne-Marie Cazabat,² and Martine Ben Amar²

¹*Nordic Institute for Theoretical Physics, Roslagstullsbacken 23, 10691 Stockholm, Sweden*

²*Laboratoire de Physique Statistique, Ecole Normale Supérieure, UPMC Univ Paris 06, Université Paris Diderot, CNRS, 24 rue Lhomond, 75005 Paris, France*

Recent experiments [1, 2] demonstrated that thin nematic films, spread on liquid substrates, exhibit a long-wavelength periodically deformed state as stripes, squares, chevrons up to the thickness of 20 nm. The formation of these instability patterns can be attributed to the response of the system to the antagonistic boundary conditions. Although being extensively studied in the last two decades [3, 4], these new observations cannot be explained completely by the existing theories. To get a theoretical insight on the experimental findings, we consider the onset of stripe and square instabilities in ultrathin nematic films within the continuum theory of liquid crystals [5]. In the linear approximation, we find analytical expressions for the critical thickness as well as for the critical wavenumber and discuss the role of the surface-like terms entering the free energy.

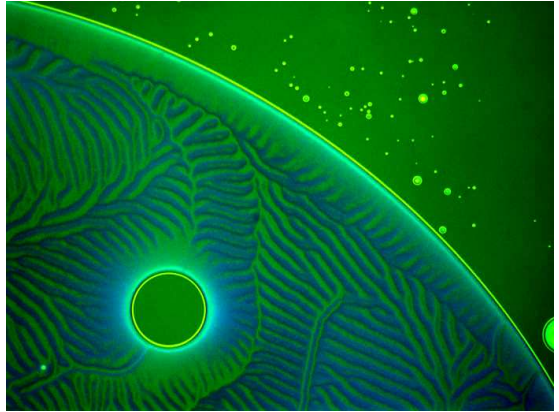


FIG. 1. Polarised-light microscopy image 1.8×1.3 mm of periodically distorted 6CB/water LC at 27°C . The thickness of nematic film is $h \approx 0.2 \mu\text{m}$ and the periodicity of stripes, the distance between two stripes, is $L \approx 40 \mu\text{m} \gg h$. The alternation of colour (dark and light) is associated with violent reorientation ($\sim \pi/2$) of the director in the plane of the image.

O.M. acknowledges financial support through ANR-07-BLAN-0158 fund.

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Cell motility: a viscous fingering analysis of active gelsMartine Ben Amar,¹ Oksana Manyuhina,² and Gaetano Napoli³¹Laboratoire de Physique Statistique, Ecole Norm. Sup., UPMC Univ Paris 06, Université Paris Diderot, CNRS, 75005 Paris, France²Nordic Institute for Theoretical Physics, Roslagstullsbacken 23, 10691 Stockholm, Sweden³Dipartimento di Ingegneria dell'Innovazione Università del Salento, Via per Monteroni - Edificio "Corpo O", I-73100 Lecce, Italy

The symmetry breaking of the actin network from radial to longitudinal symmetry has been identified as the major mechanism for keratocytes (fish cells) motility on solid substrate. For strong friction coefficient, the two dimensional actin flow which includes the polymerisation at the edge and depolymerisation in the bulk can be modelled as a Darcy flow, the cell shape and dynamics being then modelled by standard complex analysis methods. We use the theory of active gels to describe the orientational order of the filaments which varies from the border to the bulk. We show analytically that the reorganisation of the cortex is enough to explain the motility of the cell and find the velocity as a function of the tensorial order parameter in the bulk.

O.M. acknowledges financial support through ANR-07-BLAN-0158 fund.

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Self-assembly in solution of silica-based hybrid materials: contribution of in-situ SAXS studiesS. Manet,¹ M. Impéror-Clerc,¹ N. Baccile,² F. Michaux,² C. Gervais,² F. Babonneau,² M. J. Stebé,³ F. Meneau,⁴ C. Rochas,⁵ C. L. P. Oliveira,⁶ J. S. Pedersen,⁷ D. Durand,⁸ and V. Zholobenko⁹¹Laboratoire de Physique des Solides, Université Paris Sud, Orsay, France²Laboratoire de Chimie de la Matière Condensée de Paris, Collège de France, Paris, France³Laboratoire de Physico-Chimie des Colloïdes, Nancy Université, Vandoeuvre lès Nancy, France⁴SWING, Synchrotron Soleil, Gif-sur-Yvette, France⁵D2AM, ESRF, Grenoble, France⁶Instituto de Física, Universidade de São Paulo, Brasil⁷Department of Chemistry, University of Århus, Denmark⁸IBBMC, Université Paris Sud, Orsay, France⁹Chemistry Department, Keele University, UK

Surfactant templated mesoporous silica powders have been extensively studied in the past 15 years by exploiting the self-assembly properties of amphiphilic molecules in aqueous medium. The large success of these systems mainly relies on the apparent simplicity that enables to design porous networks with different architectures and pore sizes. However, a better control of the final nanostructure (2D-hexagonal, 3D-cubic) requires a deeper understanding of the interaction mechanisms between the templating agents and the network-forming species.

This work will show our latest experiments using in-situ Small Angle X-ray Scattering (SAXS) performed with highly brilliant synchrotron radiation to follow the formation mechanism of templated silica powders in the presence of different types of surfactants (non-ionic triblock copolymers, nonionic fluorinated surfactants, cationic surfactants with different polar head groups) and silica precursors. This type of experiments give access to a lot of information about the cooperative self-assembly of these systems and the nanostructure formation. We will emphasize how the inorganic precursor affects the micelles in solution (prior to, during and after hydrolysis of the precursor) and how the micelles shape is linked to the final nanostructure of the hybrid material.

Transport of Finite-sized Colloidal Tracers Through Random Structures

Christian Scholz, Frank Wirner, and Clemens Bechinger

2. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Transport and flow phenomena in porous media occur in various fields of science and engineering, ranging from agricultural, biomedical, chemical and petroleum engineering to soil sciences [1]. Despite the huge interest on this topic, relations between flow and transport properties of porous media and the corresponding microstructure are not fully understood.

Here we present an experimental system which allows us to determine flow and transport properties of quasi-two-dimensional porous PDMS structures [2], with full knowledge of the microstructure and real space visualization of fluid flow and particle transport.

Fig. 1 illustrates the experimental setup. The applied pressure gradient is adjusted by the height of two water columns connected to the sample.

By varying the applied pressure and spatial properties of the sample structures the flow rate and thus the Reynolds number (Re) and Péclet number (Pe) can be varied to cover a large range of transport regimes.

