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- Ilse van der Kraaij-Quick
- Wim Bouwman

ESS organisation (ESS, Sweden)

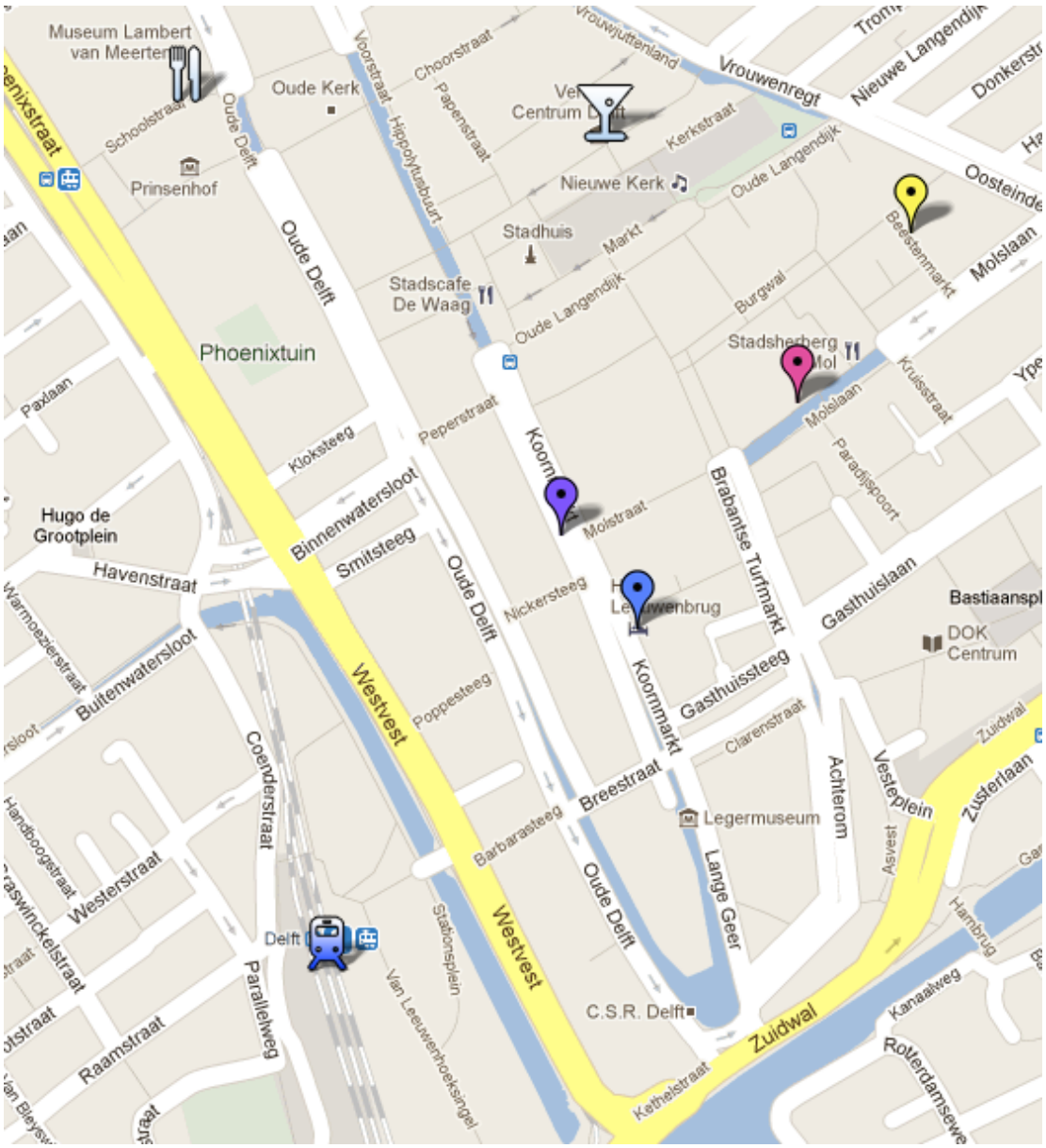
- Sofie Ossowski
- Axel Steuer

Location:

Delft University of Technology, Building 34
Faculty Mechanical, Maritime and Materials Engineering
Lecture hall D: James Watt, Mekelweg 2, 2628CD Delft
the Netherlands.

Contact:
Neutronfood@tudelft.nl

Maps of the Centre of Delft



- Restaurant de Prinsenkelder, Schoolstraat 11
- Vermeer Centrum Delft, Voldersgracht 21
- Faculty Mechanical, Maritime and Materials Engineerin Mekelweg 2
- Reactor Instituut Delft, Mekelweg 15
- Delft train station
- Hotel Delft Centre
- Hotel De Koophandel
- WestCord Hotel Delft
- Hotel Restaurant Johannes Vermeer BV
- Hotel de Ark
- Hotel Leeuwenbrug - Delft

Programme Neutrons and Food

Sunday 29 January

17.30 **Welcome reception and Registration** at the "Vermeer Centrum Delft", Voldersgracht 21 in Delft with a guided tour starting at 18.15 hrs. The Vermeer Center offers a visual voyage of discovery through the life, work and city of Johannes Vermeer. Step into 17th century Delft, see samples from Vermeer's oeuvre, go in search of his mentor and find the stories behind the paintings.

Monday 30 January

Welcome

Chair: Wim Bouwman

8.45 Registration

9.15-9.25 Tim van der Hagen, Dean Faculty Applied Physics, Delft University of Technology
Welcome and Opening of the work shop

9.25-9.30 Wim Bouwman, plan for the work shop

Session 1: Neutrons and Food, chair: Erik van der Linden

9.30-9.45 Sofie Ossowski, Aim of work shop and status ESS

9.45-10.15 Andrew Jackson, Introduction to Neutron Scattering

10.15-10.45 Martin Leser, 'Soft' Matters in Food

10.45-11.15 Coffee break

Session 2: Large length structures, chair: Arjen Bot

11.15-11.35 Kitty van Gruijthuijsen, Towards understanding gelation in complex model mixtures

11.35-11.55 Wim Bouwman, SESANS for food

11.55-12.15 Frank Wieder, High pressure treatment of food materials: Compression monitoring by means of cold neutron radiography

12.15-12.35 Markus Strobl, Neutron Imaging and Food

12.35-12.45 1 minute poster presentations

12.45-13.30 Lunch break

13.30-14.20 Poster session

Session 3: Health and structure, chair: Thomas Gutberlet

14.20-14.50 Alan Mackie, Food Structure for Health

14.50-15.10 Dieter Middendorf, Nanoscale dynamics of food constituents by neutron scattering

15.10-15.30 Thomas Vilgis**,** Structure and Texture of Food Polymer Mixtures

15.30-16.00 Coffee break

Session 4: Cook and Chemist, chair: Wim Bouwman

16.00-17.00 Eke Mariën en Jan Groenewold, Cook and Chemist

Tuesday 31 January

Session 5: Interfaces, chair: John Webster

9.15-9.45 Annika Olsson, Neutrons for Food Packaging

9.45-10.05 Camille Loupiac, Major Role of Interfacial Water on Protein Structure and Dynamics

10.05-10.35 Peter Fischer, Stabilization of emulsions and foams: Probing interfacial properties by small angle scattering

10.35-10.55 Rob Dalgliesh, Spin-Echo SANS and Neutron reflection at the ISIS SecondTarget Station.

10.55-11.05 Conference Photo

11.05-11.25 Coffee break

Session 6: Interaction, chair: Tommy Nylander

11.25-11.55 Jan Swenson, Water Dynamics in Carbohydrate Rich Food by Quasielastic Neutron Scattering
11.55-12.15 Richard Frazier, Puroindolines and neutrons: determining the function of a family of sticky, non-stick wheat proteins
12.15-12.35 Ad van Well, Protein adsorption at the air-water interface
12.35-12.55 Maaike Nieuwland, Visualization and characterisation of protein structures at different length scales

12.55-13.45 Lunch break

Session 7: Dairy, chair: Marie Paulsson

13.45-14.15 Richard Ipsen, Some Current Issues in Dairy Technology Where Neutrons Could Play a Role
14.15-14.35 Sofie Ossowski, A neutron and light scattering study on pure κ-casein
14.35-14.55 Sreenath Bolisetty, Formation of multistranded β-lactoglobulin amyloid fibrils and their stimuli responsive magnetic behaviour in the lyotropic liquid crystals.
14.55-15.15 Andrew Jackson, Effects of high pressure on casein micelle structure

15.15-15.45 Coffee break

Session 8: Emulsions & hydration, chair: John van Duynhoven

15.45-16.15 Arjen Bot, Wall structure of self-assembled sitosterol + oryzanol tubules: a low-safa structurant of edible oils
16.15-16.45 Maria Ricci, Hydration of Trehalose and Glutathyone
16.45-17.05 Hans Tromp, Hydrogen bonds studied by wide angle neutron scattering
17.05-17.25 Vasyl Haramus, A comparative study of SANS, ultrafiltration and dialysis

19.00-22.00 Conference dinner at Restaurant "De Prinsenkelder", Schoolstraat 11, 2611 HS Delft

Wednesday 1 February

Session 9: Foams & proteins, chair: Hans Tromp

9.15-9.45 Monique Axelos, Neutrons for structural investigation of biopolymer assemblies
9.45-10.05 Fabrice Cousin, Self-assembly of Fatty acids and Neutrons : from the determination of the structure in bulk solution and at the air/water interface to the understanding of the Mechanisms of Stabilization of Smart Foams.
10.05-10.25 Sarah Rogers, Small-Angle Neutron Scattering at ISIS: Applications to Food Science
10.25-10.45 Sheila Khodadadi, Preservation of Proteins in Glassy State

10.45-11.15 Coffee break

Session 10: Conclusions, chair Sofie Ossowski and Andrew Jackson

11.15-12.15 Panel discussion, How can the ESS be a good facility of food science?
12.15-12.30 Erik van der Linden, Conclusions of the work shop
12.30 Bus to reactor
12.45-13.30 Lunch break at the Reactor Institute Delft for the visit
13.30–15.00 Visit to neutron facilities
15.15 Bus to Delft Centre

Practical Information

Coffee , tea and lunch breaks
For registered participants wearing their name badges, coffee and tea during the breaks are included in the fee. They are served in front of the lecture hall or in the Faculty room at the end of the corridor.

