Copolymers, composites and crystallization: Working with DPI for tomorrow's polyolefins

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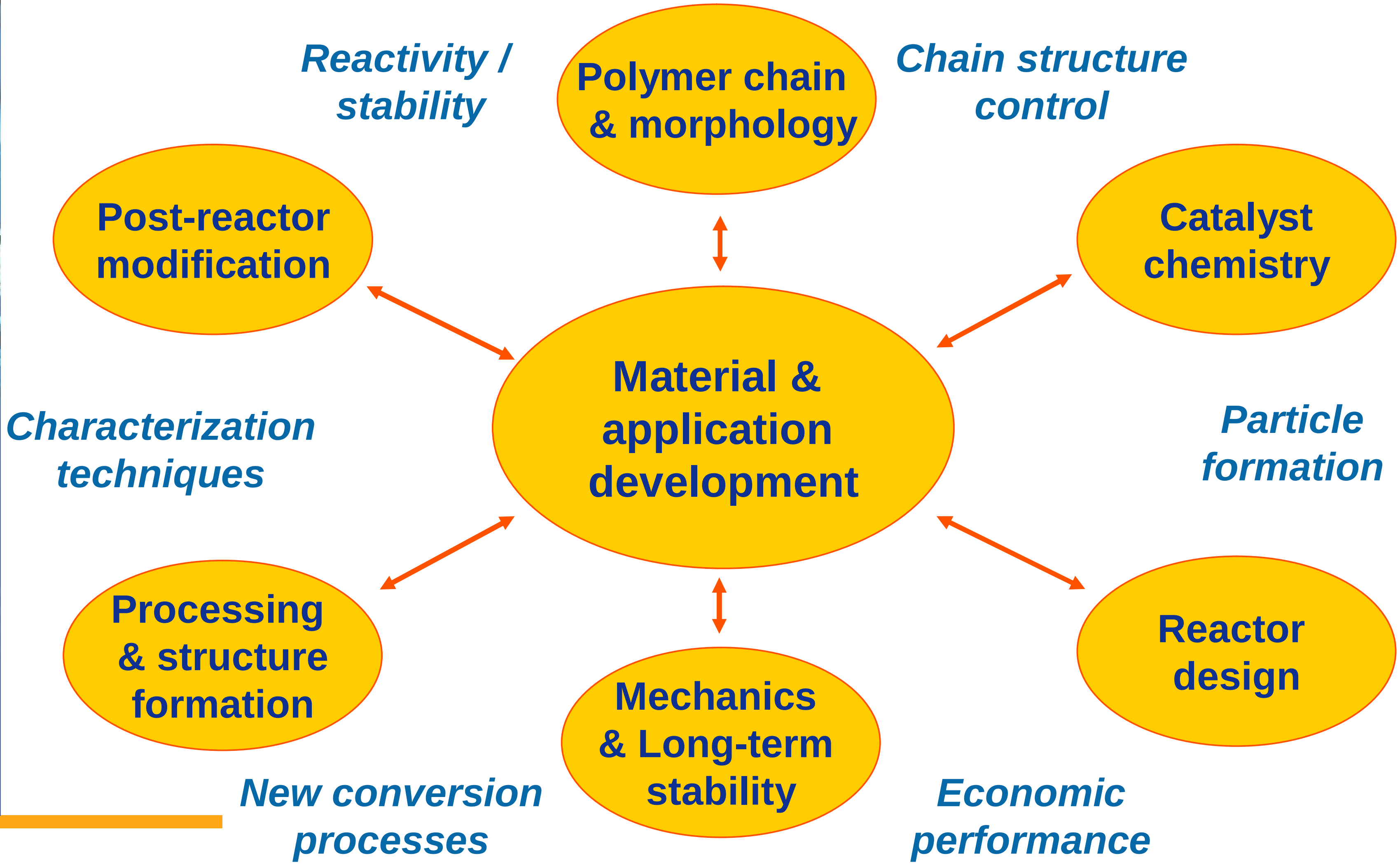
Borealis – Who we are

- More than 40 years of heritage in polyolefins
- State-of-the-art bimodal Borstar®
  PE & PP technology
- Over 55 new product launches in 2005
- EUR 6 billion revenue in sales
- 4,500 employees in 11 countries
- Four European hubs
- Expanding in Middle East and Asia

