IV. Comité scientifique et instrumental

Intervention de I. Anderson, président du CSI

Workshop “Reflection on the unique role of neutrons”

The Laboratoire Léon Brillouin
Saclay the 26-27th September 2016

Membres du comités

Roger Pynn
Kurt Clausen
Ian Anderson
Arnaud Desmedt
Christiane Alba-Simionesco
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Robert McGreevy
Virginie Simonet

Personnalités scientifiques invitées

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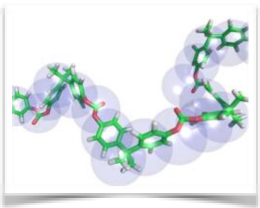
	Speaker	Theme	Scribes
Monday 26 September			
13:00 - 13:15	C. Alba-Simionesco/I.Anderson	Welcome and Context	
13:15 - 14:15	Jean Marie Tarascon	Electrochemistry, batteries	JM Zanotti/P. Judeintsein
14:15 - 15:15	Loic Barré	Petroleum industry	J. Jestin/ L. Lay-Theng
15:15 - 16:15	Liliane Léger	Soft Matter	A.Chenevière/C. Le Cœur
16:15-16:30	**Pause**		
16:30 - 17:30	François Boué	Food science	F Cousin/ C.Loupiac
17:30 - 18:30	Michael Fitzpatrick	Engineering	MH Mathon/F.Ott
18:30 - 19:30	Jean Daillant	What synchrotrons can't do	F.Porcher/ A.Bataille
20h30	**Dîner « Le Living » Massy**		
Tuesday 27 September			
08:30 - 09:30	Sanat Kumar	Materials Science	F. Cousin/J. Jestin
09:30 - 10:30	Bruno Robert	Biology	S. Longeville/S. Combet
10:30 - 11:30	Alan Tenant	Hard Matter	Y. Sidis/ J-M. Mignot
11:30 - 12:30	Christian Pfleiderer	Magnetism	I. Mirebeau/G. Chaboussant
12:30 - 13:30	**All - Buffet Lunch with LLB staff**		
13:30 - 14:30	**Committee Meeeting**		

Neutrons 101

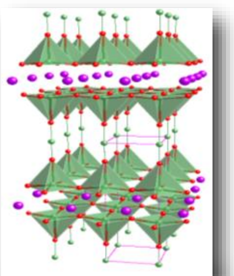
- The reason we use neutrons hasn’t changed
  - Length and time scales
  - Light atoms/contrast variation
  - Magnetism
  - Penetration
  - Precision

But the range of science has

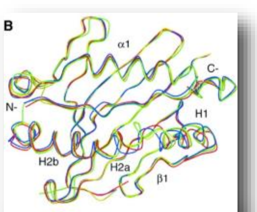
H/D Contrast in Polymers



Novel Superconductors

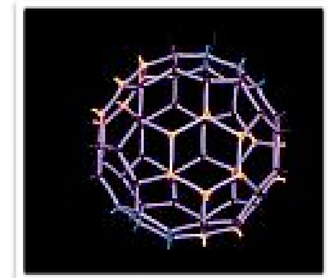


H/D Contrast in Proteins

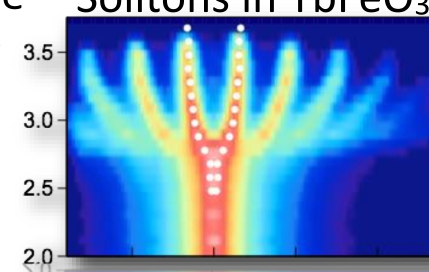


Protein/Polymer Structure
Phonons
Crystal/Chemical Structure
Liquids and Amorphous
Thin films structure
Magnons
Localised Excitations
Chemical Spectroscopy
Proton tunneling
Nanoscience
Slow dynamics
Magnetic Structure
Protein/proton dynamics