Currency and banking
There is an ATM machine located on the ground floor of the Aula of Delft University of Technology, Building 20; on the other site of the Mekelweg.

Mobile phones
Mobile phones must be switched off in the meeting rooms.

Oral Presentations
- All presentations will be held at the Delft University of Technology, Faculty Mechanical, Maritime and Materials Engineering, Lecture hall James Watt, Mekelweg 2, 2628CD Delft, the Netherlands (see map).
- Each contributed oral presentation will be 15 minutes long, followed by 5 minutes of discussion. The invited talks are 25 minutes followed by 5 minutes of discussion. The chairs of the sessions will be instructed to adhere strictly to the program. Speakers will not be allowed to exceed their allotted time for presentation, so make sure that you are able to stay within the allocated time limit.
- The presentation room will be equipped with a PC for PowerPoint slides. It is allowed to use your own laptop though we do recommend to use the computer which is already connected to the screen. In case you do want to connect your own laptop, please make sure that all screen-savers and pop-ups are turned off and that power save and sleep settings are switched off.
- Please bring your presentation on CD-ROM or memory stick. Use only standard fonts in the preparation of your PowerPoint slides.
- Please load your presentation file onto the computer in the meeting **room ultimately during the break in advance of your session.** We highly recommend that you take advantage of one of the early file loading opportunities before the meeting starts to check your presentation or to make last minute changes. Having the presentation files loaded in advance will help to ensure that the sessions run on schedule without delays.

Poster Instructions
- The poster session is:
  - Monday 30 January 13.30 – 14.20. Afterwards the posters have to be removed, but can be moved into the lecture hall for further discussion during the workshop breaks.
- Posters should not be larger than 147 cm in height and 97 cm in width
- The following information must appear at the top of the poster:
  - Title, Name(s) of Author(s), address of author(s), photograph(s) of authors.
  - The presenter of the poster must be identified with an asterisk.
- Poster boards, poster numbers and adhesive materials will be available to delegates to display
- Presenting authors are offered to opportunity to make advertisement for their poster in a one-minute presentation in the session from 12.35-12.45 using at most one slide. If you want to do this, please send the slide in PowerPoint before to neutronfood@tudelft.nl

Public Transport
Delft is a very compact city where your destination usually will not be at a great distance. Therefore, Delft is ideal for getting around by foot, bicycle or public transport. There is a dense public transport system and tram, metro or bus stops are usually around the corner. Cars are less suitable for navigating in Delft. Moreover, parking must be paid for in almost the entire city and the rates can be substantial.

How to reach the Faculty Mechanical, Maritime and Materials Engineering:
From Schiphol Airport: the easiest (and cheapest) way is to take the train directly from the airport to the Delft railway Station.
From Delft railway Station: from this station it is a short walk (10 minutes) to the Faculty Mechanical, Maritime and Materials Engineering. You can also take bus 69, 121 or 174.
More information you can find on http://www.veolia-transport.nl/netherlands-transport/ressources/documents/2/15128,Delft _Abrikaart_2010_2011_v3.pdf

Registration and Information:
You can register during the welcome reception on Sunday, January 29 at the "Vermeer Centrum Delft" and on Monday January 30, from 8.45 hrs. on at the registration desk in front of the lecture hall.
The registration desk will be open during the whole Workshop.

Registered participants and students are entitled to:
* Participation in scientific sessions
* Meeting documentation
* Admission to the welcome reception on Sunday
* Admission to the poster receptions on Monday
* Admission to the tour on Wednesday (although admission is free, pre-registration before 31 January is required for this event since maximum numbers apply and we need to have your passport number to register)
* Coffee, tea and lunch services during the scheduled breaks

Proceedings
The proceedings of the workshop will be published in the Journal of Neutron Research. Neutrons and food is a relatively new topic so would attract interest and in particular any papers which include technical or methodological innovations. The dead line for manuscripts is March 1st, 2012.

Oral presentations

Introduction to Neutron Scattering

Andrew J Jackson[1]
[1]*European Spallation Source ESS AB, Stora Algatan 4, Lund 221 00, Sweden*

Neutrons are a powerful tool for the study of the structure and dynamics of materials and biological systems. As such, application to food science is a natural extension of the use of neutron scattering. A general introduction to neutron scattering will be presented, along with a description of the neutron scattering techniques that might be most applicable to food science. In particular, small angle scattering, reflectometry, diffraction, inelastic scattering and imaging will be presented.

'Soft' Matters in Food

Martin E. Leser

Nestle Research, Product Technology Center Marysville, Ohio, USA

The increasing importance of health & wellbeing from a healthcare system perspective urges Food Industry to speed up their research and development work of new innovative products, which allow the consumers to better sustain or promote their personal health and wellbeing. Other key market trends are convenience, naturalness of the food, or appealing taste and aroma.

In order to develop and produce such tasty, nutritious and healthy food products the creation of new know-how on how to better tailor, design or control colloidal food structures and their interactions is required.

Although foods are complex systems, it becomes more and more evident that applying 'Soft Condensed Matter' Physics concepts allows also to better understand structure formation and dynamics in Food materials. The behaviour of 'soft' matter is dominated by one simple fact: it contains 'mesoscopic structures'of different length scales (from the nano- up to the millimetre length scale). In order to control the final product properties, it is not only necessary to couple the structural behaviour on different length scales, but also to look at the structure dynamics in these materials. Therefore, Neutron scattering methods are attracting more and more the interest of Food researchers, since they perfectly allow to study soft condensed matter principles also in the context of food, nutrition and health science.

In the present contribution some of the latest global key market trends in Food will be mentioned and used to sketch what type of questions have to be addressed and answered by the Food research community in order to describe and generate new solutions meeting the changing needs and expectations of the consumers in the future.

Towards understanding gelation in complex model mixtures

Kitty van Gruijthuijsen[1], **Wim G. Bouwman**[2], **Peter Schurtenberger**[3], **Anna Stradner**[3]
[1]*Fribourg University, Adolphe Merkle Institute, Rte de l'ancienne Papeterie 1, 1723 Marly, Switzerland, kitty.vangruijthuijsen@unifr.ch*
[2]*Delft University of Technology, Faculty of Applied Sciences, Delft*
[3]*Physical Chemistry, Lund University, Lund*

Food and materials are complex mixtures of numerous ingredients which can vary in size, solubility, and mutual compatibility. To engineer and predict properties like texture and shelf live, we need to understand how the nanostructure of these mixtures leads to (in)stability of the final products. In this area food and materials sciences have started to enormously profit from parallel developments in soft matter physics. Especially insights into model systems without specific interactions, like hard spheres, charged spheres, and ideal polymers, can easily be extrapolated to their industrial counterparts. In mixtures of these model components, steric exclusion of the polymer from an area around the colloid results in an attractive colloid-colloid interaction potential, the so-called depletion attraction. Strengthened with a good description of the interactions in our system, we aim to form physical gels at higher polymer concentrations. Light, x-ray and neutron scattering techniques are used to link the nano- and microscopic colloidal structure to the bulk properties. These insights may help in the design of chewable, but low-calorie products.

SESANS for Food

Wim G. Bouwman, J. Plomp, C.P. Duif
Delft University of Technology, Faculty of Applied Sciences, Mekelweg 15, 2629 JB Delft, the Netherlands, w.g.bouwman@tudelft.nl

Systems of practical relevance to the food industry are often hard to investigate non-invasively. This is caused by the fact that most food emulsions are opaque and soft materials. The relevant length scales are often micrometres. Spin-echo small-angle scattering (SESANS) operates at these length scales and benefits from the high penetrating power of neutrons. SESANS yields directly the scattering length density correlation function, which facilitates visual data-analysis [1].
In this presentation we show how we investigated the fat droplet structure of different emulsion gels after storage at fixed temperature or after temperature cycling. Upon temperature-cycling the fat droplet clusters increase in size, next to the droplets themselves getting larger as well [2]. We determine quantitatively the aggregation of casein micelles into yoghurt [3] and show a few other examples.