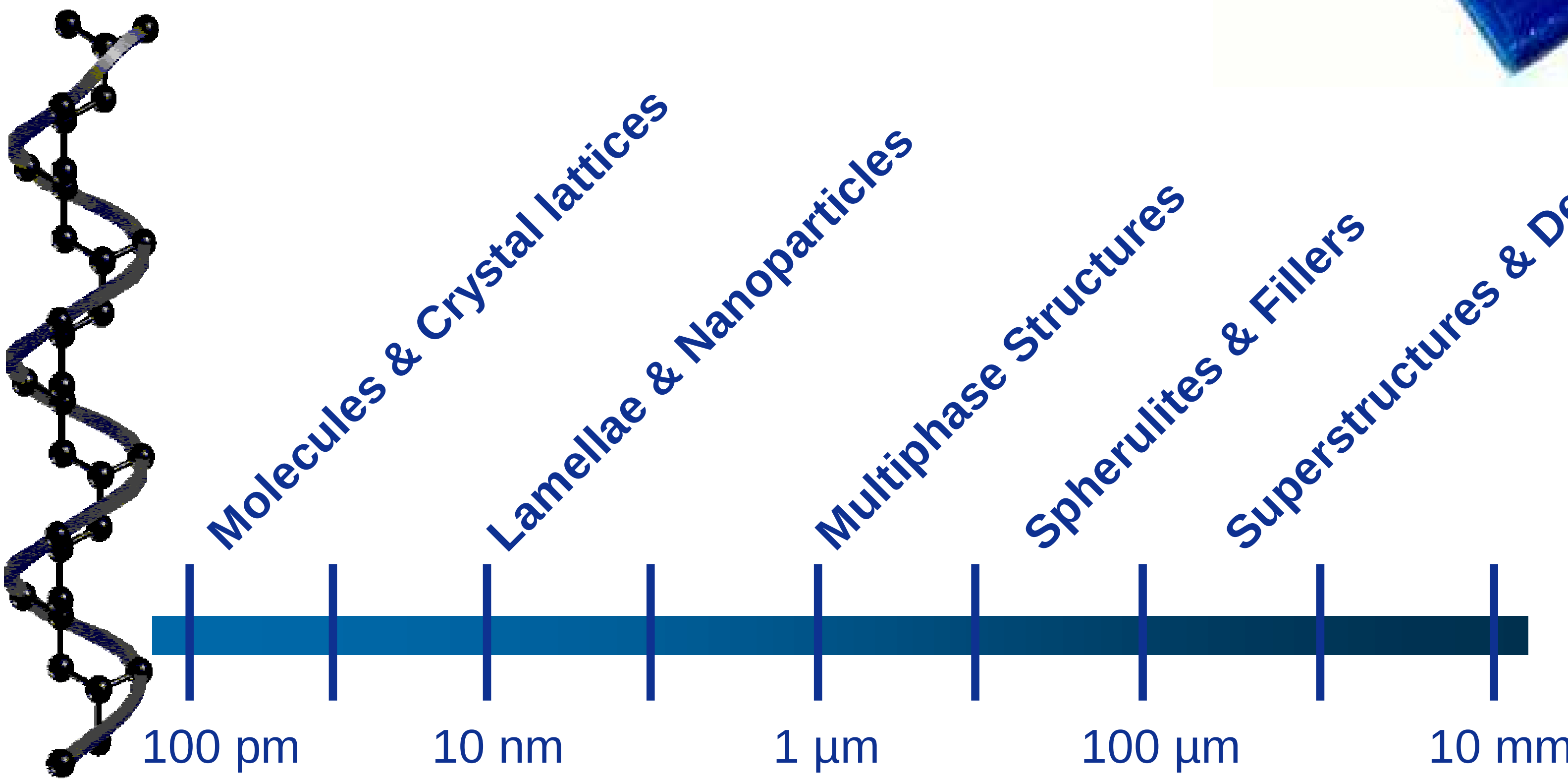
Content

- Polymer development is teamwork !
- Three examples for working with DPI:
  - Polyolefin copolymers with well-defined architecture
  - Revolutionary ways towards polymer nanocomposites
  - Understanding fundamentals of crystallization
- Stepping into the 21st century

Polymer development is teamwork !