Using digital video microscopy a detailed reconstruction of the particle trajectories inside the porous media can be performed with a temporal resolution of 2 ms and spatial resolution of $0.3 \mu\text{m}$.

Fig. 2 shows a characteristic measurement of particle trajectories inside a random porous structure consisting of monodisperse circular obstacles and their local average velocity. This allows us to study the influence of particle sizes on their transport velocities and the consequences on particle image velocimetry on the microscale.

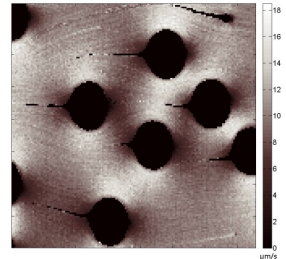
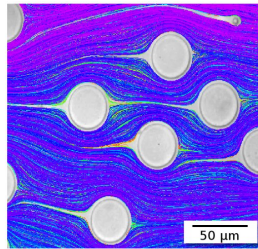


FIG. 2. Trajectories of $5.2 \mu\text{m}$ PS particles through a random microstructure (left) and corresponding local average velocity (right).

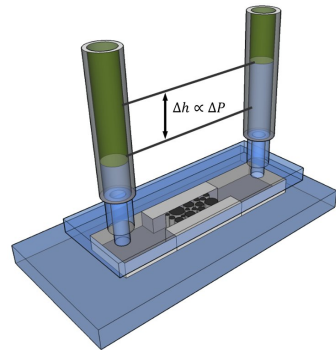


FIG. 1. A schematic of the experimental setup. Flow is driven by hydrostatic pressure as illustrated.

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Fractal geometry of point robot laser hardened material

M. Babič,¹ P. Kokol,² M. Milfelner,³ and S. Babič

¹Emo-Orodjarna d.o.o. Slovenia

²University of Maribor, Faculty of Health Sciences, Slovenia

³Tic-Lens d.o.o. Slovenia

Abstract

This article describes the fractal geometry of point robotic laser hardening microstructure at different parameter. We show the experimental results and analysis of fractal patterns that occur in point robotic laser hardening at different parameter. In the end we present fractal geometry in point robot laser hardening pattern.

Introduction

Fractals are a beautiful of mathematics and art. Perhaps this is the reason why most people recognize fractals only as pretty pictures useful as backgrounds on the computer screen or original postcard patterns. The fractal patterns look complex in robot laser hardened patterns to. Fractal structures we can find in robot laser hardened patterns to if we observed it with electron microscope. Robotic laser surface hardening heat treatment is complementary to the conventional flame or inductive hardening. In this work we have used scanning electronic microscope (SEM), search and analyze the fractal structure of the robotic laser-hardened material.

Experimental Method and Materials Preparation

We made some different patterns in material GGG 70 and GGG 70L. We research if it is possible to find a fractal structure in microstructure, when we hardening materials with different parameters of robot laser cell. Also, we wanted to know or find the fractal structure of the optimal parameters. Each sample was etching and polish (IMT Institute of Metals and Technology Ljubljana, Slovenia) and then we looked at under a microscope (JSI Jozef Stefan Institute, Slovenia). Images were made by field emission scanning electron microscope JMS-7600F JEOL company.

The surface is irregular texture with a few breaks are represented by black islets. We find fractal structure in robot laser hardened materials GGG 70. We hardened materials GGG 70 with the laser at different temperatures. So we changed parameter of temperature $T \in [1000, 1400]$ °C with steps 50 °C. In all these attempts we have made picture of microstructure. We made recordings of hardened surface area.

Conclusion

Fractal structures are also found in robotic laser-hardened patterns when viewed under sufficient magnification. We find a fractal geometry in the robotic laser hardening material. Robot laser hardening is useful in automotive and military industry. However, we can also see many problems in robotic laser hardening. One is also fractal geometry.

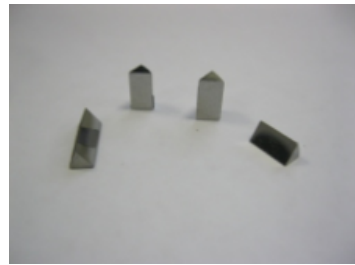


FIG. 1. Robot laser hardened patterns

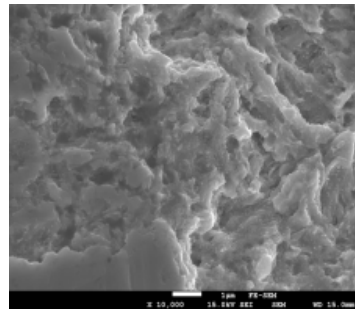


FIG. 2. Fractal geometry of robot laser hardened material

- [1] J.-M. Barbaroux, F. Germinet, and S. Tcheremchantsev, Fractal dimensions and the phenomenon of intermittency in quantum dynamics, *Duke Math. J.* 110 (2001), 161–193
- [2] B. Pesquet-Popescu and P. Larzabal, “2D self-similar processes with stationary fractional increments”, in *Fractals in Engineering*, J. Lévy Véhel, E. Lutton, and C. Tricot, Eds. Heidelberg, Germany: Springer-Verlag, 1997, pp. 138–151

Fabrication of biomimetic metallic chiral composites with true cubic symmetry

Mark D. Turner,^{1,2} Matthias Saba,³ Gerd E. Schröder-Turk,³ and Min Gu¹

¹Centre for Micro-Photonics and CUDOS, Faculty of Engineering and Industrial Sciences, Swinburne University of Technology, Hawthorn, Victoria 3122, Australia.

²CRC for Polymers, 8 Redwood Drive, Notting Hill, Victoria 3168, Australia.

³Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudstr. 7B, Erlangen, Germany.

We present the fabrication of a series of three-dimensional (3D) photonic biomimetic chiral composites using a modified direct laser writing (DLW) method to produce microstructures that preserve the cubic symmetry of the srs-network. This provides enhanced mechanical strength and superior optical properties over the standard DLW method which normally suffers from an elongation of the laser focal spot [1]. We have experimentally characterised the transmission spectra of these chiral srs-networks, which show excellent agreement with numerical simulations and recent theoretical studies [2] that predict the formation of strong circular dichroism bands. Using an electroless silver coating method, we have used these polymer cubic networks as a template for the development of cubic chiral plasmonic crystals and discuss the potential development of other exciting structures based on these methods.