References
[1] W.G. Bouwman, J. Plomp, V.O. de Haan, W.H. Kraan, A.A. van Well, K. Habicht, T. Keller, M.T. Rekveldt, Nuclear Instruments and Methods in Physics Research A **586** 9–14 (2008)
[2] A. Bot, F.P. Duval, and, W.G. Bouwman, Food Hydrocolloids **21** 844–854 (2007)
[3] L.F. van Heijkamp, I.M. de Schepper, M. Strobl, R.H. Tromp, J.R. Heringa, W.G. Bouwman, J. Phys. Chem. A **114** 2412-2426 (2010)

High pressure treatment of food materials: Compression monitoring by means of cold neutron radiography

Oliver Schlüter [1], Stefan Boguslawski [2], Dietrich Knorr [2], Frank Wieder [3], Ingo Manke [3], Nikolay Kardjilov [3]
[1] Leibniz Institut für Agrartechnik Potsdam-Bornim, Potsdam/Germany
[2] Technische Universität Berlin, Berlin/Germany
3 Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin/Germany

With the use of conventional thermal processes the properties of the complex system “food” and/or single food components could be influenced with respect to the process target. Different aggregate states are used for drying, steaming, crystallizing, melting and extracting. The phase or state changes are not only influenced by temperature but also directly affected by the acting pressure. With the application of high hydrostatic pressure there arises a new opportunity to specifically control phase changes during treatment of foods. To better understand the entire processes in-situ observation of the related changes is challenging.
Cold neutron radiography (CNR), a novel approach was used to visualize high pressure induced changes of food materials. D2O was applied as pressure transmitting medium, which has a smaller mass absorption coefficient for neutrons than H2O. Different model foods (water, olive oil, potato) were used as samples. CNR was conducted at V7, HZB, Berlin. Before compression the samples were inserted into a special sample holder for liquid food samples, separated from the pressure transmitting medium by a floating piston made of Teflon. Pressure was built up in different steps (0.1, 10, 50, 100, 150, 200, 300, 400 MPa) and at each level CNR images were taken every 15 seconds with an exposure time of 10 seconds. Teflon and D2O created positive contrast when compared to the treated sample. Visualization of the gaseous-liquid phase changes was realized and volume changes of the samples were clearly observed from the movement of the floating piston. Results and potential of the CNR technique will be discussed.

Neutron Imaging and Food

M. Strobl[1], E. Lehmann[2], N. Kardjilov[3]
[1]European Spallation Source ESS AB
P.O Box 176, SE-221 00 Lund, Sweden, markus.strobl@esss.se
[2]Paul Scherrer Institut, Villigen Switzerland
[3]Helmholtz-Zentrum Berlin, Berlin, Germany

Neutron imaging has a quite wide scope of applications ranging from industrial applications via engineering, geology, paleontology and art history to biology and agricultural research [1]. It is the latter where neutron imaging enters life science and nowadays a connection to food relevant research can be made. In particular examples can be found where neutron imaging was used to investigate the water household of plants [2,3] either focussing on the processes in the roots and the surrounding soil or the water uptake into the plant itself. Both measurements take advantage of the high sensitivity of neutron for hydrogen, one additional of its good penetration characteristics and the other of its isotope sensitivity, which allows to distinguish hydrogen and deuterium. Recently further applications which benefit from the good transmission through metals have been reported investigating the effects and process of high pressure treatment of food and hence requires a pressure cell that needs to be penetrated in order to get meaningful results. Although this list might not seem long yet, however it demonstrates a certain potential and additionally some novel methods and increased resolution capabilities in neutron imaging that might increase this potential will be discussed shortly as well.

References

[1] M. Strobl et al. Advances in neutron radiography and tomography. J. Phys. D **42** (2009) *243001*
[2] U. Matsushima, W.B. Herppich, N. Kardjilov, W. Graf, A. Hilger, I. Manke, Estimation of water flow velocity in small plants using cold neutron imaging with D_2O tracer. Nucl. Instr. Meth. A **605**, 1-2, (2009)*146-149*.
[3] A. Moradi and E. Lehmann, Neutrons reveal a zone of water increase in soil around plant roots, NMI3 Newsletter, Highlights from Access Programm, Inside NMI3, Nov 2011
[4] O. Schlüter, S. Boguslawski, N. Kardjilov, In-situ observation of pressure induced phase changes in cellular food materials, BENSC Experimental Reports (2009)

Food Structure for Health

Alan R Mackie, Peter J Wilde, Adam Macierzanka

Institute of Food Research, Norwich Research Park, Colney Lane, Norwich, NR4 7UA, UK alan.mackie@ifr.ac.uk

As the rates of diet related health problems in Europe rise, there is increasing pressure to find ways of making our food healthier. The Food Structure group at IFR is interested in the development of food structures that have improved health benefits through their behaviour in the gastrointestinal (GI) tract. The basis of this approach is the ability to tune specific structures for targeted delivery of nutrients. For example, one of the target regions for addressing satiety requires improved resistance to digestion of either protein or lipid. This in general involves structuring interfaces in order to limit the access of digestive enzymes.

Neutrons have the potential to help us understand the structures we need to form in order to control rates of digestion. These range from gelled or fibrillar protein structures to protein nanoparticles coated with polysaccharides[1, 2]. Similarly emulsion systems with surface layers that can resist enzyme penetration through steric repulsion or other principles are of much interest[3].

Another aspect of the digestion process that is of interest is how products of lipolysis and hydrophobic compounds are transported in the aqueous environment of the GI tract. Often the transport involves the formation of complex colloidal structures that must pass through the mucus barrier to the gut lining[4]. The use of neutron scattering or reflectometry in environments that have the correct level of physiological relevance could help us to improve understanding in this area.

References

1. A. Macierzanka, A. I. Sancho, E. N. C. Mills, N. M. Rigby and A. R. Mackie, Soft Matter, 2009, 5, 538-550.
2. A. R. Mackie and A. Macierzanka, Current Opinion in Colloid and Interface Science, 2010, 15, 102-108.
3. B. S. Chu, G. T. Rich, M. J. Ridout, R. M. Faulks, M. S. J. Wickham and P. J. Wilde, Langmuir, 2009, 25, 9352-9360.
4. A. Macierzanka, N. M. Rigby, A. P. Corfield, N. Wellner, F. Böttger, E. N. C. Mills and A. R. Mackie, Soft Matter, 2011, 7, 8077-8084.

Nanoscale dynamics of food constituents by neutron scattering

H. Dieter Middendorf

Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, UK

d.middendorf@bioneutron.org.uk

Neutron spin-echo, backscattering, and time-of-flight techniques can contribute unique spatiotemporal information to the characterisation of biomolecular systems [1]. However, apart from quasielastic scattering (QENS) experiments on hydration processes in polysaccharide gels [2] or plant and fruit tissues, there are as yet few studies of direct relevance to food science. With the commissioning of fast third-generation spectrometers, the scope for experiments on multicomponent systems involving perdeuterated constituents is expanding. In terms of temperature T and specific hydration *h*, there are two main regions here –

(a) $180<T<280$ K, $0.05<h<0.5$. Because of much basic research on the 'energy landscape' of slightly hydrated proteins by way of measuring proton mobilities from ~30 to 300 K, work in this region is well established. Although data on ternary systems (protein + solvent + ligand) are scarce, the supercooling and upper cryogenic regions are obviously of great interest for studies of food preservation processes.

(b) $280<T<350$ K, $0.5<h<2.0$. Experiments on fully solvated macromolecules in this T,*h*-region present challenging problems [3]. These are due to the fact that, as in most other areas of macromolecular neutron spectroscopy so far, the aim is to isolate the incoherent scattering from biomolecular components in the form of $\Delta S_{inc}(Q,\omega)$ as the 'useful' signals. This requires subtraction of the predominantly coherent D_2O buffer scattering along with that from other dynamically important components present in perdeuterated form. The necessary data subtraction and correction procedures are problematic, and there are as yet no systematic experimental or simulation studies. Some headway has been made in this area by QENS studies of 'crowded' protein solutions, but further more comprehensive work of this kind is badly needed.

The aims of this paper are: (i) to review food-related hydration studies by QENS; (ii) to discuss selected results from (a) that illustrate the way in which neutron techniques can contribute to understanding the dynamics of food preservation processes; (iii) to outline possible approaches to exploiting more fully the rich information content of neutron $\Delta S(Q,\omega)$ data from ternary biomolecular solutions.

References

[1] H.D. Middendorf, in *Neutrons in Biology*, pp. 435-460 (J. Fitter *et al*., eds.), Springer (2006).
[2] H.D. Middendorf, D. DiCola, F. Cavatorta, A. Deriu, C.J. Carlile, Biophys. Chem. **47**, 145 (1994).
[3] H.D. Middendorf, Nucl. Instr. Meth. A **600**, 282 (2009).

Structure and Texture of Food Polymer Mixtures

Neyla Chatti, Sania Maurer, Natalie Russ, Birgitta Schiedt, Thomas Vilgis

Max-Planck-Institute for Polymer Research, Ackermannweg 10, 55128 Mainz
vilgis@mpip-mainz.mpg.de

Gelling agents and hydrocolloids are basic food ingredients which are able to set up basic structure property relationships in edible systems. Together with proteins, e.g., gelatin they can act as fundamental food systems whose physical textural properties can be controlled better as in real many component foods. Therefore it appears worthwhile to construct "model systems" for the fundamental interactions and the interplays between food polymers with different properties. In this contribution we present different systems where a systematic variation of parameters can be studied. The stiffness and composition of different polymers e.g. agarose (flexible, polar), xanthan (rigid, charged), gelatin ("polyampholyte") and small carbohydrates (sugars, additional water binding). The phase behavior and the resulting structure depend on the polymer properties [1]. Pair wise combinations of such molecules at various concentrations and compositions allow for very different structures. Part of the structure formations can be drawn back to the static and dynamical properties of the hydrocolloids, other parts of the interactions with the solvent water via the competition for water [2]. The interplay between large and small scale interactions leads also new insight. It would be intriguing to support these ideas by neutron scattering techniques propping different length and time scales like in classical polymer physics.

References

[1] D.Nordqvist, T.A. Vilgis, Rheological Study of the Gelation Process of Agarose-Based Solutions, Food Biophysics, (2011) **6**, 450-461

[2] S. Maurer, A. Junghanns, T.A. Vilgis Impact of xanthan gum, sucrose and fructose on the viscoelastic properties of agarose hydrogels, (2011) preprint

Scattering in The Kitchen

Eke Marien and Jan Groenewold

Cook & Chemist, Amsterdam, The Netherlands

In the cooking process structural changes occur during cooking. These changes often occur primarily on the level of food colloids/macromolecules. The study of these changes has advanced significantly with the aid of neutron scattering techniques. For the cook these structural changes are visible only through their consequences on the optical properties of the food. It is our aim to take you on tour through some cooking processes and discuss with you what could be happening in terms of food structure, during this process. Our main goal is to give you a few do's and dont's based on science that make you a better cook.