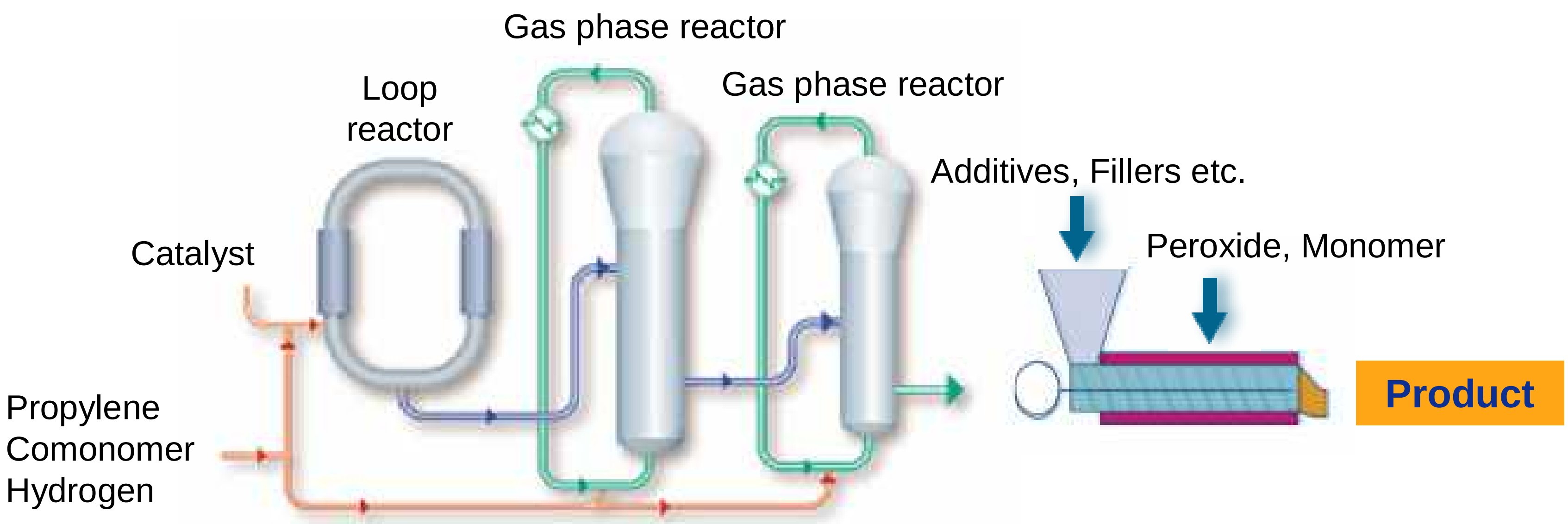
Orders of Magnitude, …



… Steps of Production

Borstar® PP as example for a “holistic view”