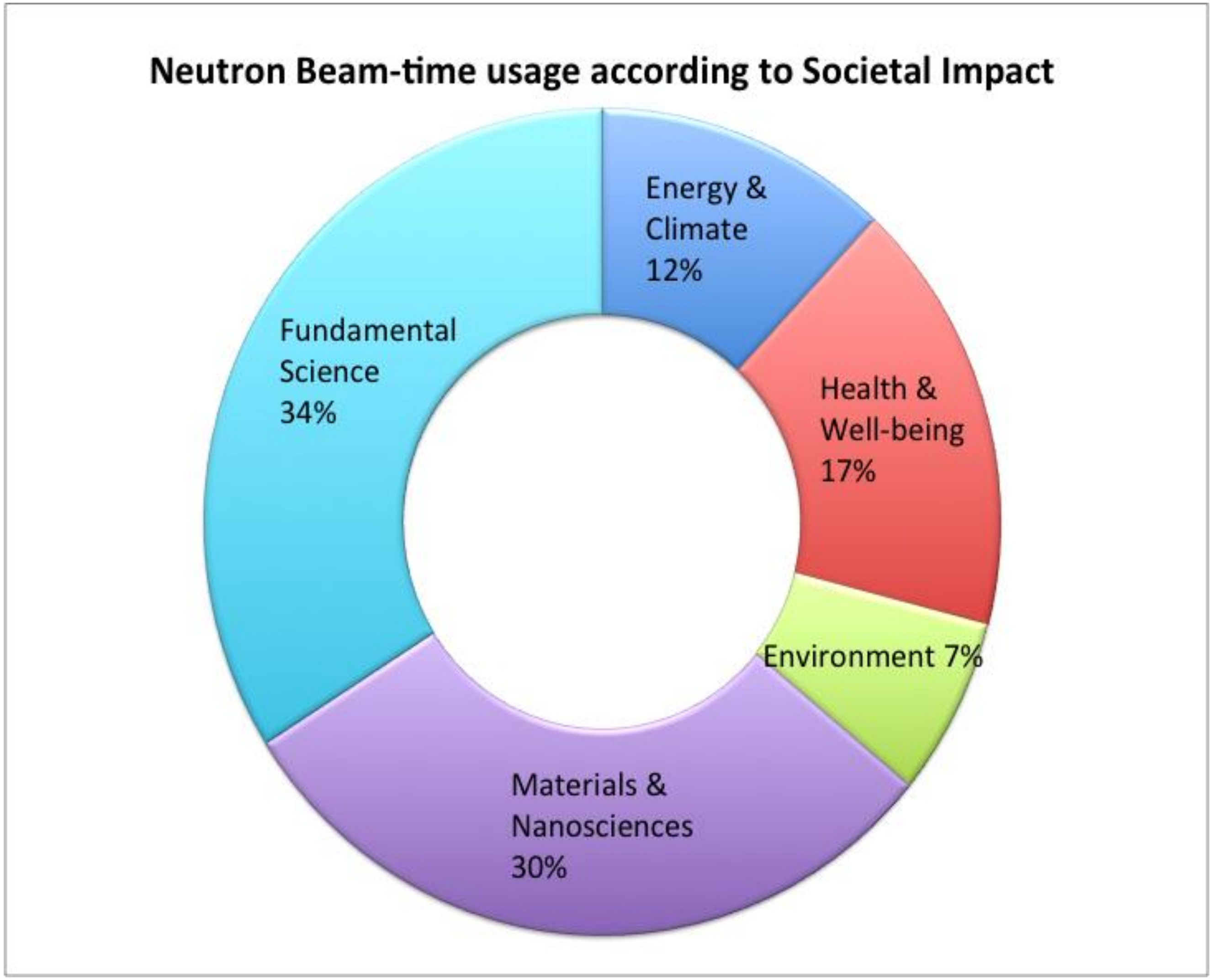
Fluerines Structure/Dynamics

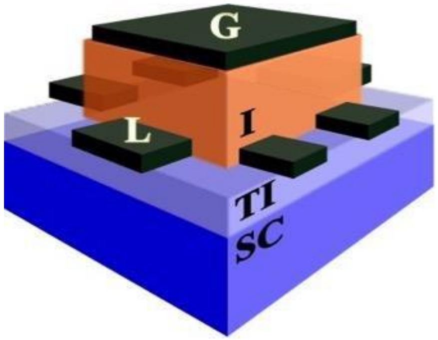


Solitons in $TbFeO_3$

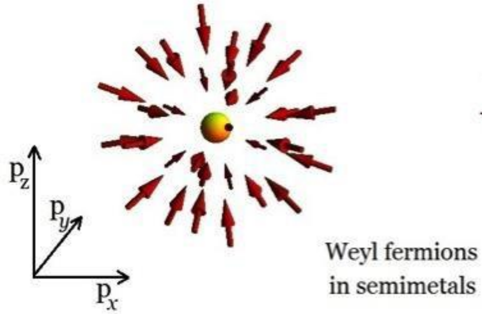


And the impact is wide ranging

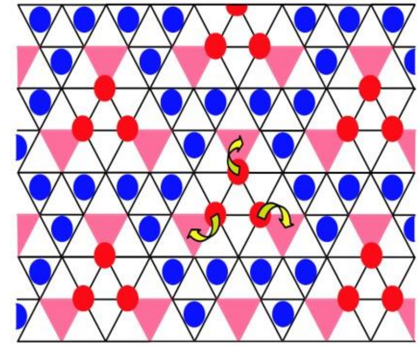




Quantum devices

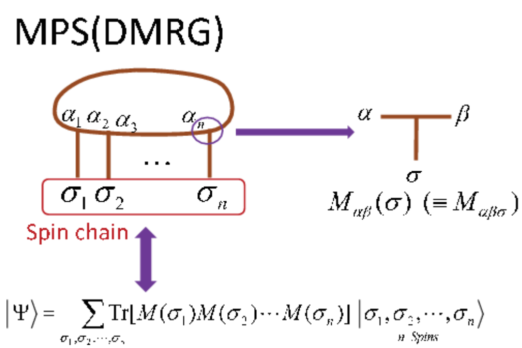


Topological materials

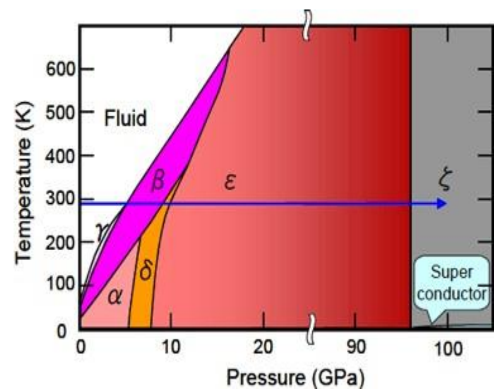


Mesoscale effects

Quantum Materials

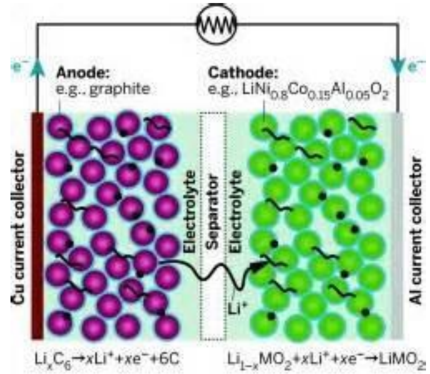


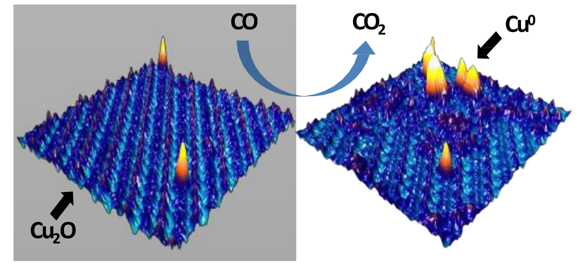
Theory and simulation



Extreme conditions

OAK RIDGE
National Laboratory
Shull Wollan Center
a Joint Institute for Neutron Sciences



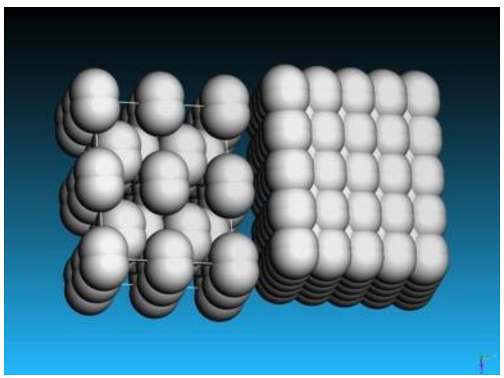


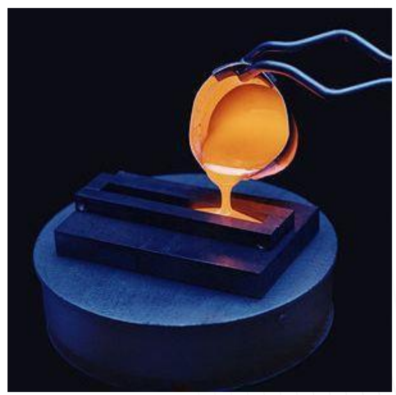
Infrastructure stewardship

Future energy and transport

Catalysis and chemical reactions

Materials Synthesis and Performance





Materials under extreme conditions

Glasses, liquids, defects and disorder

Advanced manufacturing

Quantum electronics - Functionalizing Topological Insulators

Neutrons see the interfaces

Scientific Achievement

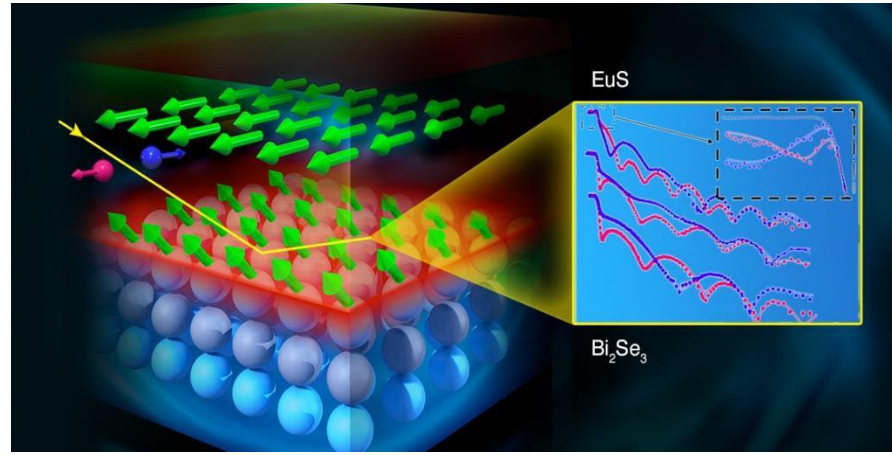
Using polarized neutron reflectometry (PNR), researchers have discovered magnetic moments in hybrid topological insulator (TI) materials at room temperature, hundreds of degrees warmer than the sub-zero temperature where the properties are expected to occur.

Significance and Impact

TIs are insulating materials *in bulk* and display conducting *surface states* protected by time-reversal symmetry, wherein electron spins are locked to their momentum. Inducing ferromagnetic surface states in TIs are thought to enable the emergence of exotic phenomena such as interfacial magneto-electric coupling, and Majorana fermions. This discovery promises new opportunities for next-generation electronic and spintronic devices such as improved transistors and quantum computing technologies.

Research Details

- The ferromagnetic state was directly observed in the top two quintuple layers (QL, where 1 QL ≈ 0.96 nm) of Bi_2Se_3 near the TI-FMI interface up to temperatures higher than 300 kelvins.
- PNR provides characterization of the depth profiles of the elemental nuclear density, the magnetization density, and is also particularly element-sensitive to Eu via the absorption density profile. This affords a very precise disentanglement of the intrinsic ferromagnetism of EuS, from its interfacial magnetism and the induced magnetization in Bi_2Se_3.