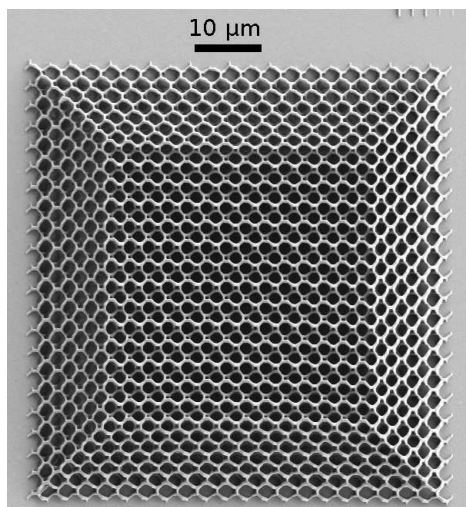


FIG. 1. SEM image of a biomimetic chiral srs-network fabricated via direct laser writing. The cubic unit cell size is 3 μm .

[1] M. D. Turner, G. E. Schröder-Turk, and M. Gu, *Opt. Express* 19, 10001-10008 (2011)

[2] M. Saba, M. Thiel, M. Turner, S.T. Hyde, M. Gu, K. Grosse-Brauckmann, D.N. Neshev, K. Mecke and G.E. Schröder-Turk, *PRL* 106, 103902 (2011)

An Interference-Priority Simulator for the Optical Near Field at Cubic Membrane Assemblies

Xiaochun Xu and Felix Margadant

MechanoBiology Institute, NUS, Singapore

Transparent cubic membranes are found in many optically active or light exposed interfaces in biology. As their lattice of folding is often comparable in magnitude with the wavelength of visible light, many conjectures have been drawn if there is a secondary (or maybe even primary) bio-physical purpose of these membranes such as channeling, guiding, or focus light or then – in the contrary – a role as angle independent interference filter which protects the tissue from higher energy radiation.

We present the design and some results of a beam propagation algorithm which simulates the interference structure generated by a cluster of highly folded cubic membranes.

For the sake of computational efficiency, the simulator jettisons diffraction contributions of higher than order 1 and hence is not useful to predict any part of the optical far field. It does however solve the time independent global interference across the membrane cluster with very few generalizations and hence makes detailed predictions about the change in transmission for different wavelengths.

We will present some results for globular clusters of cubic membrane arrangements, different biologic compartments, and assembly types. We will show some dependencies on wavelength, lipid layer, and lattice and discuss the potential meaning and biological application of such assemblies as protective filters or waveguides.

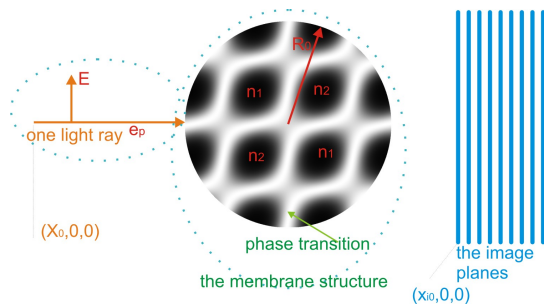


FIG. 1.

Self-assembly of low-dimensional inorganic structures in vicinity to equilibrium during sputter deposition

Yu.O. Kosminska, A.A. Mokrenko, A.S. Kornushchenko, V.B. Dyoshin, and V.I. Perekrestov

Sumy State University, R.-Korsakov St. 2, Sumy 40007, Ukraine

Currently the technologies of reproducible self-assembly of various low-dimensional structures are under considerable research attention. For further development of this scientific area the study of analogy between physicochemical principles of conservative self-organization in organic and inorganic nature appears to be rather promising. In part, the progress of supramolecular chemistry can be useful here. If to analyze comparatively organic and inorganic self-assembly, then in both cases the self-assembly can be observed in vicinity to thermodynamical equilibrium, and, as a consequence, extreme minimization of the free energy of structural elements and highly selective growth take place.

Following the idea of quasi-equilibrium self-assembly, in the present work the authors set the problem to study experimentally the possibility of selective formation of complex low-dimensional inorganic structures, using the technology of quasi-equilibrium steady-state condensation of weakly volatile ion-sputtered substances in highly purified inert medium. For that purpose the technique was developed, being realized on the basis of dc planar magnetron sputtering [1] and accumulative ion-plasma system (AIPS) [2, 3]. The feature of quasi-equilibrium condensation consists in that the atoms are condensed only if they realize the strongest chemical bonds with the growth surface to minimize the free energy.

Thus, it has been shown on the example of a number of metals (Cu, Ni, Cr, Ti, Al), silicon and carbon that under approaching the equilibrium the self-assembly of various low-dimensional structures occurs, which possess complex 2D or 3D architecture or developed surface topology. Structural elements of the layers can have identical forms and sizes, their characteristic dimensions being of an order of several units and tens both of micrometres and nanometres. Specifically, among the main structures obtained there are metal individual nanoclusters (Fig. 1a), 3D nanoclusters networks (Fig. 1b), various fractal forms (Fig. 1c,d), and whisker systems as well. Besides, when using AIPS [2], porous metal and carbon structures were produced with various 3D architecture (Fig. 1e,f). Condensation of silicon by means of AIPS revealed formation of continuous layers with developed surface topology in the form of convex and concave ellipsoids of revolution.

The principal physical mechanisms, responsible for structure formation near equilibrium, have been suggested on the basis of experimental results and several mathematical models created. The results of the present work can be used for developing new self-organized technologies, based on wide spectrum of physicochemical processes. Here, great assistance can be provided by investigations of self-organization mechanisms in organic systems.

The work was supported partly by The Ukrainian State Agency For Science, Innovation and Informatization.

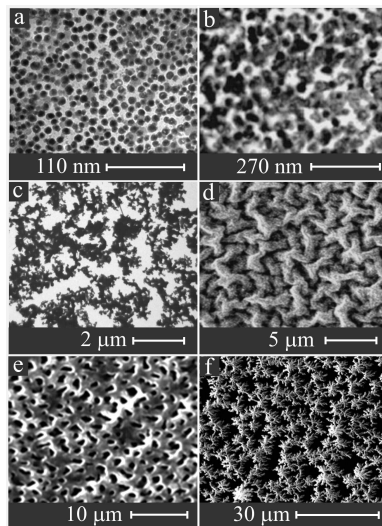


FIG. 1. TEM (a,b,c) and SEM (d,e,f) images of the *ex-situ* grown condensates: copper (a,b), nickel (c,d), aluminium (e), carbon (f).