Catalysis | **Polymerisation** | **Extrusion**

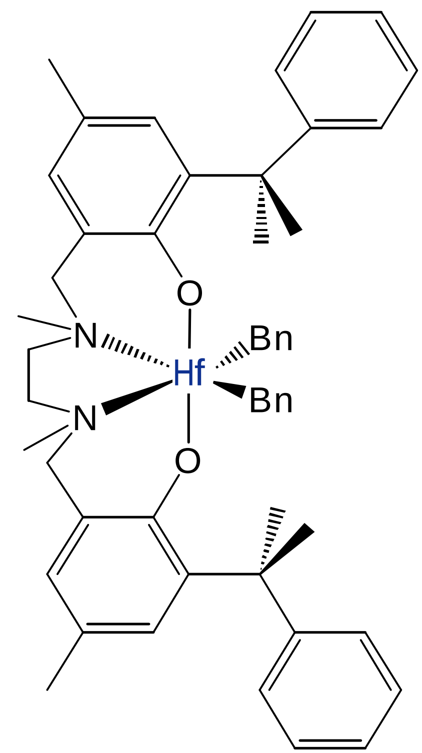


Molecule design | **Composition design** | **Property design**

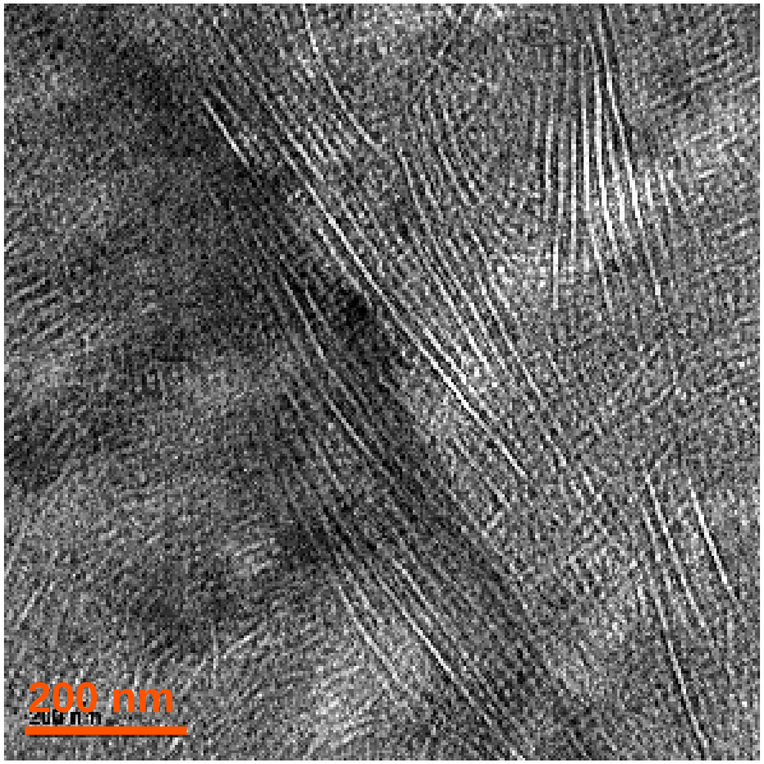
Tailored reactor materials

Polyolefin copolymers with well-defined architecture

- Di- and triblock copolymers are ideal compatibilizers – but so far not accessible for polyolefins
- New development in DPI – iPP-EPR(-iPP) as well as iPP-PE(-iPP) etc. di- and triblocks accessible from phenoxyimine catalyst
- Living polymerization allows excellent structure & molecular weight control
- Question of phase structure and performance in polyolefin blends (PP/PE, PP/EPR, …)