Schematic of the PNR experimental set up for Bi_2Se_3EuS bilayer films and measured and fitted (solid lines) reflectivity curves for two neutron spin-polarization. The inset is an expanded view of the reflectivity below its critical edge that is sensitive to the distribution of the Eu ions due to the absorption cross section and the magnetic moment.

F. Katmis, V. Lauter, F. Nogueira, B. Assaf, M. Jamer, P. Wei, B. Satpati, J. Freeland, I. Eremin, D. Heiman, P. Jarillo-Herrero, and J. Moodera, *Nature*, **2016.**

Work was performed at ORNL's SNS Magnetism Reflectometer instrument, BL-4A, a DOE Office of Science User Facility.

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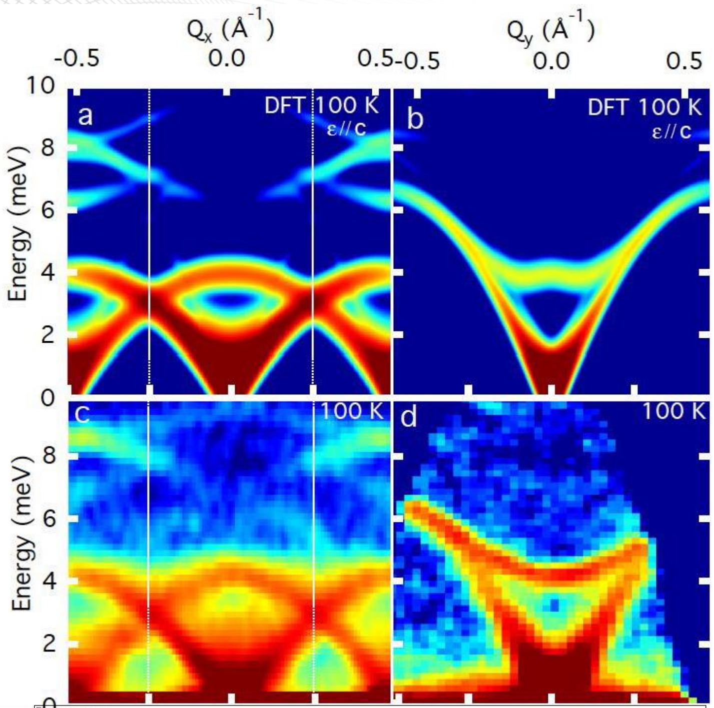
Joint Institute for Neutron Sciences

Thermoelectrics – neutrons see transport

Electronic Orbitals Drive Phonon Anharmonicity of SnSe



a,b: DFT calculations of phonon S(Q,E) for SnSe along [H02] and [0K2]. **c,d:** INS data measured on CNCS at 100K.

C. Li*, J. Hong*, A May, D. Bansal, S. Chi, T. Hong, G. Ehlers, and O. Delaire. *Nature Physics.* (2015).

Scientific Achievement

The origin of the anisotropic, ultralow thermal conductivity in high-efficiency thermoelectric SnSe was explained with neutron scattering and simulations.

Significance and Impact

Understanding the chemical origin of the anharmonic phonon potential will enable the design of highly efficient thermoelectrics.

Research Details

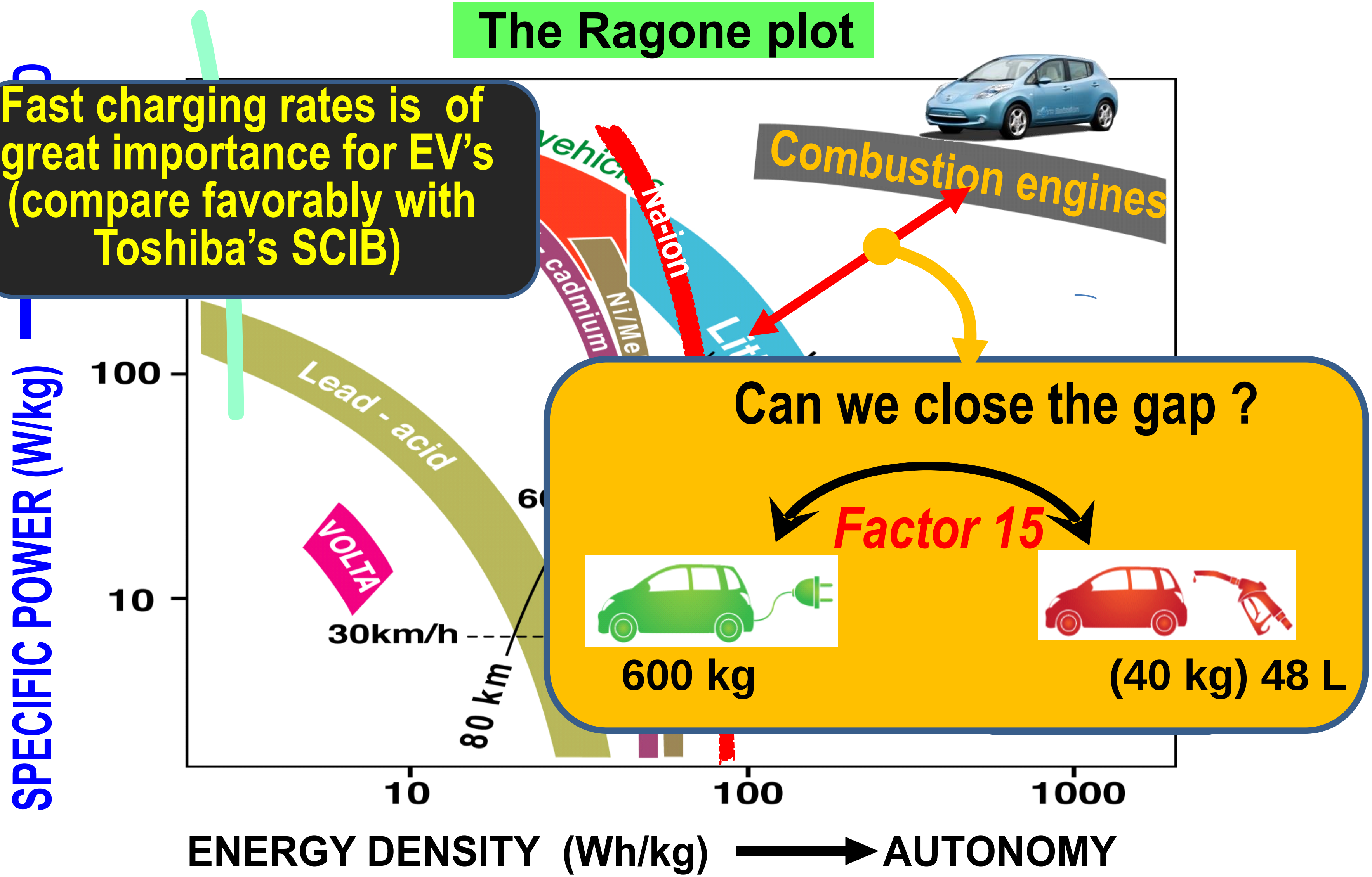
- S phonon dispersion and intensities were mapped on single-crystals of SnSe with instruments at SNS and HFIR, and computed with DFT.
- The instability of resonantly-bonded *p*-orbitals couples with Sn 5*s* lone pairs, causing anharmonicity and the structural distortion at 800K.

Work was performed at ORNL's Spallation Neutron Source and High Flux Isotope Reactor, which are DOE user facilities. Simulations used resources of the Oak Ridge Leadership Computing Facility, also a DOE user facility.

OAK RIDGE National Laboratory

Shull Wollan Center a Joint Institute for Neutron Sciences

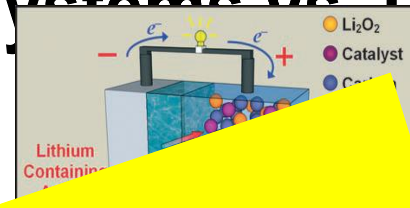
Battery technologies: Power rate comparison



Why so much excitement ? What are they ?
metal air systems vs. Li-ion

Li-S

Li-air



Battery	Cell Voltage	Theoreti...
Toda... $½C_6Li$...		
Zn/air $Zn + ½O_2$...		
Li/S $2Li + S = Li_2$...	2.2	2567
Li/air (non-aqueous) $2Li + O_2 = Li_2O_2$	3.0	3505

What is the reality ?