Neutrons for Food Packaging

A. Olsson[1]

[1]*Lund University, Faculty of Engineering, Design Sciences, Packaging Logistics*
Box 118, 221 00 Lund, Sweden, annika.olsson@plog.lth.se

The development of new packaging materials for food is a key for, longer shelf life, better protection and distribution of safe, nutritious food that ends up in good condition for consumption. In this paper/speech some important aspects will be regarded: 1) the industrial needs for stronger and yet lighter materials, 2) the evolution and industrial needs for biomaterial and nanotechnology in packaging material and 3) the interaction of packaging material and food items, 4) the need to make consumer confidence in and authority approvals of the new materials.

Major Role of Interfacial Water on Protein Structure and Dynamics

Domimique Champion[1], **Camille Loupiac**[1], **Daniela Russo**[2], **Jean-Marc Zanotti**[3]
1- Equipe EMMA, Université de Bourgogne, France
2- CNR-IOM, c-o Institut Laue Langevin, Grenoble, France
3- Laboratoire Léon Brillouin, CEA-CNRS, Saclay, France

Properties of the food matrices need to be studied as a function of parameters as temperature, high pressure, water content, and small co-solute nature (salt, sugars …). It is expected that this will contribute to an improved knowledge of molecular mechanisms underlying physical phenomena such as barrier properties, diffusion, phase transitions and structural rearrangements of the different food macromolecules. The talk will present some of our recent results on **protein hydration** and stability, with a specific focus on **protein structure and dynamics in concentrated systems** in relationship with a potential change of functionalities. The physical state of the proteins in the matrix has to be followed during processes and storage. We will present some of our recent results on this topic on whey protein powders, purified and dried beta-lactoglobulin in presence of various solutes (salt, sugar). Different biophysical tools (Neutron Scattering, DSC, sorption isotherms) were used. One of the main conclusions of our work emphasized the **major role of interfacial water on protein structure and dynamics**. We still need to better understand how this interfacial water affects or impacts the protein properties (functionality changes) and how we can modulate the effect of this pool of water molecules to better control protein conformation.

Stabilization of emulsions and foams: Probing interfacial properties by small angle scattering

Varvara Mitropoulos[1], Thomas Geue[2], Peter Fischer[1]
[1]ETH Zurich, Institute of Food, Nutrition and Health, Schmelzbergstrasse 9, 8092 Zurich, Switzerland, pefi@ethz.ch
[2]Paul Scherrer Institute, Laboratory for Neutron Scattering, 5232 Villigen PSI, Switzerland

Interfacial stabilization by adsorption layer of proteins, small molecular weight surfactants, and particles is ubiquitous in numerous food products and discussed as potential encapsulation method [1, 2]. To establish the link between morphology and mechanical properties of the adsorption layer this study focuses on a set of recombinant proteins called designed ankyrin proteins [3, 4]. The modular construction allows a polymer-like extension of a protein with the same building block and a controlled adjustment of its bulk and interfacial properties. Using small angle scattering and interfacial rheology we are able to correlate the protein size and stability to the resulting adsorption layer morphology, layer viscoelasticity, and capsule mechanics.

References

[1] Erni, P., E.J. Windhab, and P. Fischer, Emulsion Drops with Complex Interfaces: Globular Versus Flexible Proteins. *Macromolecular Materials and Engineering*, (2011) **296** 249-262.
[2] Mitropoulos,V., E.J. Windhab, and P. Fischer, The interfacial behavior of designed ankyrin repeat proteins. *Soft Matter*, (2011) **7** 7612-7615.
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Spin-Echo SANS and Neutron reflection at the ISIS Second Target Station.

Robert Dalgliesh[1]
[1] ISIS, Science and Technology Facilities Council, Rutherford Appleton Laboratory, Harwell Oxford, Didcot, OX11 OQX, United Kingdom, Robert.Dalgliesh@stfc.ac.uk

The ISIS Second Target Station and it's reflectometer instrumentation has significantly decreased the time taken to acquire data over a broad dynamic range. This has enabled the study of the dynamics of monolayer films of proteins and surfactants on time scales of a few tens of seconds to a few minutes. The development of Spin-Echo SANS on the OffSpec instrument has enabled the dynamics of surfactant aggregation and emulsions to be studied at lengths of 100nm-5μm. It is currently possible to access time scales of approximately 10 minutes but a new detector will allow measurement times to be reduced to ~1 minute. The current status of measurements for food science will be reviewed and future possibilities discussed. The review will also include the development and capabilities of the Larmor instrument which is currently under construction.

Water Dynamics in Carbohydrate Rich Food by Quasielastic Neutron Scattering

Jan Swenson
Department of Applied Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden, jan.swenson@chalmers.se

The water dynamics in carbohydrate rich food, such as white bread, strawberry and red onion, has been elucidated by quasielastic neutron scattering (QENS). The aim of the studies has been twofold; to determine how the water dynamics is affected by the geometrical confinements and molecular interactions in the host materials and to understand how this interfacial water influences the dynamical properties of the host materials. We find that the water dynamics is of jump-diffusion character and that it can be described by a stretched relaxation function. The relaxation rate and the associated diffusion constant are strongly dependent on the hydration level, as well as the structure and/or dynamics of the food "matrix" [1,2]. In fresh white bread the diffusion constant of water is almost a factor 10 lower than for bulk water [2], whereas in strawberry and red onion at a similar hydration level the water dynamics is only a factor 2-3 slower compared to bulk water [1]. In the case of strawberry and red onion it is also clear that the dynamics of the interfacial water and the pure food material (mainly sugar) are interrelated [1].

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Puroindolines and neutrons: determining the function of a family of sticky, non-stick wheat proteins

Richard A. Frazier[1], Luke A. Clifton[2], Michael R. Sanders[1,3], Rebecca J. Green[3]
[1]Department of Food and Nutritional Sciences, University of Reading, PO Box 226, Whiteknights, Reading RG6 6AP, United Kingdom, r.a.frazier@reading.ac.uk
[2]ISIS Spallation Neutron Source, Science and Technology Facilities Council, Rutherford Appleton Laboratory, Didcot, United Kingdom
[3]Reading School of Pharmacy, University of Reading, Reading, United Kingdom

The puroindolines (PINs) are a family of proteins that occur in wheat primarily to act in plant seed defence against fungal pathogens. They are also closely linked to the milling properties of different wheat varieties, acting as genetic markers of hard or soft endosperm texture, which defines the end-use quality of wheat. The PINs occur as two isoforms, PIN-a and PIN-b, which both feature a tryptophan-rich domain that is thought to be the site of interaction with lipid membranes. The PIN isoforms differ in the number of Trp-residues within this domain, 5 in PIN-a and 3 in PIN-b. Point mutations in the gene encoding PIN-b introduce single residue substitutions in the Trp-rich domain (Gly46 to Ser46 and Trp44 to Arg44), which have significant impact on endosperm texture through governing the level of adhesion between starch granules and gluten proteins. Using a combination of surface-sensitive techniques, including neutron reflectometry, we have characterised the lipid membrane interactions of PINs and focused on the role of tryptophan in their ability to penetrate lipid membranes [1-3]. Through these studies we have determined the impact of residue substitutions on the synergistic interactions of PINs with lipid membranes, which link both to determination of endosperm texture and to anti-pathogenic activity. We have expanded these studies to consider the solution structure of PINs [4], and synergistic activity with other co-localised plant seed defence proteins and peptides in wheat [5].

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Protein adsorption at the air-water interface

Ad A. van Well
[1]Delft University of Technology, Faculty of Applied Sciences, Mekelweg 15, 2629 JB Delft, the Netherlands, a.a.vanwell@tudelft.nl

Foams are stabilised by amphiphilic molecules that decrease the surface tension. In food materials this role is often played by proteins. The structure, i.e. the protein volume-fraction profile at the interface can be determined by means of neutron reflectometry. We studied the adsorption of two different types of proteins, β–casein and β-lactoglobulin. The former has little secondary structure and behaves like a random polymer, while the latter can be considered the be a rigid globular protein.

We measured the structure, using contrast variation, as a function of bulk concentration and compared the β-casein results with numerical self-consistent field theory calculations. The kinetics of the protein-layer formation is followed using an overflowing-cylinder. First results of this technique will be discussed.

Visualization and characterisation of protein structures at different length scales.

Maaike Nieuwland[1,2], **Arno Alting**[1,3], **Anneke Martin**[1,2], **Harmen de Jongh**[1,4]
[1]*Top Institute Food and Nutrition (TIFN), PO box 557, 6700 AN Wageningen, The Netherlands*
[2] *TNO, PO box 360, 3700 AJ Zeist, The Netherlands*
3 NIZO food research, PO Box 20, 6710 BA Ede, The Netherlands
4 Wageningen University and Research centre, Food Physics Group, PO Box 8129, 6700 EV Wageningen, The Netherlands

Some Current Issues in Dairy Technology Where Neutrons Could Play a Role

Richad H. Ipsen
Dairy Technology, Department of Food Science, University of Copenhagen, Rolighedsvej 30, 1958 Frederiksberg C, Denmark

Neutron scattering has a long history as a tool for structural elucidation in dairy relevant systems, most notably for probing the casein micelle architecture [1]. Recent applications include e.g. following and characterizing milk gelation [2] and characterizing adsorption of surfactants at interfaces [3].
However, milk is a highly complex fluid and dairy products are diverse and subject to a wide range of processing regimes. Hence, much is still unknown or unclear when it comes to a more fundamental understanding of the structural phenomena governing dairy product quality and research and development in academia and industry has an ever growing need for tools for structural elucidation.
A number of issues illustrating this will be presented, including processing of concentrated casein micelle systems, whey protein aggregation (including self-assembly) and the interactions of milk proteins with polysaccharides and surfactants.
The emphasis will be on the importance of a continuous dialogue between fundamental understanding of molecular function and a more applied approach.