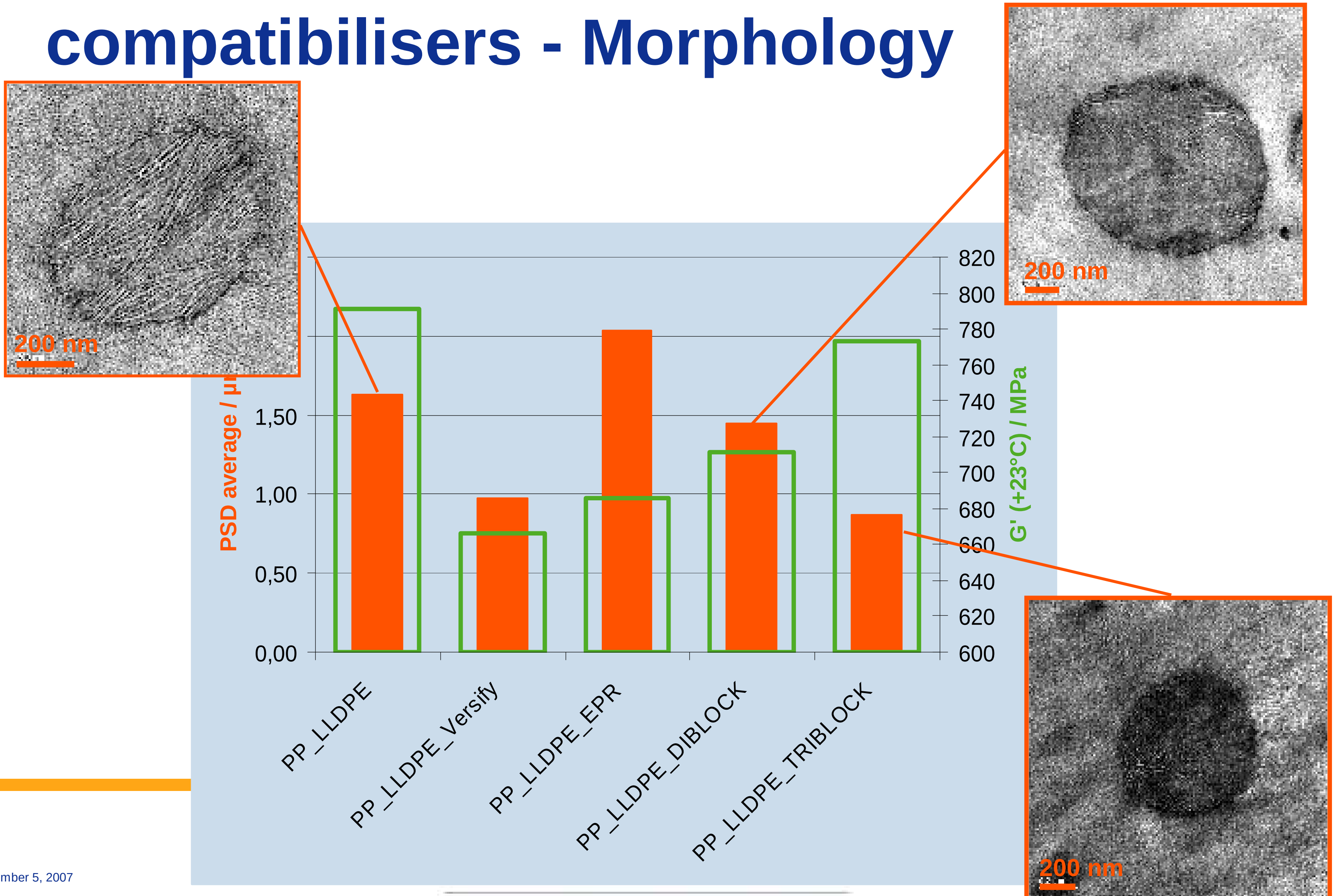


Morphology of di- and triblock systems

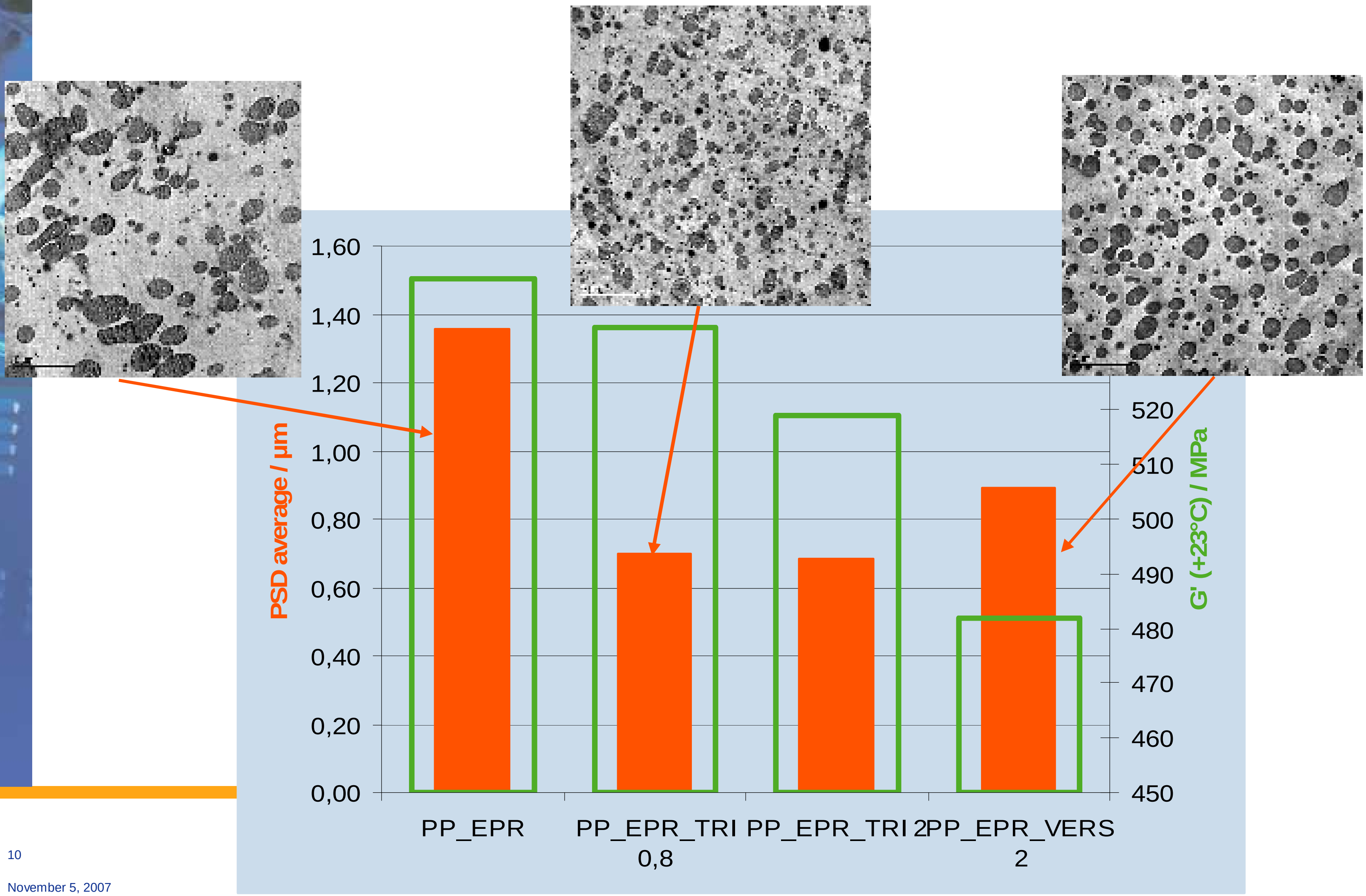


PP/EPR-Diblock **PP/EPR/PP-Triblock**

PP/PE blends with different compatibilisers - Morphology

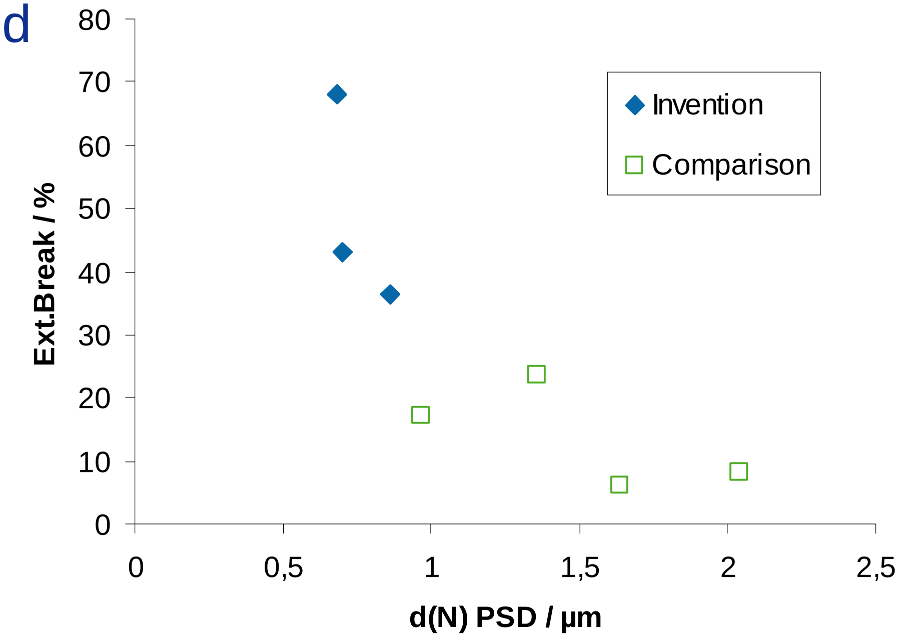


Triblock action in PP/EPR blends



Patent application filed …

- „Compatibilized polyolefin compositions" – EP 07115376.1 (DPI NoPOComp, ID 07.008) filed August 31st 2007