Still a few decades to have commercial Li-air cells.

The Li-S will reach the market place sooner

Bruce PG, Freunberger SA, Hardwick LJ, Tarascon JM, Nature Materials, 11, 19-29, 2012.

Conclusions-Messages

- **Humungous progresses in developing characterization techniques**
  - → Competition is fierce
  - → Our old models of running large instruments must be revised to satisfy users.
  - → X-ray synchrotrons (Use of the 11BM service: Mail-in)
  - → Neutrons is becoming similar with two programs at Oakridge NOMAD and POWGE

"Adequate balance between pushing the frontiers of Neutron and satisfying today's researchers needs"

- **In-operando Neutrons.**
  (Need time and lines dedicated to battery research, PSI,Berlin ,,,)

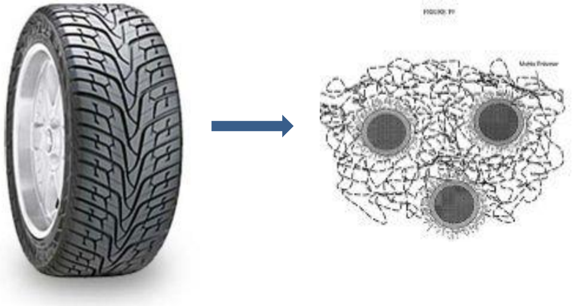
- **In short, writing proposal should not be the only way to have access to neutron facilities.**

Soft Matter and Neutrons

- Neutral Polymers and Polyelectrolytes in bulk and at interfaces

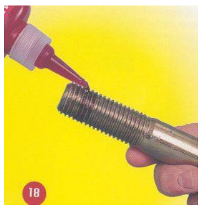
  -> Adhesion, Friction and Mechanical Reinforcement

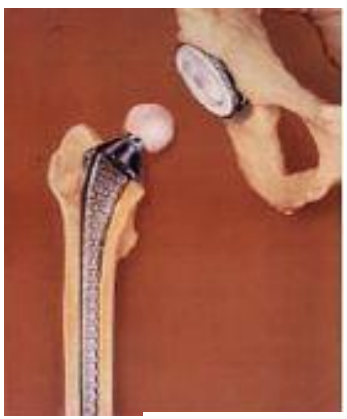
- Why?
  - The internal structure of a surface attached polymer layer rules its ability to interpenetrate with a bulk polymer
  - This will rule **adhesion, friction**, and more generally all mechanisms **of stress transmission** at an interface
  - Manipulating this internal structure allows one to adjust **adhesion** and **friction** and **mechanical reinforcement** by micro- or nano-particles

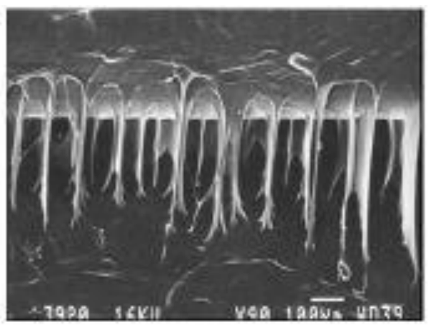


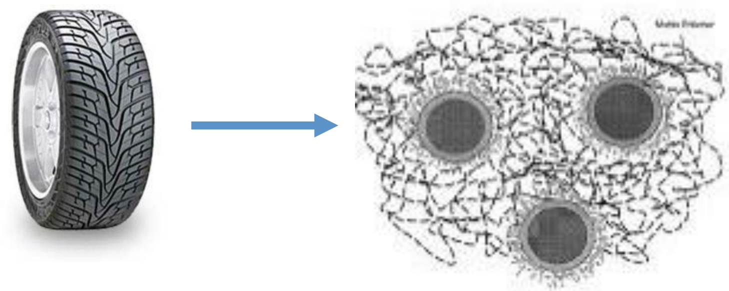
Why is it important?

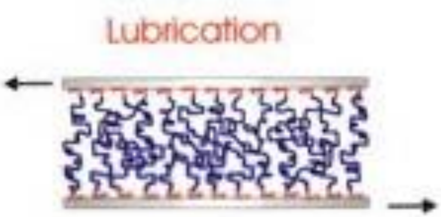
Polymer chains attached to a surface: An every day situation

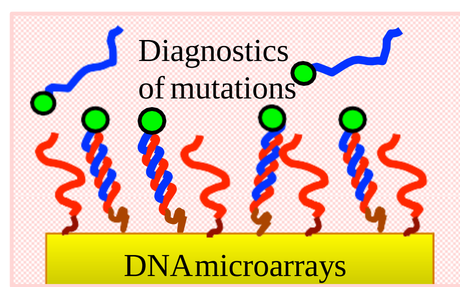


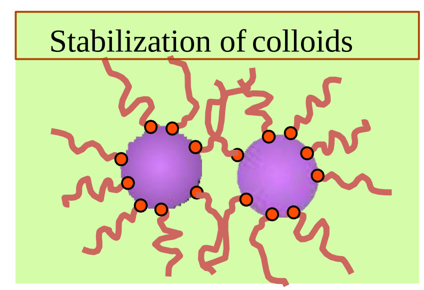






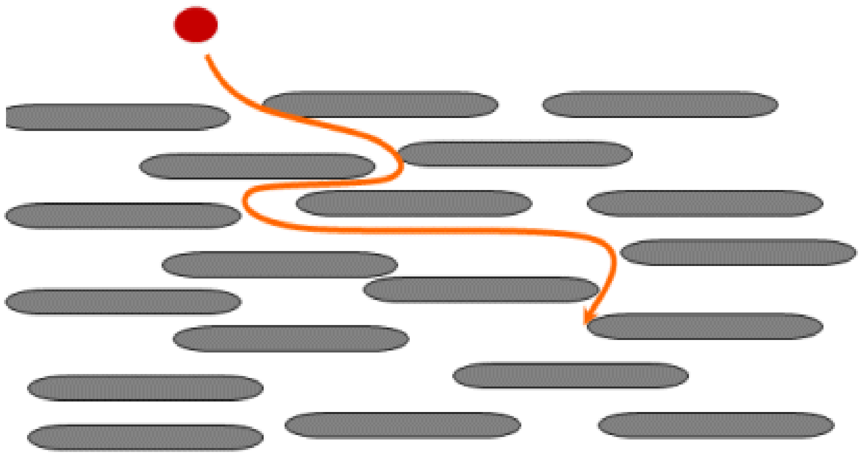






Selective Gas Separation Membranes
- Sanat Kumar

$$J_s = \bar{P}(p_h - p_l)/\delta$$



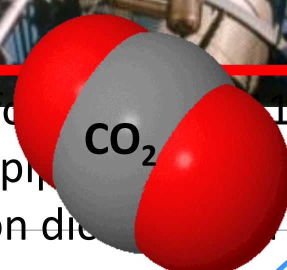
$$P = D \times S$$

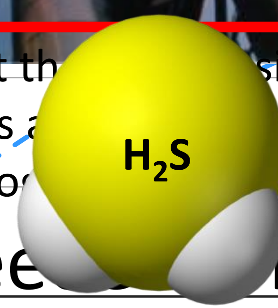
Diffusion Coefficient

Solubility

$$\alpha_{ij} = \frac{P_i}{P_j} = \frac{D_i S_i}{D_j S_j}$$

Motivation





The corrosion that was f… 103 at th… site was likely caused by a combination within the pi… robes a… taminants as moisture, chlorides, oxygen, carbon di… hydro…