- [1] V.I. Perekrestov, A.S. Kornushchenko, Yu.O. Kosminska, JETP Lett. 86, pp.767–771 (2007)
- [2] V.I. Perekrestov, A.I. Olemskoi, Yu.O. Kosminska, A.A. Mokrenko, Phys. Lett. A 373, pp. 3386–3391 (2009)
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Minimal surface scaffold designs for tissue engineering

Sebastian C. Kapfer,¹ Stephen T. Hyde,² Klaus Mecke,¹ Christoph H. Arns,³ and Gerd E. Schröder-Turk¹

¹Institut für Theoretische Physik, Fried.-Alexander-Universität Erlangen-Nürnberg, Staudstr. 7, 91058 Erlangen, Germany

²Applied Maths, Research School of Physics and Engineering, The Australian National University, Canberra, 0200 ACT, Australia

³School of Petroleum Engineering, The University of New South Wales, Sydney NSW 2052, Australia

Triply-periodic minimal surfaces are shown to be a more versatile source of biomorphic scaffold designs than currently reported in the tissue engineering literature. A scaffold architecture with sheetlike morphology based on minimal surfaces is discussed, with significant structural and mechanical advantages over conventional designs. These sheet solids are porous solids obtained by inflation of cubic minimal surfaces to sheets of finite thickness, as opposed to the conventional network solids where the minimal surface forms the solid/void interface. Using a finite-element approach, the mechanical stiffness of sheet solids is shown to exceed that of conventional network solids for a wide range of volume fractions and material parameters. We further discuss structure-property relationships for mechanical properties useful for custom-designed fabrication by rapid prototyping. Transport properties of the scaffolds are analyzed using Lattice-Boltzmann computations of the fluid permeability. The large number of different minimal surfaces, each of which can be realized as sheet or network solids and at different volume fractions, provides design flexibility essential for the optimization of competing design targets.

GEST and SK acknowledge financial support through the Deutsche Forschungsgemeinschaft (DFG) under grant SCHR1148/2-1. KM gratefully acknowledges the support of the Cluster of Excellence 'Engineering of Advanced Materials' within the Exzellenzinitiative of the DFG. We also acknowledge travel support by the German Academic Exchange Service (DAAD) and the Australian Group of Eight (Go8) Universities through a joint funding scheme.

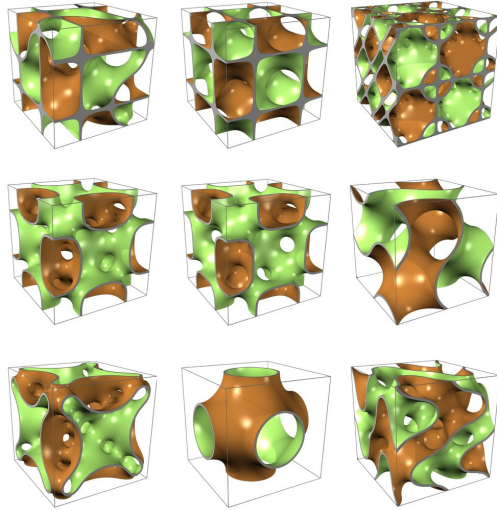


FIG. 1. Examples of periodic minimal surfaces. Shown are (from top left to bottom right) translational unit cells of $C(Y)$, Diamond, $C(D)$, Batwing, F-RD, Gyroid, Manta 35, Primitive, and Fischer-Koch S.

Fractal modelling of the interplay between heterogeneous media separated by irregular interfaces. Application to wetting fronts in porous media invading heterogeneous distributions of chemicals

Miguel Ángel Martín

Universidad Politécnica de Madrid, Spain

The wetting front zone where water invades and advances into an initially dry soil plays a crucial role in solute transport through the unsaturated zone. The leaching of chemicals by wetting fronts is influenced by two major factors, namely: the irregularity of the fronts and heterogeneity in the distribution of chemicals.

Recently, irregularity and heterogeneity have been dealt with in Soil Science by using fractal concepts and techniques. The fractal nature of wetting fronts within a range of scales has been demonstrated and fractal theories used to describe fingering structures as well as estimate the effective surface tension at the wetting front during infiltration (Adler, 1985; Chang et al., 1994; Onody et al., 1995. On the other hand, variability in the distributions of chemicals, nutrients, pollutants and soil properties such as pore space geometry, have been parameterized and modelled by *multifractal analysis* (Muller, 1995; Kravchenko et al., 1999, Caniego et al. 2001, 2003, 2005, among others) which provides theoretically a continuum spectrum of dimensions characterizing heterogeneity.

The fractality of wetting fronts and the heterogeneity (multifractality) of distributions of chemicals provide a phenomenological basis for dealing with a special aspect of leaching, namely: the physical interplay between a stationary geometric structure, the fractal curve modelling the wetting front, and a heterogeneous distribution of chemicals around it which is assumed to be multifractal. Such an interplay must influence leaching of chemicals, the dispersion of solutes throughout the soil, the mobilization of adsorbed contaminants such as radionuclides by rainfall events as well as other transport processes.

Clearly, the dimensionality of wetting fronts must interplay with the heterogeneity of any adsorbed nutrients or chemicals present; therefore, the fractal dimension of the front appear to be an effective measure of the interplay. However, how to manage the heterogeneity factor is far from clear even if the surrounding distribution is multifractal.

Moreover, similar problem arises in a wide number of biological and physical scenarios where irregular interfaces separates highly heterogeneous media.

Thus, such important questions as the following remain open: (a) which heterogeneity parameters of the distribution should be used and (b) how can the parameters used to characterize both structures help evaluate the mass-geometry interplay? To our knowledge, no connection between the structures described above has been established to date nor have the previous questions been raised and/or answered in this or any other context. This work presents a theoretical framework for studying the physical interplay between a stationary wetting front of fractal dimension D and a multifractal distribution of chemicals around it with a singularity spectrum $f(a)$. The proposed modelling approach and the results it provides can be useful with a view to obtaining supplementary information about the leaching process and its prediction, as well as in other biological and physical scenarios.

Star-Polyphile Bicontinuous Cubic Phases with De-Mixed Hydrocarbon, Fluorocarbon Bilayer

Liliana de Campo,¹ Minoo J. Moghaddam,² Trond Varslot,¹ Nigel Kirby,³ Chris Garvey,⁴ and Stephen Hyde¹

¹*Applied Maths, ANU, Australia*

²*CSIRO, North Ryde, Australia*

³*Australian Synchrotron, Melbourne, Australia*

⁴*ANSTO, Sydney, Australia*

The triphilic star-polyphiles presented here are short-chain oligomeric molecules with a star-shaped arrangement of hydrophilic, hydrocarbon and fluorocarbon chains. As a consequence of their star-shaped geometry, these polyphiles can only self-assemble along one-dimensional lines, and not along surfaces, which opens the path to a wealth of possible novel nanostructures [1–3].