- Combination of iPP with different polyolefin & di/triblock protected
- Morphology-related toughness enhancement demonstrated
- Very efficient at low molecular weight – better processability



November 5, 2007

Reference

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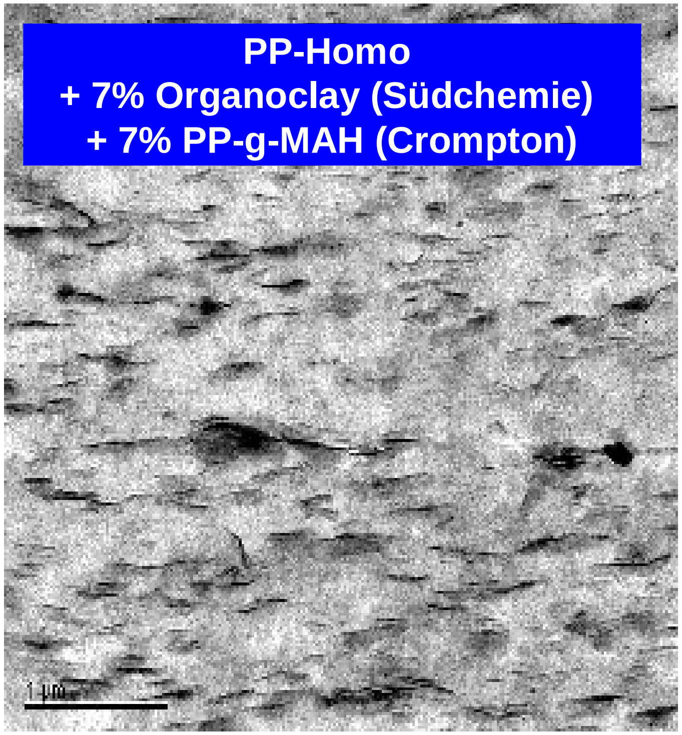
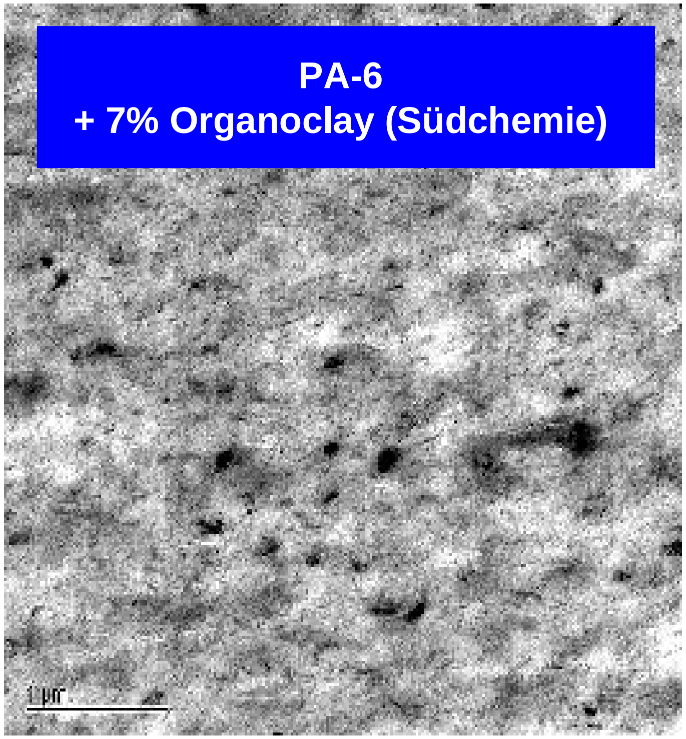
… next steps to be decided