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A neutron and light scattering study on pure κ-casein

Sofie Ossowski[1,2*], Tommy Nylander[2], Marie Paulsson[3], Carl Holt[4], Marc Obiols-Rabasa[2] and Lionel Porcar[5]

[1]*European Spallation Source ESS AB, Sweden; sofie.ossowski@esss.se*
[2] *Physical Chemistry Lund University, Sweden*
[3]*Food Technology, Lund University, Sweden;*
[4]*University of Glasgow, UK;* [5]*Institute Laue Langevin, Grenoble, France*

The casein micelle of milk is a colloidal polydisperse particle comprising the four caseins, α_{S1}-, α_{S2}-, β- and κ-caseins, together with about 7% by dry weight of calcium and inorganic orthophosphate (Pi) in the form of nm-sized amorphous calcium phosphate nanoclusters (CPN) [1-3]. Three of the four caseins (α_{S1}-, α_{S2}- and β-casein) are involved in the sequestration of the CPN through their phosphorylated sequences whereas the κ-casein somehow limits the micelle size and forms an outer, diffuse, layer [4]. Our studies aim to reveal the substructure of the native casein micelle, which still is not yet fully known. As a part of this we have studied pure κ-casein, to be reported here, as well as simplified model system consisting of β- and κ-caseins and calcium phosphate CaP.

The self-association of κ-casein was studied with SANS and light scattering, covering the concentration range over the previously reported critical micelle concentration (CMC). The aim was to investigate the monomer <-> multimer equilibrium as our previous SANS data suggested formation of very large aggregates. Furthermore we investigated if D_2O has any effect on the monomer <-> multimer equilibrium. Previous report suggested that the micellation of κ-casein was not affect by temperature. Here we report a significant difference for the hydrodynamic radius for 6°C and 25°C. These results was confirmed by complimentary cryo-TEM investigation on the temperature effect on κ-casein assembly.

Dynamic Light Scattering (DLS) show that κ-casein is temperature sensitive. Samples prepared at 25°C give rise to a hydrodynamic radius (R_h) of about 25-30nm, while samples prepared at 6°C gives significantly smaller R_h of about 16-18nm. No significant difference was observed between proteins dissolved in H_2O and D_2O buffer. The CMC is in accordance with the literature for κ-casein in H_2O buffer, namely about 0.5mg/ml. Further data analysis is required to reveal if D_2O has an effect on the CMC.

Cryo-TEM showed that temperature sensitivity of κ-casein self-assembly can be related to fibril formation. Previous studies report that κ-casein incubated at 37°C give rise to fibril formation, but claimed that no fibrils were formed at room temperature [5]. We incubated κ-casein at 6°C, 25°C and 37°C and could see fibrils at 37°C and 25°C, while at 6°C only micelles was observed. Fibrils were in the size range of 10-15nm thick and roughly 100nm long. κ-casein dissolved in D_2O buffer and stored at 25°C also resulted in fibrils, although with a larger fraction of micelles compared to when the protein was dissolved in H_2O.

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Formation of multistranded *β*-lactoglobulin amyloid fibrils and their stimuli responsive magnetic behaviour in the lyotropic liquid crystals.

Sreenath Bolisetty[1], Jozef Adamcik[1], Amar-Yuli Idit[1] and Raffaele Mezzenga [1]*

[1] *ETH Zurich, Food and Soft Materials Science, Department of Health Science and Technology, Schmelzbergstrasse 9, CH-8092 Zürich, SWITZERLAND*

We investigated snapshots of the fibrillation and aggregation kinetics of multi-stranded *β*-lactoglobulin amyloid protein fibrils at pH 2 and 90 °C by combining scattering (SANS, DLS, DDLS) as well as atomic force microscopy (AFM) [1]. Scattering techniques clearly demonstrate the structural conversion and time evolution of *β*-lactoglobulin monomers (2 wt %) into semi-flexible protein fibrils upon heating at 90°C. AFM allowed resolving the critical steps for the formation of single protofilaments, their alignment driven by liquid crystalline interactions and the twisting of the final fibrils due to the intra-molecular electrostatic interactions, leading to the development of multistranded twisted ribbon fibrils [2]. In further, *β*-lactoglobulin fibrils were titrated with a sulfated polysaccharide (k-carrageenan) to determine the morphology and mechanism of complex formation. SANS and microscopy indicated the complex formation of spherical aggregates attached along their contour length of the multistranded twisted protein fibrils, arranged in a necklace configuration [3].

In addition, we investigated the encapsulation of the *β*-lactoglobulin fibrils, fibrils coated with magnetic nanoparticles into the three different types of lyotropic liquid crystalline (LLC) meso phases. Mesophases composed of glycerol monolinoleate, linoleic acid and water yielding respectively lamellar, inverse bicontinuous cubic and inverse columnar hexagonal symmetries [4]. The impact of fibrils confinement within the LLC on their secondary structure, spatial organization and their response to an external magnetic field stimulus [5] was studied by combining small angle X-ray and neutron scattering (SAXS, SANS), ATR-FTIR and AFM techniques.

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Effects of high pressure on casein micelle structure

Andrew J Jackson[1] and Duncan J McGillivray[2]

[1]*European Spallation Source ESS AB, Stora Algatan 4, Lund 221 00, Sweden*
[2]*Department of Chemistry, The University of Auckland, Auckland 1142, New Zealand*

The structure of casein micelles in milk is still much debated. Here we present the results of making *in-situ* structural measurements using ultra-small-angle and small-angle neutron scattering while subjecting casein micelles to pressures up to 350MPa.

Modelling of the small angle scattering data across multiple isotopic water compositions reveals both reversible and irreversible breakdown of the casein micelle into component "sub-micelles". The pressure sensitivity of the micelles appears to be mediated by the presence of non-casein proteins.

Wall Structure of Self-Assembled Sitosterol + Oryzanol Tubules: A Low-SAFA Structurant of Edible Oils

Arjen Bot,[a] Elliot P. Gilbert,[b] Wim G. Bouwman,[c] Hassan Sawalha,[d] Vasyl M. Garamus,[e] Paul Venema,[d] Erik van der Linden,[d] Ruud den Adel,[a] and Eckhard Flöter.[a]

[a] Unilever Research and Development Vlaardingen, The Netherlands; [b] Bragg Institute, Australian Nuclear Science and Technology Organisation, Menai, Australia; [c] Delft University of Technology, The Netherlands; [d] Wageningen University, The Netherlands; [e] Helmholtz Zentrum Geesthacht, Germany

The structure of oil-continuous food products, such as margarine or butter, is based on a network of small crystallites of triglycerides (also known as triacylglycerols or TAGs). Surprisingly, few alternative structuring routes for food grade oils are known that are not based on the crystallisation behaviour of fatty acids [1]. One of the rare exceptions is the mixture of γ-oryzanol with β-sitosterol, which self-assembles in a helical ribbon, thus creating tubules with a diameter of ~7 nm and a wall thickness of ~1 nm. The tubules can aggregate to form transparent gels in triglyceride oils [2]. In emulsions, however, the presence of water interferes with tubule self-assembly in these systems by preventing the formation of intermolecular hydrogen bonds between β-sitosterol and γ-oryzanol and promoting β-sitosterol monohydrate formation, leading to structures that give rise to 'normal' sharp crystallographic reflections (as opposed to the broad scattering signals from the tubules) [3].

To study the structure of the tubules more closely, a neutron scattering study was performed using a range of deuterated and non-deuterated organic solvents. It was found that the walls of the tubules can be modelled as consisting of two layers: an inner higher proton-density layer and an outer lower-proton density. The lower density layer can be interpreted as the protruding ferulic acid moieties that are part of the oryzanol molecules. This confirms the structure that was earlier proposed previously on the basis of circumstantial evidence.

The data also sheds light on the effect of water on tubule structure in emulsion gels. It can be shown that certain subtle effects on shape of the scattering pattern are related to the choice of the organic phase in the emulsion gel, and not to interference of water with the tubular wall structure, as was surmised previously.

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Hydration of Trehalose and Glutathyone

Maria Antonietta Ricci, Fabio Bruni, Sara Pagnotta, Ernesto Scoppola
Dipartimento di Fisica E. Amaldi, Universita' degli Studi Roma Tre,via della Vasca Navale 84, 00146 Roma, Italy, riccim@fis.uniroma3.it

Neutrons are a powerful tool for studies of the hydration of biologically relevant molecules. In this paper the cases of trehalose and glutathyone are reported as examples of two extreme situations.
Indeed trehalose is found to form very few hydrogen bonds with water, at odds with the glutathyone molecule.

Hydrogen bonds studied by wide angle neutron scattering

R. Hans Tromp
NIZO food research, Kernhemseweg 2, 6718 ZB Ede, The Netherlands

H/D substitution offers a unique way to obtain separately partial radial distribution functions $g_{HH}(r)$, $g_{XH}(r)$ and $g_{XX}(r)$ ['X' being any atom except H]. In the past this method has been applied on various liquids containing hydrogen bond networks. Examples are water, phosphoric acid, concentrated salt solutions and liquid and glassy glucose. An overview of the results will be given, and the possibilities and the limitations of the technique will be discussed.