These molecules form a number of liquid crystalline structures when mixed with water. Among those, some display SAXS patterns that resemble mesostructures found in amphiphile-water systems with bulky hydrophobic chains, but neutron contrast variations show that the three chains are in fact separated into three separate nanodomains. [4]

In this contribution, we would like to focus on the structure of their bicontinuous cubic phases. We will present some of our models, which are based on their phase behaviour, geometric considerations, and synchrotron and neutron studies, to establish the most likely underlying structures.

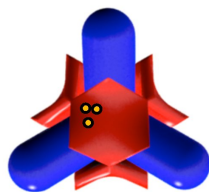


FIG. 1. Structure of a conventional diamond type bicontinuous cubic liquid crystal (blue: hydrophilic channels, red: hydrophobic membrane, yellow: center of a few arbitrary surfactant molecules).

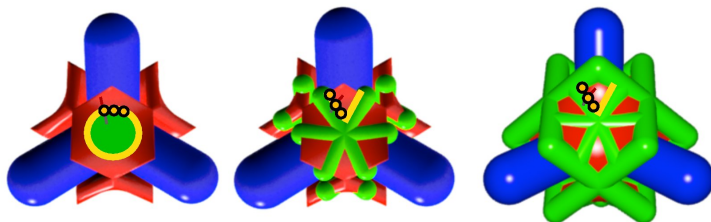


FIG. 2. In star-polyphiles, the hydrophobic domain separates into a hydrocarbon region (red) and fluorocarbon region (green). The pattern of segregation in the bilayer is the result of the delicate balance between various competing driving forces, like minimization the hydrocarbon/fluorocarbon interface, the necessity to cover the whole hydrophilic/hydrophobic interface homogeneously, and the preferred packing arrangement of hydrocarbon (more splayed) vs. fluorocarbon chains (parallel, locally flat curvature).

[1] S. T. Hyde and G. E. Schroeder, *Curr. Op. Coll. Interf.*, pp. 5-14 (2003)

[2] J. J. K. Kirkensgaard and S. T. Hyde, *PCCP* 11, pp. 2016-2022 (2009)

[3] S. T. Hyde, L. de Campo and Ch. Oguey, *Soft Matter* 5, pp. 2782-2794 (2009)

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PO25

Linnéa Andersson

Permeability, pore connectivity and pore throat control of macroporous alumina evaluated with X-ray micro-CT

Linnéa Andersson

Dept of Materials and Environmental Chemistry, Stockholm University, Sweden

F. Akhtar, A. Jones, M. Knackstedt, and L. Bergström

We have regulated the permeability in macroporous alumina materials by manipulating the connectivity of the pore phase and the sizes of the smallest constrictions between connected pores. The alumina materials were produced by a novel method that combines gel casting with expandable polymeric microspheres (EPS) as a sacrificial templating material. Templating with particle-coated EPS significantly increased the fraction of isolated pore clusters, and reduced both the sizes and the number of connections with neighboring pores, as determined by 3D evaluation with X-ray micro-computed tomography (micro-CT). The simulated permeability was reduced by as much as two orders of magnitude when templating with the particle-coated EPS compared to templating with un-coated EPS in materials of similar porosities. 3D visualisations of snapshots from the simulated flow fields and flow velocities, and the pore structure are also shown. We also show that with water-based porosimetry the pore size distribution and throat size distribution of these macroporous ceramics can be evaluated by one single extrusion and intrusion cycle.

PO26

Douglas Cleaver

Molecular simulation of the gyroid cubic phase

Doug Cleaver,¹ Laurence Ellison,¹ and Gerd Schröder-Turk²¹*Materials and Engineering Research Institute, Sheffield Hallam University, UK*²*Inst Theor Phys., Alexander-Friedrich Universität, Erlangen, Germany*

By performing standard molecular dynamics (MD) simulations on purely repulsive pear-shaped objects, we have observed free self assembly of the 3d periodic soft solid gyroid cubic phase. For weakly tapered objects, increasing the system density only gives conventional nematic and lamellar (or smectic bilayer) phases. At intermediate taperings, however, a very different, highly curved supramolecular structure becomes apparent. This can best be visualised by depicting each particle blunt-end as a single dot and using cluster identification algorithms to construct wireframes. With this simplified representation, two interpenetrating 3d networks become apparent, characterised by a series of triply bonded nodes. This is the Gyroid phase, well known in experimental block copolymer and lyotropic systems, but never previously observed in hard-particle MD simulation.

A bicontinuous mesophase geometry with hexagonal symmetry

Gerd E. Schröder-Turk,¹ Sebastian Kapfer,¹ Walter Mickel,¹ Trond Varslot,² and Liliana de Campo²

¹Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

²Department of Applied Mathematics, Research School of Physical Sciences and Engineering, The Australian National University, 0200 ACT, Australia

We report that a specific realization of Schwarz' triply-periodic *hexagonal minimal surface* is isotropic with respect to the Doi-Ohta interface tensor and simultaneously has minimal packing and stretching frustration similar to those of the commonly found cubic bicontinuous mesophases. This hexagonal surface, of symmetry $P6_3/mmc$ with a lattice ratio of $c/a = 0.832$, is therefore a likely candidate geometry for self-assembled lipid/surfactant or copolymer mesophases. Furthermore, both the peak position ratios in its powder diffraction pattern, and the elastic moduli closely resemble those of the cubic bicontinuous phases. We therefore argue that a genuine possibility of experimental misidentification exists.

[1] G.E. Schröder-Turk, T. Varslot, L. de Campo, S.C. Kapfer and W. Mickel, A bicontinuous lipid mesophase geometry with hexagonal symmetry, *Langmuir*, doi: 10.1021/la201718a (2011)

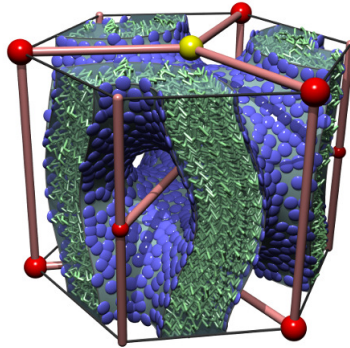


FIG. 1. An illustration (not a simulation) of the hypothetical hexagonal bicontinuous mesophase.