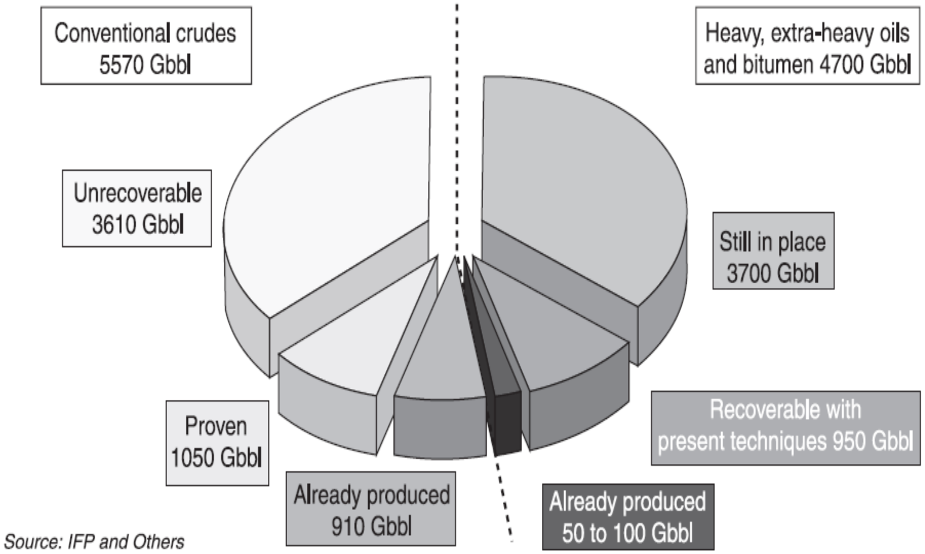
New Technology is nee… r significant

Natural Gas Processing

United States Energy Information Association Annual Energy outlook 2013, 2014,2015

National Transportation Safety Board Pipeline Accident Report NTSB/PAR-03/01.

HEAVY OILS : AN IMPORTANT RESOURCE FOR THE RENEWAL OF OIL RESERVES



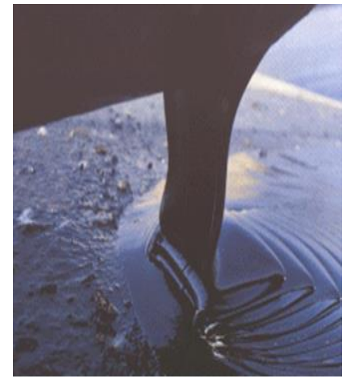
Oil & Gas Science and Technology – Rev. IFP, Vol. 59 (2004)

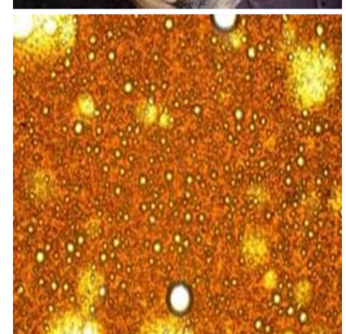
- Half of proved reserves
- Petroleum Industry : need to
  - produce
  - transport
  - refine
- Most of the issues are related to the heaviest and most polar fraction of crude oil : the Asphaltenes

INDUSTRIAL ISSUES RELATED TO HEAVY FRACTIONS

RESPONSIBLE OIL AND GAS

- **Bulk Properties**
  - Density
  - Blackness
  - Viscosities
- **Stability / deposition**
  - Phase separation
  - Transport
  - (In)ability to diffuse in porous media
  - Clogging (wellbore vicinity, catalyst, pipes..)
- **Surface properties**
  - Emulsions Stability
  - Affect rock wettability
  - Inhibit hydrate plugs