A comparative study of SANS, ultrafiltration and dialysis

Kathleen Oehlke[1], Vasyl Haramus[2], Anja Heins[1], Heiko Stöckmann[1], Karin Schwarz[1]
[1]Institute of Human Nutrition and Food Science, University of Kiel, 24118 Kiel, Germany
[2]Helmholtz-Zentrum Geesthach:t Zentrum für Material- und Küstenforschung, Max-Planck-Strasse, 21502 Geesthacht, Germany

The partitioning of SDS and CTAB in o/w emulsions was investigated by ultrafiltration (UF), dialysis and small-angle neutron scattering (SANS). It was possible to measure the monomeric and the micellar concentrations of the emulsifiers in the filtrate and permeate in the UF and dialysis experiments, respectively. In addition, the interfacial concentration was calculated as the difference to the initial concentration. SANS experiments provided data, from which the micellar concentrations were obtained, followed by the calculation of the interfacial concentrations.
The three methods were compared on the basis of the area, which is occupied by each emulsifier molecule at the interface. Micellation started at total emulsifier concentrations of approx. 10 mM in emulsions containing either CTAB or SDS. At saturation (>10 mM SDS in a 10% o/w emulsion), the area per SDS headgroup at the interface was between 48 and 64 $Å^2$, depending on the method. In emulsions with CTAB, saturation of the interface was not achieved. The minimum headgroup area was determined by UF to be 33 $Å^2$ at a concentration of 30 mM CTAB in a 10% o/w emulsion.

Neutrons for structural investigation of biopolymer assemblies

M.A.V. Axelos
INRA, Biopolymères Interactions Assemblages
Nantes - France
Monique.axelos@nantes.inra.fr

We report on the use of neutron scattering to investigate the structure of biopoplymer assemblies used to create foams, gels, new surfactant …in connection with their for food applications. Examples are given 1) on the structural determination of different whey proteins aggregates formed under conditions that coupled heating and shear flow in a plate heat-exchanger at high temperature and for short holding time [1], 2) on the in-situ structure of three-dimensional aqueous foams stabilized by surfactant molecules, proteins, polysaccharide – surfactant or polysaccharide – protein complexes [2,3].

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Detemination of the Structure of Polyectrolyte/proteins Complexes by SANS : from synthetic deuterated polyelectrolyte to Polysaccharides

Fabrice Cousin[1], François Boué[1]
[1] *Laboratoire Léon Brillouin, CEA Saclay, 91191Gif-sur-Yvette, France, fabrice.cousin@cea.fr*

The determination of the structure of polysaccharides/proteins complexes of opposite charges is of major importance in many situations in food science, as it enables to determine the mechanisms of formation of complexes as a function of physic-chemical parameters (pH, ionic strength, concentrations, flexibility of chains, etc...) and the subsequent properties of soluble complexes (colloidal stability, viscosity of solutions...). As the typical scales probed by SANS match the relevant scales of the system, it is *a priori* a tool of choice for such structural determination. It becomes especially powerful if one uses the contrast matching method to solve the structure of the solvent/polyelectrolytes/proteins system. However, this last experiment necessitates a difficult step of deuteriation, which is very costly (in time and/or money) or even impossible for proteins and polysaccharides. In this presentation, we will show how such difficulty can be overcome if one starts form a model polyelectrolyte/protein system, close to the polysaccharide/protein of interest, with a synthetic polyelectrolyte for which the deuteration step is easy. The refined structural determination of the structures of the model system thanks to the contrast matching will reveal the main trends of physicochemical parameters on complexation mechanisms, which will be a strong basis for the protein/polysaccharide system without deuteriation. This will be illustrated by SANS experiments on systems made of lysozyme, a positively charged protein, and either PSS, a synthetic polyelectrolyte [1-6], or polysaccharides (pectin [7] and hyaluronan [8]).

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Small-Angle Neutron Scattering at ISIS: Applications to Food Science

Sarah E. Rogers[1], Richard K. Heenan[1], Ann E. Terry[1] and Stephen M. King[1]
[1]*ISIS Facility, STFC, Harwell Science & Innovation Campus, Didcot, OX11 0QX, UK*

Small-Angle Neutron Scattering (SANS) is a powerful technique for determining microstructure in the dimension range of a few nanometres to hundreds of nanometres. SANS on a pulsed source has the significant advantage of a wide simultaneous Q range which is ideal when studying systems containing a broad range of lengthscales as is often the case in food science.

At ISIS there are currently two operational SANS beam lines, *Loq* and *Sans2d*, and a focussing beam line, *Zoom*, is under construction [1]. The complementary design of these three beamlines and the extensive range of sample environment available, potentially allows a wide variety of scientific problems in food science to be studied. In this paper the different characteristics of each beam line will be discussed along with actual and possible applications relevant to food science.

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Preservation of Proteins in Glassy State

Sheila Khodadadi[1], Susan Krueger[1], Evgenyi Shalaev[2], Marcus T. Cicerone[3], Joseph E. Curtis[1]

[1]Center for Neutron Research, NIST, MD, USA, sheila.khodadadi@nist.gov; [2]Department of Pharmaceutics, University of Minnesota, MN, USA; [3]Polymer Division, NIST, MD, USA

Polyhydroxy compounds, including carbohydrates (sugars) and sugar-alcohols, are well-known cryo- and lyo-protectors, which minimize destabilization of proteins and biological systems during freezing and drying processes. However, freeze-destabilization of proteins is commonly observed even in presence of sugars. There are several mechanisms proposed for freeze-destabilization of proteins, including different freeze-concentration effects [1], cold-denaturation [2], and destabilization of proteins due to interfaces between ice crystals and remaining unfrozen solution [3]. However, essential details of processes leading to freeze-induced unfolding and aggregation of protein molecules are still elusive.

Methods to elucidate high order structure of proteins in amorphous solid (glassy) phase are limited. Small Angle Neutron Scattering can be employed to study the tertiary structure of proteins in such systems. Different experimental and theoretical approaches to provide phenomenological and quantitative insights into the mechanism of destabilization-aggregation of the model protein in different glasses will be discussed.

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The partitioning of emulsifiers in o/w emulsions: A comparative study of SANS, ultrafiltration and dialysis

Kathleen Oehlke[1], Vasyl Haramus[2], Anja Heins[1], Heiko Stöckmann[1], Karin Schwarz[1]

[1]Institute of Human Nutrition and Food Science, University of Kiel, 24118 Kiel, Germany
[2]Helmholtz-Zentrum Geesthach:t Zentrum für Material- und Küstenforschung, Max-Planck-Strasse, 21502 Geesthacht, Germany

The partitioning of SDS and CTAB in o/w emulsions was investigated by ultrafiltration (UF), dialysis and small-angle neutron scattering (SANS). It was possible to measure the monomeric and the micellar concentrations of the emulsifiers in the filtrate and permeate in the UF and dialysis experiments, respectively. In addition, the interfacial concentration was calculated as the difference to the initial concentration. SANS experiments provided data, from which the micellar concentrations were obtained, followed by the calculation of the interfacial concentrations.

The three methods were compared on the basis of the area, which is occupied by each emulsifier molecule at the interface. Micellation started at total emulsifier concentrations of approx. 10 mM in emulsions containing either CTAB or SDS. At saturation (>10 mM SDS in a 10% o/w emulsion), the area per SDS headgroup at the interface was between 48 and 64 $Å^2$, depending on the method. In emulsions with CTAB, saturation of the interface was not achieved. The minimum headgroup area was determined by UF to be 33 $Å^2$ at a concentration of 30 mM CTAB in a 10% o/w emulsion.

Poster presentations

P1.

Investigating the Structure-Function Relations of Modified and Native Herring Protamine

Marcia M. English[1], Allan T. Paulson[1]
[1]Dalhousie University, Department of Process Engineering and Applied Science, Halifax, NS, B3J2X4 Canada.
allan.paulson@dal.ca

Protamine is an inexpensive cationic antimicrobial peptide (CAP) isolated from fish sperm and it contains 31 amino acid residues, 20 of which are arginine [1]. Although protamine has exhibited broad spectrum antimicrobial activity against some food-borne pathogenic Gram-negative and Gram-positive bacteria its non-specific binding to negatively charged food components reduces its antimicrobial activity [2]. The mechanism of action of protamine has not been fully elucidated and one of our objectives is to chemically modify protamine by (1) lipophilization and (2) with 1,2-cyclohexanedione to reduce the charge on the peptide, and determine how these changes affect the peptide's mechanism of antimicrobial activity.

Using neutron reflectometry we would like to answer the following questions: (1) Do native and modified protamine samples have the same membrane translocating mechanism in Gram-negative bacteria? (2) Are membrane transport proteins (porins) involved in protamine internalization in Gram-negative bacteria?

Preliminary results show lipophilization of clupeine (herring protamine) at the N-terminal proline residue of the YII fraction. In addition, lipophilized clupeine tested against human common cancer cells (HT29) was non-toxic at concentrations up to 100 µg/mL.

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P2.

Spin-Echo Small-Angle Neutron Scattering for the Study of Food Systems

W.G. Bouwman[1], J. Plomp[1], C.P. Duif[1], F.P. Duval[2] and A. Bot[2]
[1]*Department Radiation, Radionuclides & Reactors, Faculty of Applied Sciences, Delft University of Technology, Mekelweg 15, NL-2629 JB Delft, The Netherlands*
[2]*Unilever Research & Development Vlaardingen, Olivier van Noortlaan 120, NL-3133 AT Vlaardingen, The Netherlands*

Systems of practical relevance to the food industry are often hard to investigate non-invasively. This is caused by the fact that most food emulsions are opaque and soft materials. The relevant length scales are often micrometers. Spin-echo small-angle scattering (SESANS) operates at these length scales and benefits from the high penetrating power of neutrons1,2. SESANS yields directly the scattering length density correlation function, which facilitates visual data-analysis3.
With SESANS we investigated the fat droplet structure of different emulsion gels after storage at fixed temperature or after temperature cycling. Upon temperature-cycling the fat droplet clusters increase in size, next to the droplets themselves getting larger as well.
We present a basic model to show how SESANS exposes the processes occurring in the cartoon below: The emulsion is initially a dispersion of polydisperse spherical fat droplets. After cycling they can aggregate into larger droplets as indicated in the higher cartoon, or into network, as indicated in the lower cartoon. The difference in structure comes out clearly in the density correlation function (as measured by SESANS).