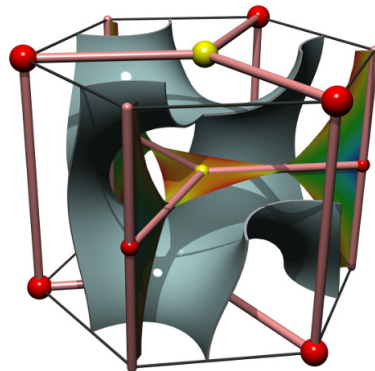


FIG. 2. Unit cell with medial surface construction used to quantify domain width variations.

Correlations between the cell nuclei in artificially grown tissues

S. Kaliman,¹ A. S. Smith,¹ F. Rehfeldt,² and C. Jayachandran²

¹Cluster of Excellence, Friedrich-Alexander Universität, Erlangen, Germany

²Third Institute of Physics, Georg-August-Universität, Göttingen, Germany

Correlations between the cell nuclei in artificially grown tissues The stability and viability of the tissue is related to the mechanical properties of the extracellular matrix. A tissue exerts contractile forces through adhesive contacts onto the extracellular matrix modulating the tension in the matrix itself. These effects have been relatively well characterized on a level of a single cell. However, the relation between the response of a single cell and the response of the tissue to changes in the environment is not yet understood. Here, large scale coordination of cells within the tissue is enabled by biochemical signaling, the role of which is, at present, equally elusive.

The difficulty in studying the above issues is the lack of quantitative measures that will allow for the understanding of the structure–function relationship in systems such as cells and tissues where a biophysical and biochemical processes are altered by the adoptable spatial structure. However, in order to relate the morphology to properties such as elasticity, permeability, tension or pressure Minkowski functionals, defined in the framework of integral geometry could be used. They are able to provide a clear distinction between anisotropy as a measure for non-sphericity or non-cubicity of the cell, and alignment as the orientation of an anisotropic structure with a given reference direction. We use these tools to determine how the sizes of the nuclei depend on a function of the density of stem cells and the elasticity of the underlying matrix. Furthermore, we quantify the decay of correlations in alignment of the cell nuclei within the culture and make an attempt to connect these observations to the polarizations of the cell bodies.

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Structure of wing scales in the Madagascan Sunset moth (*Chrysidia rhiphearia*)

Anna M. Carnerup and Stephen T. Hyde

Applied Mathematics Dept., Research School of Physics and Engineering, Australian National University, Canberra, 0200, AUSTRALIA

This beautiful moth has strikingly colourful wing patterns, that span the visible spectrum. Optical and scanning electron micrographs reveal that these colours are caused by a variety of optical effects, from corrugated scales to ultrastructured chitin assemblies within the wing scales. An earlier study proposed that the structure responsible for colouring within the most vivid regions of the wings is due to a lamellar arrangement of chitin-rich sheets, separated by randomly arranged pillars, much like a pillared clay [1]. We have looked more closely at scales from various coloured regions and found a more interesting story. (Here we ignore the complex woven fibre arrays that characterise the ribs on the upper faces of coloured – and uncoloured – scales.) In fact, all coloured scales we have looked at contain pseudo-rectangular lattices of galleries (occasionally forming quasi-hexagonal domains) whose walls contain arched openings linking adjacent chambers. These arches are most often tapered towards the lower (internal) faces of the scale, though in some examples, the openings between adjacent galleries are elliptical windows. These galleries form the skeletal foundations of all coloured scales. Occasionally, this completes the morphology of the scale. However, in most cases, one-dimensional crystals composed of lamellar stacks are indeed observed (whose lattice parameters vary from about 200-300nm.). However these lamellae are pillared by catenoidal supports that form a quasi-regular triangular lattice, giving a three-dimensional rhombohedral crystalline array. The number of lamellar intergrown within the galleries vary, resulting in variable in-filling of the galleries. Green scales are typically full (5-7 lamellae), red, yellow and blue scales less so (2-3). Intermediate examples partially fill the galleries from the "ground" up.

These rhombohedral pillared lamellar patterns bear an interesting comparison to the **srs** nets [2] found in some butterfly wing-scales. The latter arrays likely result from templating by membranes folded according to the geometry of the (sponge-like) gyroid minimal surface. The single chitin network results from chitin polymerisation within one domain of the bicontinuous pattern. The pillared lamellar patterns likewise fill the continuous complementary volume generated by a three-dimensional pattern composed of parallel meshes, each formed by inflating a simple hexagonal (**hcb** [3]) net. The genesis of the 3D rhombohedral chitin structure found in these scales can therefore be explained by templating within a giant rhombohedral mesh phase present during growth of the scales. It is worth noting that an identical geometry is found *in vitro* in lyotropic liquid crystals: namely "rhombohedral mesophases", formed by lecithin-water mixtures and soaps, first identified by Luzzati and co-workers [4]. We therefore suggest that these pillared lamellae are formed within the pupa in response to membrane folding equivalent to that found in rhombohedral mesh mesophases (albeit at a much longer length scale). To our knowledge, this morphology has not been reported previously; in addition to templating by bicontinuous ("sponge") morphologies, mesh morphologies are likely also present in some species during the pupal stage of development.

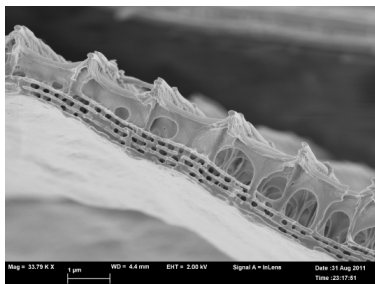


FIG. 1. Scanning electron micrograph of a coloured wing-scale of *C. rhiphearia* showing the galleries linked by arches and 3-4 lamellae, pillared by a trigonal array of catenoidal pillars.

- [1] S. Yashoika and S. Kinoshita, Optics Express 15, pp. 2691–2701 (2007)
- [2] S.T. Hyde, M. O'Keeffe and D.M. Proserpio, Angewandte Chemie International Edition 47, pp. 7996–8000 (2008)
- [3] rcsr.anu.edu.au
- [4] E.Luzzati, T. Gulok-Krzywicki and A. Tardieu, Nature 217, p. 1028 (1968) and Nature 218, pp. 1031–1034, (1968)

What encodes the diversity and ordering of self-organized monolayers?