- Development may be relevant for a number of areas
- Soft/elastic polyolefins with good sterilisation resistance among targets
- Possibilities for scale-up to be checked (catalyst, process, particle formation, …)

Revolutionary ways towards polymer nanocomposites

- Dispersion is the predominant problem in PO nanocomposites …

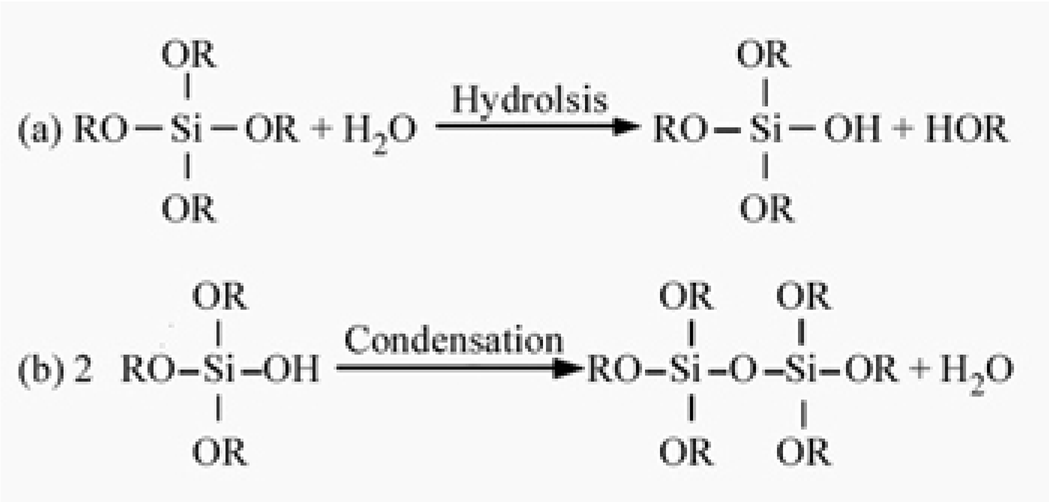


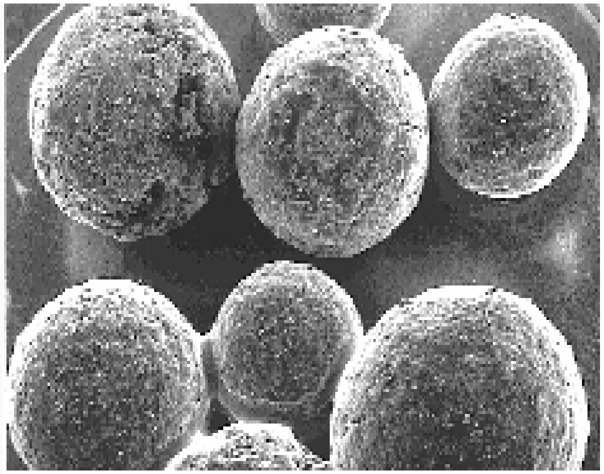


- … effectively hindering commercialization & success!

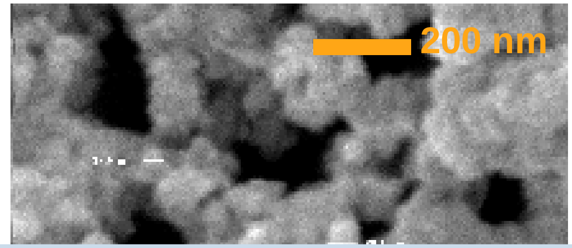
In-situ pathways to PO Nanocomposites

- … from the **Nanofiller**: Polymerization around well-dispersed nanoparticles (PA-6 – polycondensation, PO – catalytic, …)
- … from the **Polymer**: Adsorption of a precursor to polymer powder followed by particle formation (e.g. hydrolysis of silane)