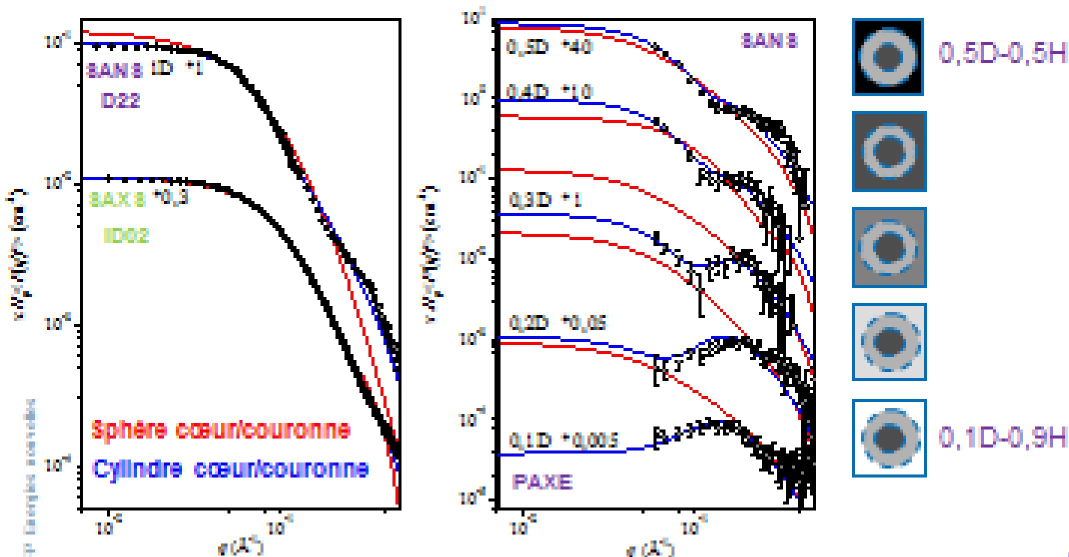
Properties

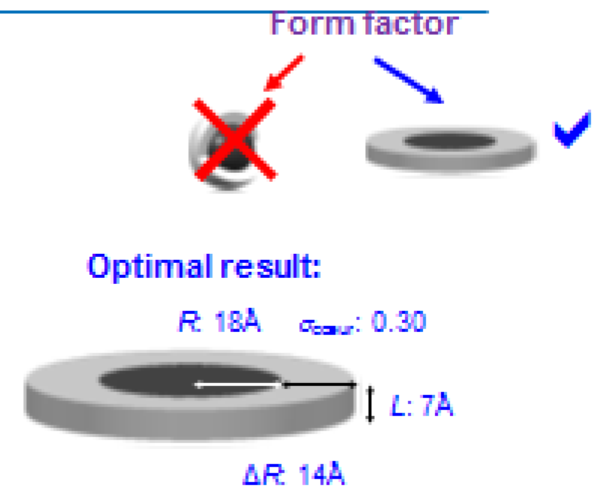
S.A.X/n/L.S

X/n/L Reflectivity

Structure

Small scale structure



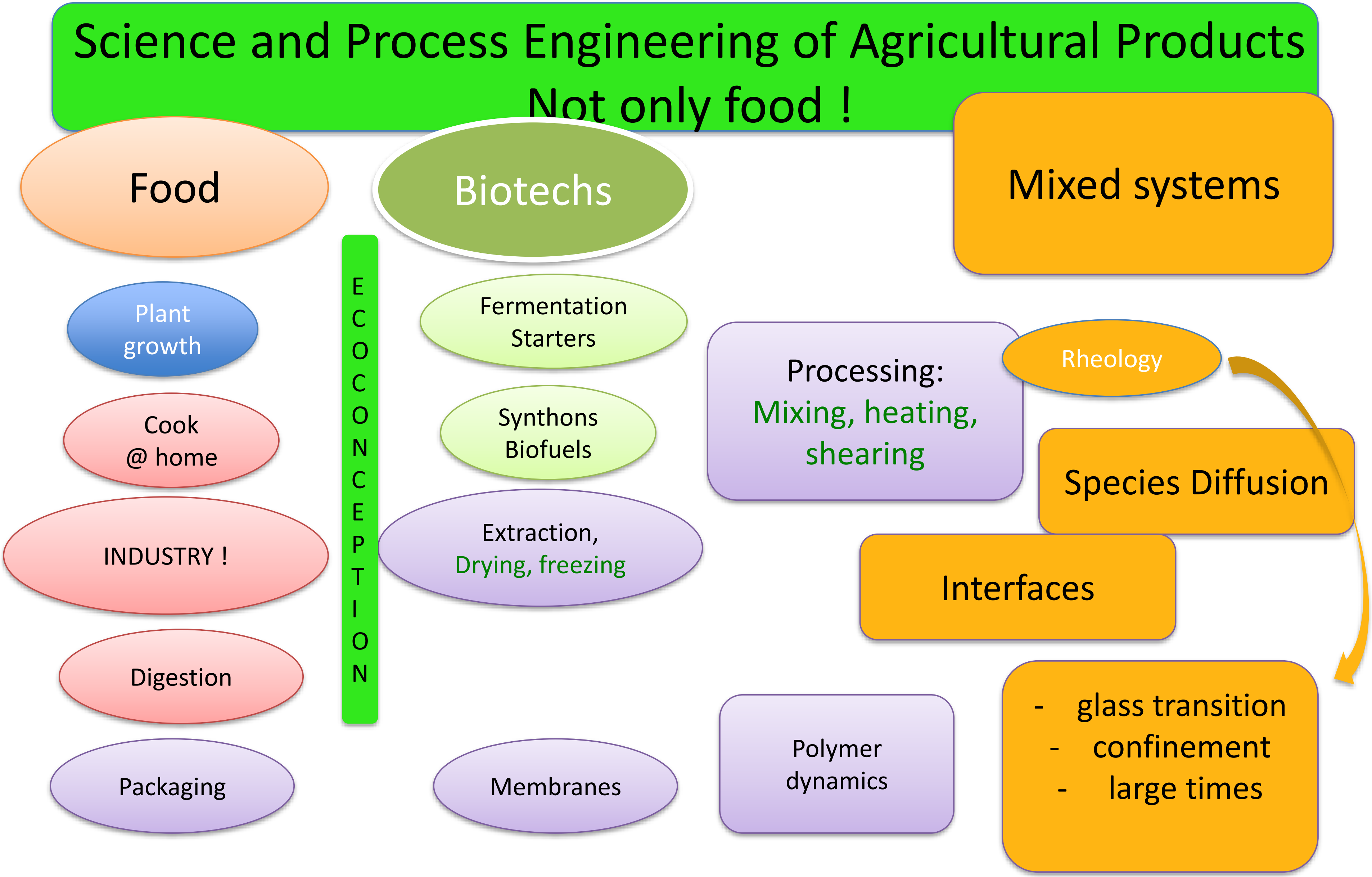


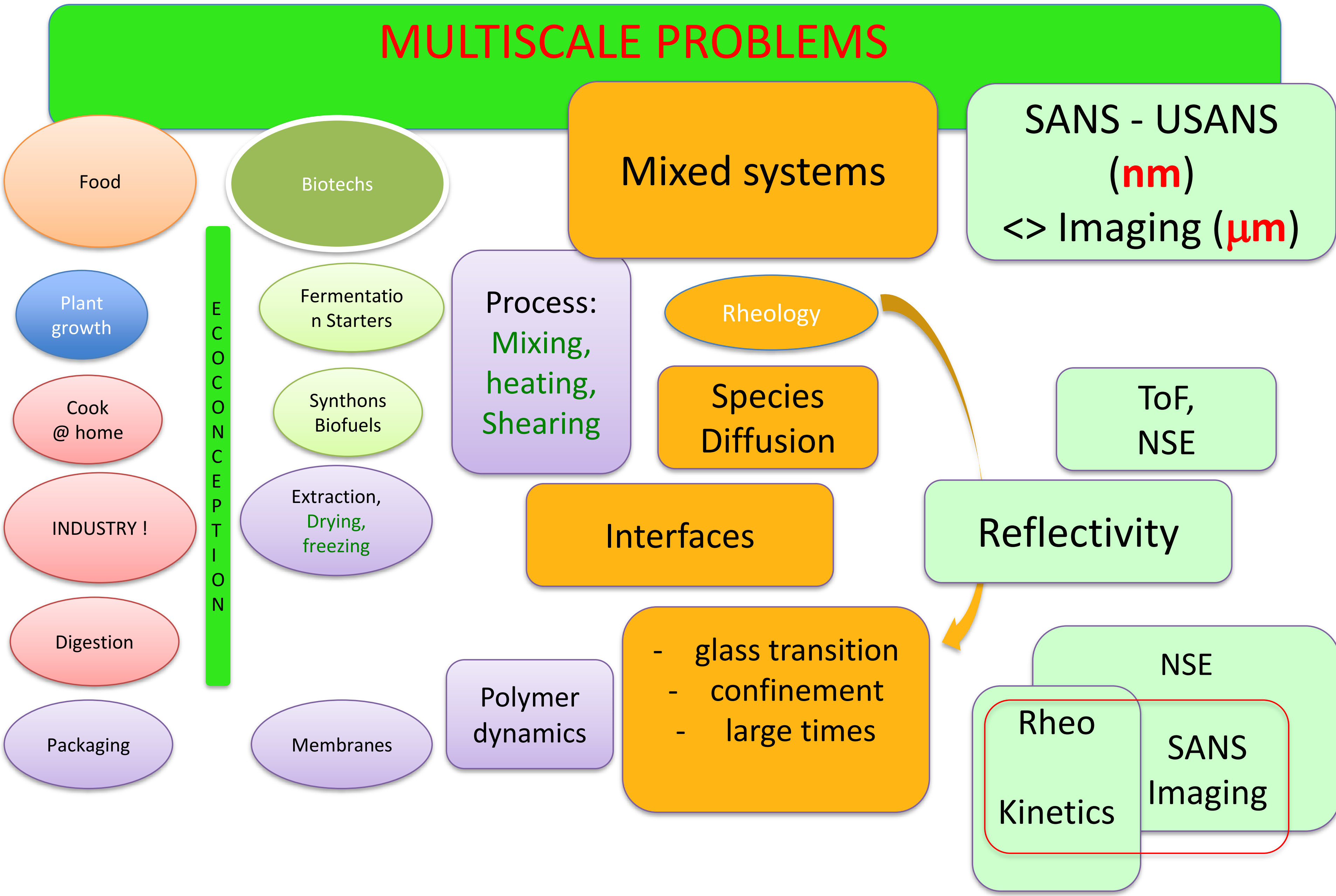
⇨ Mass : 10 000 g/mol

⇨ Diffusion Coefficient : $(1 \pm 0{,}2) \times 10^{-10}$ m²/s

Eyssautier et col. J. Phys. Chem. B 2011

Sample environment and size are critical


Science and Process Engineering of Agricultural Products
Not only food !
Food
Biotechs
Mixed systems
Plant growth
Cook @ home
INDUSTRY !
Digestion
Packaging
ECOCONCEPTION
Fermentation Starters
Synthons Biofuels
Extraction, Drying, freezing
Membranes
Processing: Mixing, heating, shearing
Rheology
Species Diffusion
Interfaces
Polymer dynamics
- glass transition
- confinement
- large times


MULTISCALE PROBLEMS
Food
Biotechs
Mixed systems
SANS - USANS
(nm)
<> Imaging (µm)
Plant growth
ECOCONCEPTION
Fermentation Starters
Process:
Mixing,
heating,
Shearing
Rheology
Cook @ home
Synthons Biofuels
Species Diffusion
ToF, NSE
INDUSTRY !
Extraction,
Drying,
freezing
Interfaces
Reflectivity
Digestion
- glass transition
- confinement
- large times
NSE
Rheo
Kinetics
SANS
Imaging
Packaging
Membranes
Polymer dynamics

Various components

- Polysaccharides : starch, cellulose
- Pectins, xyloglucans, many others (xanthan gum)!
- Proteins (structure: meat, plant; function: enzymes, bioactive peptides)
- Lipids (food, cell membranes)
- Smaller molecules : tanins, pesticides
- Nanoparticles!

Size Matters!!!