C. Rohr,¹ M. Balbás Gamba,² K. Gruber,¹ E. C. Constable,³ E. Frey,² T. Franosch,⁴ and B. A. Hermann¹

¹Walther-Meissner-Institute (WMI) of Low Temperature Research of the Bavarian Academy of Science and Faculty of Physics/Center for Nano Science (CeNS), Germany Walther-Meissner-Strasse 8, 85748 Garching b. München, Germany

²Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for Nano Science (CeNS), Department of Physics, LMU München, Theresienstraße 37, 80333 München, Germany

³Department of Chemistry, University of Basel, Spitalstrasse 51, 4056 Basel, Switzerland

⁴Institut für Theoretische Physik, FAU Erlangen, Staudtstraße 7, 91058 Erlangen, Germany

The a priori prediction of patterns formed from self-organized molecules is of crucial importance for the deliberate application of monolayers for surface functionalization. We used scanning tunneling microscopy (STM) to image self-organized monolayers of Fréchet dendrons, which display a large variety of 2D ordering motifs, even for a single molecule. We analyzed the ordering of the different phases of this high complexity system by molecular mechanics (MM) simulations. We conceived an elegant interaction-site model, which condenses the essential molecular properties determined by molecular mechanics modeling (MM), which in a Monte Carlo (MC) approach successfully predicts the various ordering motifs. With this model we could confirm that geometry as well as a few salient weak interaction sites fully encode the observed variety of structural motifs. Because of the simplicity of our approach it should be applicable to a wide variety of self-organized systems.

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- [3] C. Rohr, M. Balbás Gamba, K. Gruber, C. Höhl, M.S. Malarek, L.J. Scherer, E.C. Constable, T. Franosch, and B.A. Hermann, *Chem. Comm.* 47, 1800 (2011).

Organisation and scientific committee

Dr Gerd E Schröder-Turk

Institut für THEoretische Physik
Friedrich-Alexander-Universität Erlangen-Nürnberg
Staudtstraße 7
D-91058 Erlangen
Germany

Phone: +49 9131 85 28448

Fax: +49 9131 85 28444

e-mail: gerd.schroeder-turk@physik.uni-erlangen.de

Prof Stephen T Hyde

Department of Applied Mathematics
Research School of Physical Sciences and Engineering
The Australian National University
Canberra
0200 ACT
Australia

Phone: +61 2 6125 4553

Fax: +61 2 6125 0732

e-mail: stephen.hyde@anu.edu.au

Venue

Hotel Zora

Primošten hoteli d.o.o.
Raduča bb
22 202 Primošten
Croatia

Participants

Filipa Alves, Instituto Gulbenkian de Ciencia Oeiras, Biophysics and Genetics of Morphogenesis, Portugal
Michael Anderson, The University of Manchester, Centre for Nanoporous Materials, UK
Linnéa Andersson, Stockholm University, Dept of Materials and Environmental Chemistry, Sweden
Matej Babic, EMO-ORODJARNA D.O.O., Slovenia
Maria Barbi, Universite Pierre et Marie Curie, LPTMC, France
Marina Čalogović, University of Zagreb, Faculty of Science and Mathematics, Croatia
Toen Castle, Australian National University, Applied Maths, Australia
Debby Chang, Lund University, Physical Chemistry, Sweden
Xiao Changhong, Stockholm University, Department of Materials and Environmental Chemistry, Sweden
Shunai Che, Shanghai Jiao Tong University, School of Chemistry and Chemical Engineering, China
Douglas Cleaver, Sheffield Hallam University, Materials and Engineering Research Institute, UK
Robert Corkery, YKI, Sweden
Liliana De Campo, Australian National University, Applied Mathematics, Australia
Yuru Deng, National University of Singapore, Yong Loo Lin School of Medicine, Singapore
Tomonari Dotera, Kinki University, Department of Physics, Japan
Johan Engblom, Malmö University, Faculty of Health and Society, Sweden
Myfanwy Evans, Friedrich-Alexander Universität Erlangen-Nürnberg, Institut für Theoretische Physik, Germany
Helge-Otto Fabritius, Max-Planck-Institut für Eisenforschung, Dept. Microstructure Physics and Metal Forming, Germany
Peter Falkman, Malmö University, Faculty of Health and Society, Sweden
Thomas Franosch, Friedrich-Alexander Universität Erlangen-Nürnberg, Institut für Theoretische Physik, Germany
Karsten Grosse-Brauckmann, Universität Darmstadt, Mathematik, Germany
Jemal Guven, University of Mexico (UNAM), Instituto de Ciencias Nucleares, Mexico
Laurent Helden, Universität Stuttgart, 2. Physikalisches Institut, Germany
Sascha Hilgenfeldt, University of Illinois at Urbana-Champaign, Mechanical Science and Engineering, USA
Stephen Hyde, Australian National University, Applied Mathematics, Canberra, Australia
Marianne Impéror-Clerc, Université Paris-Sud, Laboratoire de Physique des Solides, France
Randall Kamien, University of Pennsylvania, Department of Physics and Astronomy, USA
Sebastian Kapfer, Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Theoretische Physik, Germany
Birgit Kaufmann, kaufmann.birgit@gmail.com, Purdue University, Mathematics and Physics, USA
Kriszian Kertesz, Research Institute for Technical Physics and Materials Science, Nanostructures, Hungary
Jacob Kirkensgaard, University of Copenhagen, Basic Sciences and Environment LIFE, Denmark
Sepp Kohlwein, University of Graz, Institute of Molecular Biosciences, Austria