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P3.

PEARL: the new NL neutron diffractometer at Delft

Lambert van Eijck[1], Ad van Well[1], Katia Pappas[1]
[1]*Delft University of Technology, Faculty of Applied Sciences, Mekelweg 15, 2629 JB Delft, the Netherlands, l.vaneijck@tudelft.nl*

We are designing and constructing a neutron powder diffractometer for the Delft research reactor. The high penetration depth of neutrons enables to do in-situ diffraction experiments of the bulk of the investigated material. Neutron diffraction is especially sensitive to light elements like carbon, nitrogen and phosphor and can easily distinguish between neighbouring elements in the Periodic Table. Furthermore, by deuteration the exact location of hydrogen can be established. Using a new conceptual optimisation routine [1] the instrument is designed for medium resolution in *d*-spacing range $0.7<d<7$AA and will be competitive (neutron flux 10^5-10^6 n/cm^2/s on the sample position). We foresee to be operational for the Dutch user community in 2013.

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P4.

Futures study on food, medicines and health

Ellen S.M. Willemse
Stichting Toekomstbeeld der Techniek, Prinsessegracht 23, 2514 AP The Hague, The Netherlands,
willemse@stt.nl, www.stt.nl

Ultimate goal of the project is to raise awareness of the importance of long term future visions for policy making. More specifically, it aims to provide government, business, education and research organisations with insights in possible futures they may use for their long term strategic decision making. In this case in particular related to food, medicines and health.

The study is based on the assumption that the future is open but not void [1, 2]. It looks at possible future roles of food and medicines in the prevention of disease. Future in this case is the long term future, more than 20 years from now. The first phase of the study consisted of desk research, expert interviews and discussion meetings. It has resulted in a paper that describes relevant trends and uncertainties, with focus on the situation in The Netherlands.

Relevant trends are many, ranging from the increasing incidence of (multiple) chronic diseases [3] to the growing use of medicines [4] and ever broader possibilities for application of nanotechnology in food and medicines [5]. Uncertainties are also many and include food price instability [6], risks associated with new technologies [7], internet hypes and changing political agendas. Based on the trends and uncertainties found, imaginary news items have been drawn up to give an impression of what the future could be like.

In the second part of the study, the news items will be elaborated upon to create a more complete set of future images. These will subsequently be used to discuss possible societal consequences with stakeholders. Possible subjects for discussion sessions include ethical issues, business models, research models and legislation.

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P5.

Origin of wheat dough viscoelastic properties

Birgitta Schiedt[1], Andreas Baumann[2], Julia Mann[1], Beatrice Conde-Petit[2], Thomas Vilgis[1]
[1]Max-Planck-Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany, schiedt@mpip-mainz.mpg.de
[2]Bühler AG, Corporate Technology 9240 Uzwil, Switzerland

Wheat dough is a highly complex material possessing unique viscoelastic properties, which are largely due to gluten, specific wheat storage proteins forming a macropolymer upon hydration and kneading [1]. Into this continuous polymer matrix, a high amount of starch granules is embedded as filler particles. One may thus identify three contributions to the overall elastic properties of dough, resulting from starch/ starch, starch/ protein and protein/ protein interactions, each dominating at different length scales. They therefore can be separated by performing rheological measurements at different deformation levels. Their relative importance can also be probed via the use of starch/ gluten model systems in which the volume ratio of matrix and filler is varied.
However, the protein's contribution concerning the exact molecular structure of the gluten network including the molecular conformation of the proteins (β-sheets, amount of unfolding,...) as well as the relative importance of different types of covalent (disulphide bonds) or non-covalent (hydrogen bonds, hydrophobic interactions) bonds and entanglements is still not fully understood. Some more insight into the network's as well as the protein's structure can possibly be gained by the application of SANS.
Challenging questions that have so far been investigated by us via amplitude dependent oscillatory shear measurements on native wheat dough as well as on model doughs are the nature of changes going on in the gluten network during the course of mixing as well as by protein aggregation occurring during heat treatment of flour.

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P6.

Self-assembly of Fatty acids and Neutrons : from the determination of the structure in bulk solution and at the air/water interface to the understanding of the Mechanims of Stabilization of Smart Foams

A.L. Fameau[1], F. Cousin[2], A. Saint Jalmes[3], F. Boué[2], F. Ott[2], B. Novales[1], J.P. Douliez[1]
[1]Biopolymères Interactions Assemblages, INRA Nantes, rue de la Géraudière, 44316 Nantes, France
[2]Laboratoire Léon Brillouin, CEA Saclay, 91191Gif-sur-Yvette, France, fabrice.cousin@cea.fr
[3]Institut Physique de Rennes, Université Rennes 1, 35042 Rennes, France

We have recently shown that foams produced from aqueous solutions of fatty 12-hydroxy stearic acids have outstanding properties [1]. First, they have an unprecedented lifetime as they have revealed to be stable over months at ambient temperature. Second they stability can be triggered by an external parameter, the temperature, as foams can be destabilized in a span of a few minutes if the temperature is increased upon a given threshold. The stability is recovered if the temperature is decreased back down to the threshold. This is of particular interest in the context of green chemistry as the fatty acids can be extracted from agricultural resources
We will show how neutron scattering was fundamental to understand the mechanism of stabilization/destabilization properties of the foams. In a first time, SANS has enabled to determine that the fatty acids form multilamellar tubes with a length of several micrometers and melt into micelles at high temperature [2]. In a second time, specular Neutron Reflectivity experiments have shown that such multilamellar tubes adsorb at the air/water interface [3]. Finally, *in situ* SANS experiments performed directly within the foam have revealed that the tubes stay intact within the foam in the Plateau borders, which provide its exceptional stability to the foam and that the melting of tubes *within* the foam upon heating enables the temperature-triggered destabilization [1].

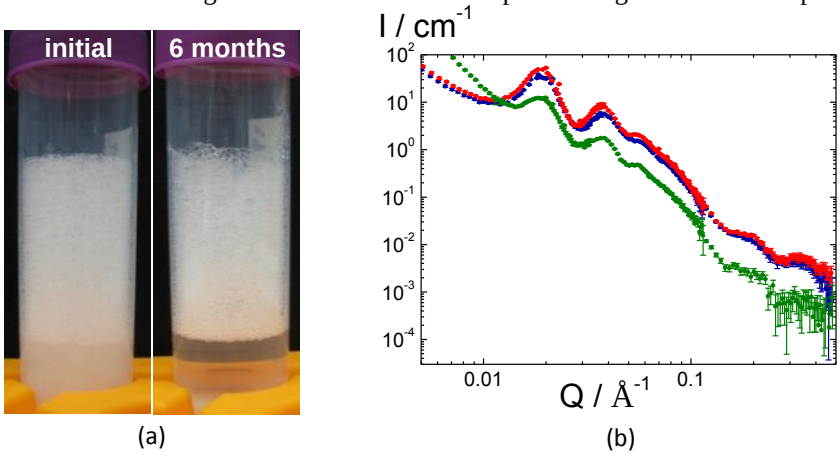

Figure 1: (a) Photos of foams taken at different times. (b) *In situ* SANS experiments in foams : data recorded for the foam (green), the stock solution (blue), and the drained solution (red).

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P7.

Intensified protein structuring for more sustainable food – Development of a continuous process

G. Krintiras[1], G. D. Stefanidis[1], A. I. Stankiewicz[1]
[1]*Delft University of Technology, Faculty of Mechanical, Maritime and Materials Engineering, Leeghwaterstraat 44, 2628 CA, Delft, The Netherlands,*
g.krintiras@tudelft.nl

Meat production is extremely inefficient with respect to use of land, water and raw materials. As consumers, we obtain only 10% of the necessary proteins that are initially present in the cereals fed to animals. Furthermore, to produce one kilogram of meat, two orders of magnitude more water is needed, compared to cereals.

A proven solution to that problem is the introduction of meat replacers to our daily diet. Meat replacers are products that contain high amounts of plant proteins like soya. Today's processes are not providing high quality meat replacers and that is due to no dedicated equipment for their production.

For this reason we are focusing of the development of a continuous process that is dedicated to the production of meat replacers. The first of its series, a shear cell developed in the University of Wageningen and in the group of Food Structuring. The device is comprised by a bottom and top cone and in between the two cone plates there is sufficient area to place the protein dispersion. This area is called the shearing zone [1].

By means of rotation of the bottom cone the homogeneous dispersion resting in the shearing zone is being subjected to a continuous shear flow. The shear flow will align the proteins to the direction of the flow and by using an enzymatic cross-linker the protein dispersion is solidified. The result is a fibrous meat-like structure.

The overall goal of this project is to develop and deliver a continuous process for the production of finely fibrous/structured, plant-based protein food products, meant as sustainable replacers for meat. Achieving this goal is not trivial, as the quality of the shear flow field is essential to the generation of the right textural properties. Imposing flow for transportation of the material through the equipment may well inhibit the formation of a good structure.

The shear cell (batch system) is the starting point towards the development of a continuous process. The new device is a Couette cell based on a two coaxial cylinder configuration with the inner cylinder rotating. Rotation induces a simple shear flow in the protein dispersion resulting in the alignment of the proteins followed by a solidification stage.