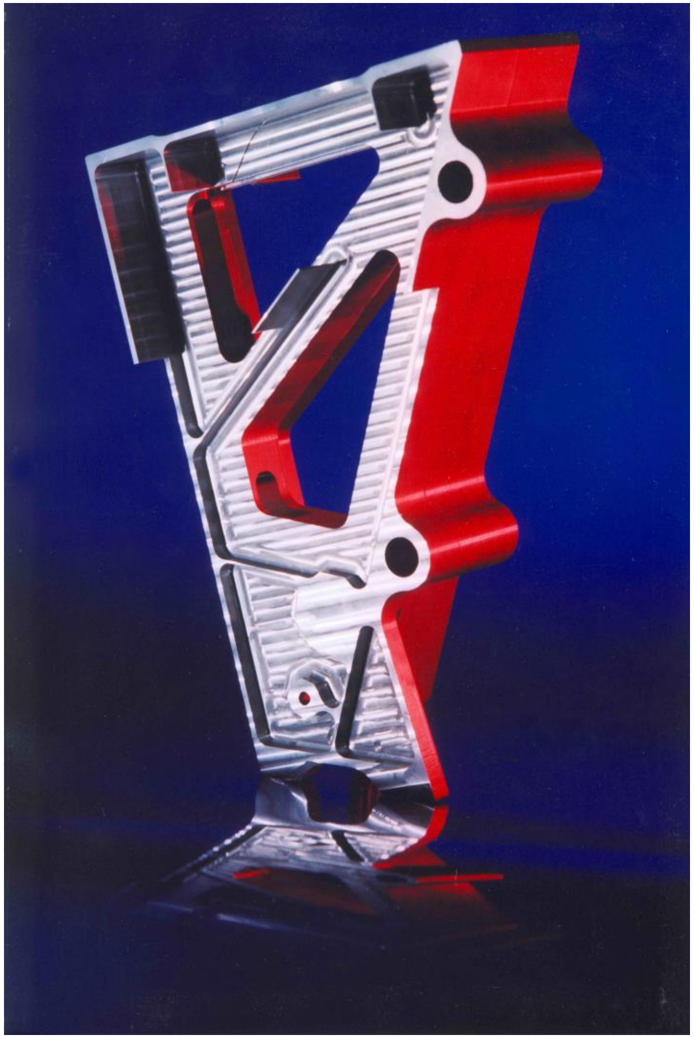
- Polysaccharides : starch, cellulose
- pectins, xyloglucans, many others (xanthan gum)!
- Proteins (structure :meat, plant,
- function : enzymes, bioactive peptides)
- Lipids (food, cell membranes)
- Smaller molecules : tanins, pesticides
- Nanoparticles!

- All sizes
- All mixed
- All interact !

- Same as soft matter!
- < > « noble » biology : more sample (quantities)!

Residual stress measurement

Technique often depends on the value of the problem, or, more accurately, the budget available to solve the problem



- £10^2
  - Can I stop using this production step that costs £1 per part?
- £10^3
  - I have a new problem with components failing a residual stress acceptance criterion
- £10^4
  - I have a critical residual stress problem on a product development path

Coventry University

Residual stress measurement

Technique often depends on the value of the problem, or, more accurately, the budget available to solve the problem

- £10^5
  - I have a major development programme where the residual stresses are critical

but the value could be.....

- £10^7 - 10^8
  - If I can't prove it's safe this power plant will be closed down / aircraft will be grounded or development stalled

Coventry University

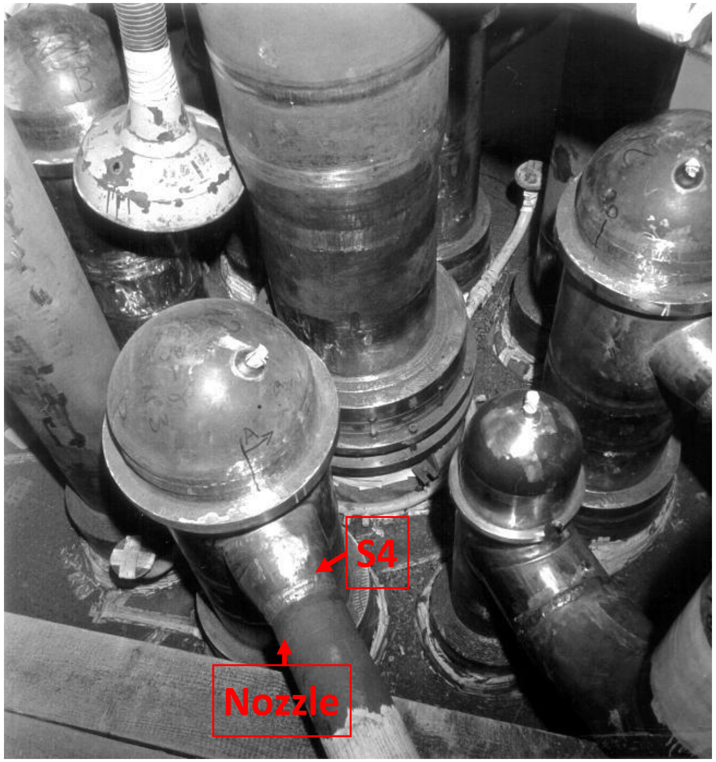
Typical costs

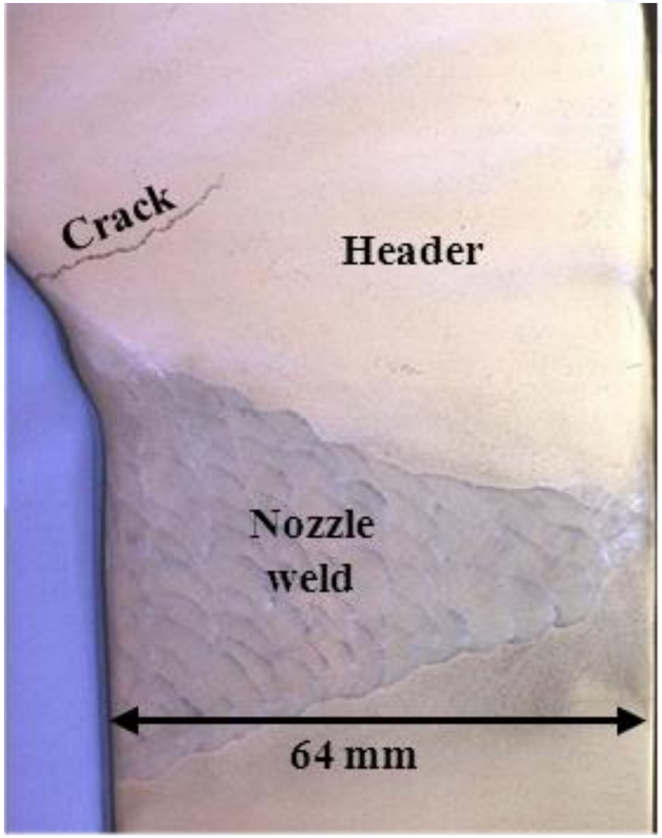
• Surface X-rays	£10^2 - £10^3
• Incremental hole drilling	£10^2 - £10^3
• Neutrons, synchrotron X-rays, contour method Deep Hole Drilling	£10^4 - £10^5

- Access to neutron and synchrotron facilities is not prohibitively expensive because
  - Possible to collaborate with the facilities or university groups to study the engineering science underpinning an application problem
  - Staffing associated with sample preparation, characterization, experimentation and analysis are often the highest costs, even for "simple" measurements