Participants

Iuliia Kominska, Sumy State University, Department of Nanoelectronics, Ukraine
Jan Kuriplach, Charles University, Low Temperature Physics, Czech Republic
Halim Kusumaatmaja, University of Cambridge, Department of Chemistry, UK
Kåre Larsson, Camurus AB, Lund, Sweden
Alfie Lethbridge, University of Exeter, School of Physics, UK
Rafael Lopez, Universidad de Granada, Geometria y Topologia, Spain
Stephen Luke, University of Exeter, Physics, UK
Robert Magerle, Technische Universität Chemnitz, Fakultät für Naturwissenschaften, Germany
Oksana Manyuhina, Nordic Institute for Theoretical Physics, Sweden
Siewert-Jan Marrink, University of Groningen, Netherlands
Miguel Martin, Universidad Politécnica de Madrid, Applied Mathematics, Spain
Elisabetta Matsumoto, Princeton University, Center for Theoretical Science, USA
Klaus Mecke, Friedrich-Alexander-Universität Erlangen-Nürnberg, Theoretische Physik, Germany
Kell Mortensen, University of Copenhagen, Basic Sciences and Environment LIFE, Denmark
Ricardo Mosna, Universidade Estadual de Campinas, Department of Applied Mathematics, Spain
Martin Mueller, Universite Paul Verlaine Metz, Physics, France
Ryo Nakazawa, Keio University, Applied Chemistry, Japan
Matthew Nixon, University of Exeter, School of Physics, UK
Tommy Nylander, Lund University, Physical Chemistry, Sweden
Christophe Oguey, LPTM, Universite de Cergy-Pontoise
Drew Parsons, Australian National University, Applied Mathematics, Australia
Caroline Pouya, University of Exeter, Physics, UK
Pavel Prybytak, Sheffield Hallam University, Materials and Engineering Institute, UK
Ling Qin, University of Manchester, Chemistry, UK
Stuart Ramsden, Australian National University, Dept. of Applied Maths and ANU Supercomputer Facility, Australia
Miguel Reyes, Dpto. Matemática Aplicada, Universidad Politécnica de Madrid
Nicolas Rivier, Universite de Strasbourg, ICPM, France
Matthias Saba, Friedrich-Alexander-Universität Erlangen-Nürnberg, Theoretical Physics, Germany
Jean-François Sadoc, Université de Paris-Sud, Laboratoire de Physique des Solide, France
Yasuhiro Sakamoto, Osaka Prefecture University, Nanoscience and Nanotechnology Research Center, Japan
Vinodkumar Saranathan, Edward Grey Institute, University of Oxford, Zoology, UK
Alan Schoen, Southern Illinois University/Carbondale, Electrical Engineering, USA
Christian Scholz, Universität Stuttgart, 2. Physikalisches Institut, Germany
Gerd Schröder-Turk, Friedrich-Alexander-Universität Erlangen-Nürnberg, Theoretische Physik, Germany
John Seddon, Imperial College London, UK
David Siegel, Givaudan Inc., USA

David Smith, Institute Ruder Boskovic, Croatia

Ana-Suncana Smith, Universität Erlangen-Nürnberg, Theoretische Physik & Eng. of Advanced Materials, Germany

Doekele Stavenga, University of Groningen, Computational Physics, Netherlands

Björn Stuhrmann, FOM Institute AMOLF Amsterdam, Biological Soft Matter, Netherlands

Osamu Terasaki, Stockholm University, Materials and Environmental Chemistry, Sweden

Carsten Tschierske, University Halle, Chemistry, Germany

Mark Turner, Swinburne University, Centre for Micro-Photonics, Australia

Daniel Van Opend Bosch, Universität Erlangen-Nürnberg, Dept. Materialwissenschaften & Werkstofftechnik, Germany

Peter Vukusic, University of Exeter, Physics, UK

Bodo Wilts, University of Groningen, Computational Physics, Netherlands

Xia Wu, Max-Planck-Institut für Eisenforschung GmbH, Dept for Microstructure Physics and Metal Forming, Germany

Xiaochun Xu, National University of Singapore, MechanoBiology Institute, Singapore

Anan Yaghmur, University of Copenhagen, Department of Pharmaceutics and Analytical Chemistry, Denmark

Tatyana Zykova-Timan, Cambridge University, Chemistry, UK

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Monday**09:00 – 10:55**

Chair: Kristen Grosse-Brauckmann

Opening words
 Alan Schoen IL
 Elisabetta Matsumoto CT
 Christophe Oguey CT

10:55 – 11:15 Coffee break

11:15 – 13:00

Chair: Robert Corkery

Doekele Stavenga
 Caroline Pouya IL
 Xia Wu CT

13:00 – 15:30 Lunch break

15:30 – 16:55

Chair: Sascha Hilgenfeldt

Klaus Mecke
 Rafael Lopez IL
 CT

16:55 – 17:20 Coffee break

17:20 – 18:30

Chair: Osamu Terasaki

Toen Castle
 Anan Yaghnur CT
 Tatyana Zykova-Tirman CT

Tuesday**09:00 – 10:50**

Chair: John Seddon

Yuru Deng
 Krisztian Kertesz IL
 Vinodkumar Saranathan CT

10:50 – 11:15 Coffee break

11:15 – 13:00

Chair: Doekele Stavenga

Siewert-Jan Marrink
 Matthias Saba IL
 Martin Müller CT

13:00 – 14:30 Lunch break

14:30 – 16:00

Chair: Alan Schoen

Karsten G-Brauckmann
 Birgit Kaufmann IL
 CT

16:00 – 17:30**Poster Session**

(with coffee, wine and snacks)

Wednesday**09:00 – 10:55**

Chair: Stephen Hyde

The Yves Bouligand Lecture
 Jean Francois Sadoc IL
 Kell Mortensen CT
 Tomonari Dotera CT

10:55 – 11:15 Coffee break

11:15 – 13:00

Chair: Vinod Saranathan

John Seddon
 Halim Kusumaatmaja IL
 Maria Barbi CT

13:00 – 15:30 Lunch break

15:30 – 16:55

Chair: Marianne Imperor

Peter Vukusic (S. Luke)
 Osamu Terasaki IL
 CT

16:55 – 17:20 Coffee break

17:20 – 18:30

Chair: Tomonari Dotera

Robert Magerle
 Jemal Guven CT
 Filipa Alves CT

Thursday**09:00 – 10:55**

Chair: Yuru Deng

Marianne Imperor-Clerc
 Nicolas Rivier IL
 Stuart Ramsden CT

10:55 – 11:15 Coffee break

11:15 – 13:00

Chair: Klaus Mecke

Randall Kamien
 Sascha Hilgenfeldt IL
 Michael O'Keefe CT

13:00 – 14:30 Lunch break

14:30 – 16:20

Chair: Kell Mortensen

Kåre Larsson
 Shunai Che IL
 David Siegel CT

16:20 – 16:45 Coffee break

16:45 – 18:00

Chair: Robert Magerle

Robert Corkery
 Jacob Kirkensgaard CT
 Carsten Tschierske CT

20:00

Conference Dinner

Friday**09:00 – 10:20**

Chair: Randall Kamien

Douglas Cleaver
 Tommy Nylander CT
 Oksana Manyuhina CT

10:20 – 10:50 Coffee Break

10:50 – 12:10

Chair: Gerd Schroeder-Turk

Bodo Wlits
 Björn Stuhmann CT
 Debby Chang CT
 Closing remarks CT