In this work we will present the influence of the operating conditions (e.g. rotational speed, temperature, process time) and the structural characteristics of the couette cell (e.g. device geometry, wall surface roughness, shearing zone thickness) on the product quality (e.g. water holding content, fine fibers) and the structure formation mechanisms.

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P8.

Soybean oleosomes

Gustav Waschatko[1], Ann Junghans[1], Sania Maurer[1], Birgitta Schiedt[1], Thomas A. Vilgis[1]
[1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany, waschatko@mpip-mainz.mpg.de

Soy Foods have rising popularities in European countries, due to ecological or health benefits, lactose intolerance or allergies against milk proteins.
Traditional soy meals like soymilk, tofu or yuba contain small oil droplets, which are known for a long time in botany, where they are called oleosomes or oil bodies. [1] Their micelle like structure is filled with triacylglycerides, surrounded by a monolayer of phospholipids and unique umbrella shaped proteins called oleosins, which are sticking hairpin like in the oil phase. The anchor contains the longest hydrophobic amino acid sequence known to date (about 70 amino acids in the middle of the sequence). The exterior hydrophilic part of the oleosomes (N- and C-terminal domains) shields the phospholipids and is, because of its pH-dependend charge, responsible for the extraordinary stability of oleosomes against coalescence and creaming.
However oleosomes can burst under certain conditions (dry heat and interfaces) resulting in a system containing free oleosins, which might undergo conformational changes as reaction to rupture. Neutron scattering can be an appropriate method to investigate whether this leads to oleosin aggregates or they are concerning the spatial arrangement or the secondary structure of the protein.

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P9.

Non-triglyceride structuring of edible oils and emulsions

Ruud den Adel, Arjen Bot, Eli Roijers and Echard Flöter
Unilever Research & Development, Vlaardingen, The Netherlands

The structure of oil-continuous products, such as margarine or butter, is based on a network of small crystallites of triglycerides (also known as triacylglycerols or TAGs). Low molecular weight structuring agents that can serve as an alternative to crystallising triglycerides in edible oils have raised considerable interest in recent years. The requirement that potential structurants should at least hold the promise to be allowed in food applications is a severe limitation. Nevertheless, several systems have been identified [1], amongst which the class of γ-oryzanol + sterol organogelators is the most intriguing representative [2].
Small-angle X-ray scattering (SAXS) studies demonstrated that mixtures of β-sitosterol and γ-oryzanol form tubules in triglyceride oil with a diameter of 7.2±0.1 nm and a wall thickness of 0.8±0.2 nm [3]. Mixtures of β-sitosterol and γ-oryzanol in emulsions at 16% total sterols show scattering data containing reflections of mainly β-sitosterol mono-hydrate crystals. Evidence for the formation of tubules is not found in these emulsion systems, indicating that transitions from anhydrous and hemi-hydrate to monohydrate formation prevent this self-assembled supra-molecular ordering. Intermolecular hydrogen bonding is playing an important role in the formation of the tubules and hydration of sterols might exclude the appearance of this bonding [4].
The stability of the tubules in the presence of water is critical for the applicability of these organogelling systems in the structuring of food emulsions. A decrease of the water activity by salt suppresses the hydration of sterols and promotes tubule formation.

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P10.

Neutrons for Mars

Marika Kok
Mars Chocolate, Taylorweg 5, 5466 AE Veghel, the Netherlands, marika.kok@effem.com

Headquartered in Mount Olive, New Jersey, U.S., Mars Chocolate is one of the world's leading chocolate manufacturers and employs more than 13,000 people across 110 sites worldwide. Our iconic brands include M&M'S®, SNICKERS®, DOVE®, GALAXY®, MARS®, MILKY WAY® and TWIX®.

Some of the main components in our chocolate products are chocolate, caramel and nougat.
Proteins play an important role in creating the desired taste and texture in all these components.

I would like to have your input on the following questions:

- **Is it possible to use neutron scattering to increase understanding of the structure of our components?**
- **Is it possible to discriminate between different proteins?**

List of Presenting Authors

List of Participants

Name	Email	Country	Affiliation
Monique Axelos	monique.axelos@nantes.inra.fr	France	INRA, Biopolymères Interactions Assemblages
Menno Blaauw	M.Blaauw@tudelft.nl	Netherlands	Delft University of Technology
Sreenath Bolisetty	sreenath.bolisetty@agrl.ethz.ch	Switzerland	ETH, Zurich
Arjen Bot	Arjen.Bot@unilever.com	Netherlands	Unilever Research and Development
Wim Bouwman	w.g.bouwman@tudelft.nl	Netherlands	Delft University of Technology
Fabrice Cousin	fabrice.cousin@cea.fr	France	Laboratoire Léon Brillouin
Robert Dalgliesh	robert.dalgliesh@stfc.ac.uk	United Kingdom	ISIS
Ruud den Adel	ruud-den.adel@unilever.com	Netherlands	Unilever R&D Vlaardingen
Chris Duif	C.P.Duif@tudelft.nl	Netherlands	Delft University of Technology
Marcia English	marcia.english@dal.ca	Canada	Dalhousie University
Timo Faber	timo.faber@frieslandcampina.com	Netherlands	FrieslandCampina Research
Peter Fischer	peter.fischer@ilw.agrl.ethz.ch	Switzerland	ETH Zurich, Institute of Food Nutrition and Health
Richard Frazier	r.a.frazier@reading.ac.uk	United Kingdom	University of Reading
Jan Groenewold	jg@denk-werk.nl	Netherlands	Cook & Chemist
Thomas Gutberlet	thomas.gutberlet@helmholtz-berlin.de	Germany	Helmholtz-Zentrum Berlin GmbH
Vasyl Haramus	vasyl.haramus@hzg.de	Germany	Helmholtz-Zentrum Geesthacht
Richard Ipsen	ri@life.ku.dk	Denmark	University of Copenhagen
Andrew Jackson	andrew.jackson@esss.se	Sweden	European Spallation Source
Sheila Khodadadi	sheila.khodadadi@nist.gov	United States	National Institute of Standards and Technology
Marika Kok	marika.kok@effem.com	Netherlands	Mars chocolate
Nico Kos	N.J.kos@nwo.nl	Netherlands	Netherlands Organisation for Scientific Research
George Krintiras	g.krintiras@tudelft.nl	Netherlands	TU Delft
Frederik Lech	frederik.lech@wur.nl	Netherlands	Wageningen University
Martin Leser	Martin.Leser@rd.nestle.com	United States	Nestle Research, PTC, Marysville
Rik Linssen	R.J.Linssen@tudelft.nl	Netherlands	Delft University of Technology
Camille Loupiac	camille.loupiac@u-bourgogne.fr	France	Equipe EMMA, AgroSup Dijon, Université de Bourgogne
Alan Mackie	alan.mackie@ifr.ac.uk	United Kingdom	Institute of Food Research, Norwich
Eke Marien	jg@denk-werk.nl	Netherlands	Cook & Chemist
Sania Maurer	maurer@mpip-mainz.mpg.de	Germany	Max-Planck-Institute for Polymer Research
Dieter Middendorf	d.middendorf@bioneutron.org.uk	United Kingdom	Clarendon Laboratory, University of Oxford
Maaike Nieuwland	maaike.nieuwland@tno.nl	Netherlands	TIFN
Tommy Nylander	tommy.nylander@fkem1.lu.se	Sweden	Lund University
Annika Olsson	Annika.Olsson@plog.lth.se	Sweden	Lund University
Sofie Ossowski	sofie.ossowski@esss.se	Sweden	European Spallation Source
Catherine Pappas	C.Pappas@tudelft.nl	Netherlands	Delft University of Technology
Allan Paulson	allan.paulson@dal.ca	Canada	Dalhousie University
Marie Paulsson	marie.paulsson@food.lth.se	Sweden	Lund University
Jeroen Plomp	J.Plomp@tudelft.nl	netherlands	Delft University of Technology
Maria Antonietta Ricci	riccim@fis.uniroma3.it	Italy	University of Rome
Sarah Rogers	sarah.rogers@stfc.ac.uk	United Kingdom	ISIS-STFC
Birgitta Schiedt	schiedt@mpip-mainz.mpg.de	Germany	Max-Planck-Institute for Polymer Research
Paul Sokol	pesokol@indiana.edu	United States	Indiana University
Markus Strobl	markus.strobl@esss.se	Sweden	European Spallation Source
Jan Swenson	jan.swenson@chalmers.se	Sweden	Chalmers University of Technology, Göteborg
Isabella van Damme	isabella.van.damme@effem.com	United Kingdom	Mars Chocolate
Atze Jan van der Goot	Atzejan.vanderGoot@wur.nl	Netherlands	Wageningen University
Erik van der Linden	Erik.vanderLinden@wur.nl	Netherlands	Wageningen University
John van Duynhoven	john-van.duynhoven@unilever.com	Netherlands	Unilever R&D
Lambert van Eijck	L.vanEijck@tudelft.nl	Netherlands	Delft University of Technology
Kitty van Gruijthuijsen	kitty.vangruijthuijsen@unifr.ch	Switzerland	University of Fribourg
Ad van Well	A.A.vanWell@tudelft.nl	Netherlands	Delft University of Technology
Thomas Vilgis	vilgis@mpip-mainz.mpg.de	Germany	Max-Planck-Institute for Polymer Research
Dirk Visser	d.visser@lboro.ac.uk	United States	Loughborough University
Hanna Wacklin	hanna.wacklin@esss.se	Sweden	European Spallation Source

Gustav Waschatko	waschatko@mpip-mainz.mpg.de	Germany	Max Planck Institute for Polymer Research
John Webster	john.webster@stfc.ac.uk	United Kingdom	STFC ISIS facility
Ellen Willemse	willemse@stt.nl	Netherlands	Stichting Toekomstbeeld der Techniek