Coventry University

Study of creep cavitation





- **Material:**

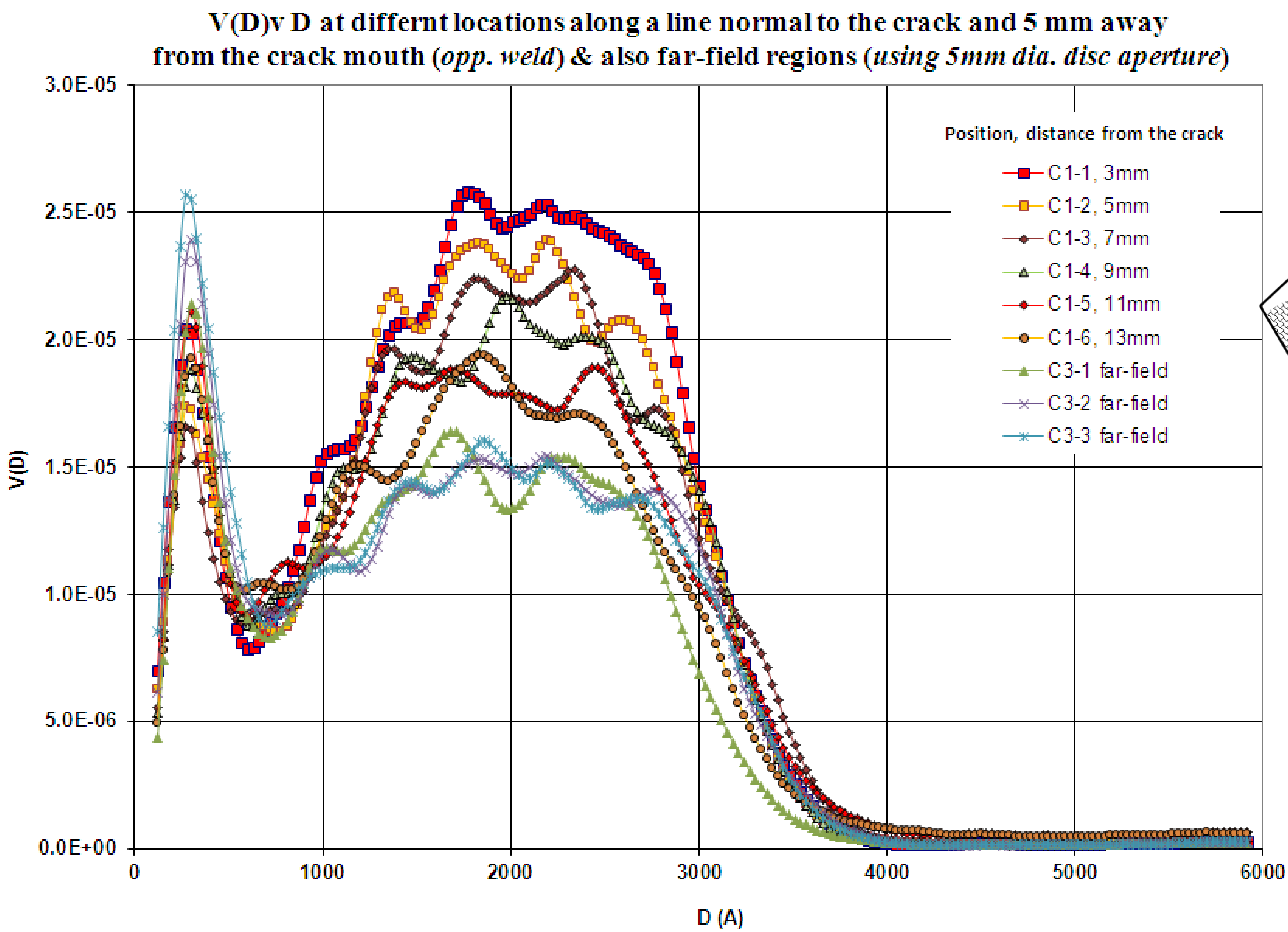
Type 316H austenitic stainless steel

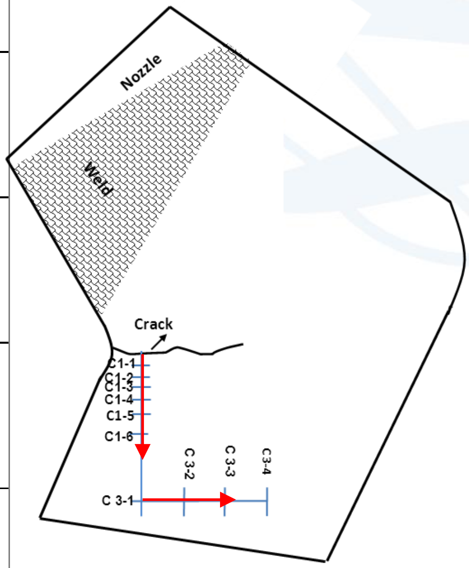
- **Service History:**

525°C for 65,000 hours

- **Crack length: <28mm**

SANS results



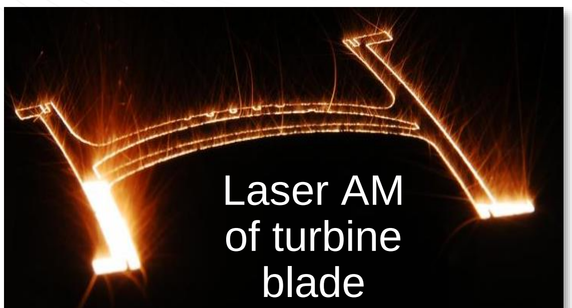


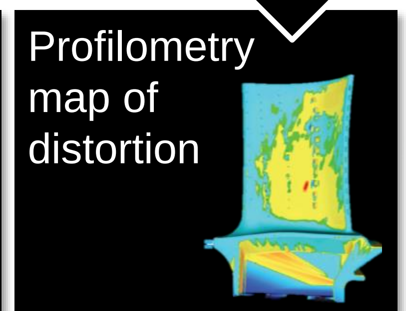
- Increase in the relative volume fraction of defects V(D) approaching the crack.

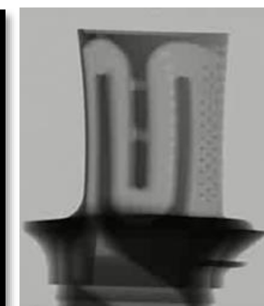
Supporting new energy-efficient manufacturing
- Laser additive manufacturing (AM)

Enables low-cost manufacturing of turbines with optimized internal cooling structures

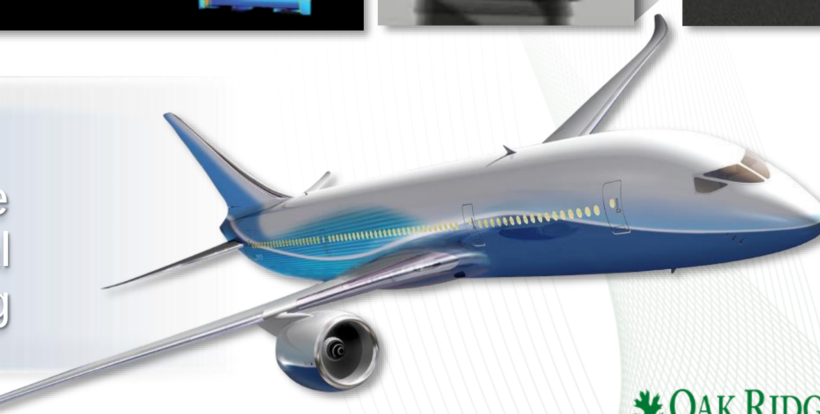
Creates large residual stress and other distortions







ORNL and Morris Technologies are using neutron scattering and imaging to improve understanding of the link between residual stress distortions and laser AM processing



Oak Ridge National Laboratory

Some take home messages

- Neutrons provide a different part of the information
  - Sometimes a critical part, sometimes not
- Materials science research is tending towards areas where neutrons are strong
  - Energy (mobile Li, H); soft matter (H, low energy dynamics)
- Neutrons have been and will be critical for discovery and characterization of emergent phenomena in complex systems
  - Magnetic skyrmions, magnetic monopoles, Weyl Fermions, quantum magnetism
- In the past neutrons have been critical for verifying techniques and concepts that can then be applied in other fields – this will not change
- There is a good mix of basic and applied research
- Capacity is as big an issue as capability
- We need to rethink access modes (fast access, dedicated instruments, programs)
  - E.g. RS2E (Research Network on Electrochemical Energy Storage)
- Size matters! Bulk analysis is often a requirement

Thanks to the participants!