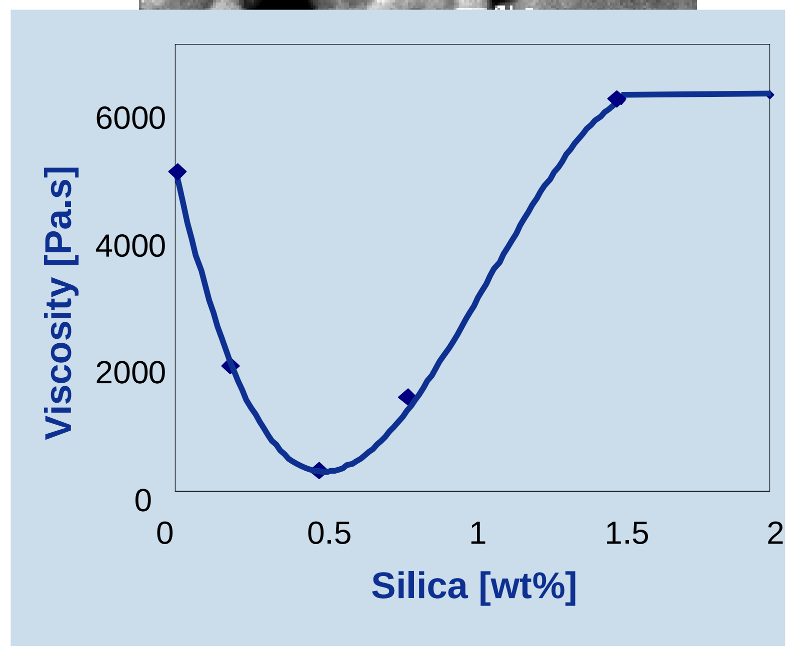


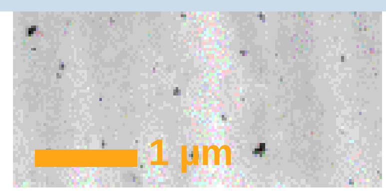


New approach to processability improvement



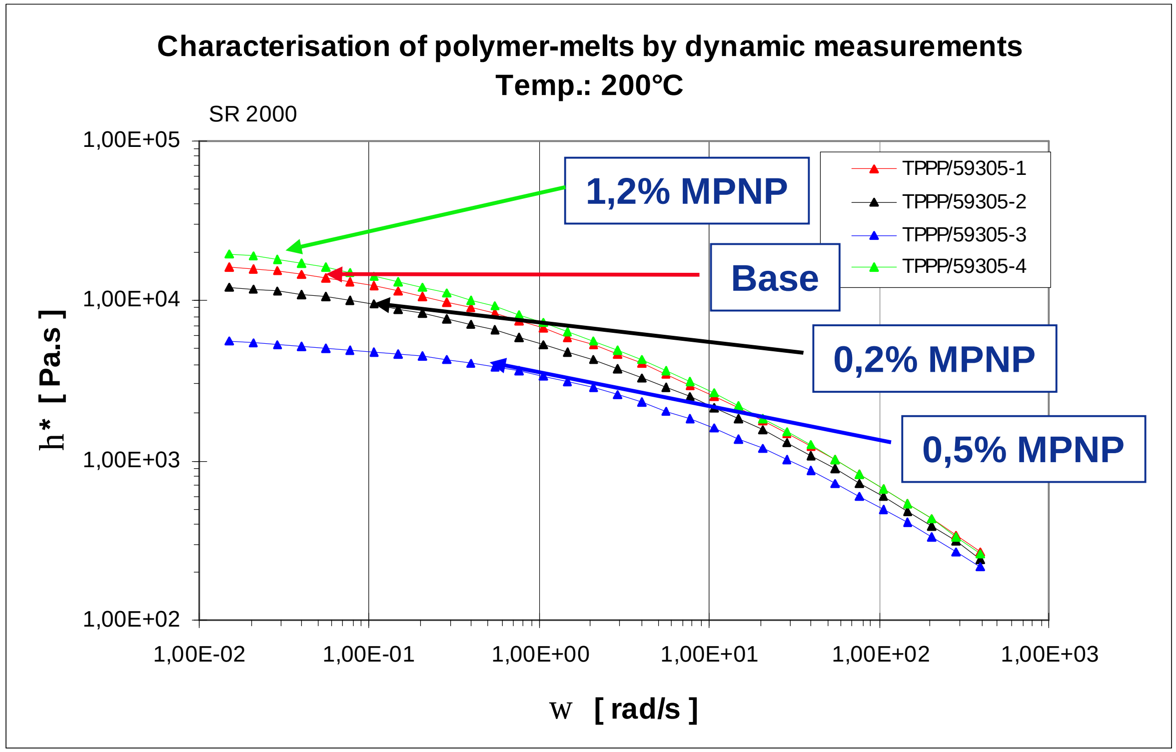
- Lab-scale development
  - In-situ preparation of mesoporous silica nanoparticles (MPNPs) by silane sorption & decomposition
  - Massive viscosity reduction at 2.000-8.000 ppm silica level, mechanics equal or improved
- Patent application filed – EP 05101388.6
- Two lines of development
  - Scale-up & application testing – Borealis
  - Scientific understanding and extension to other polymers - TUE





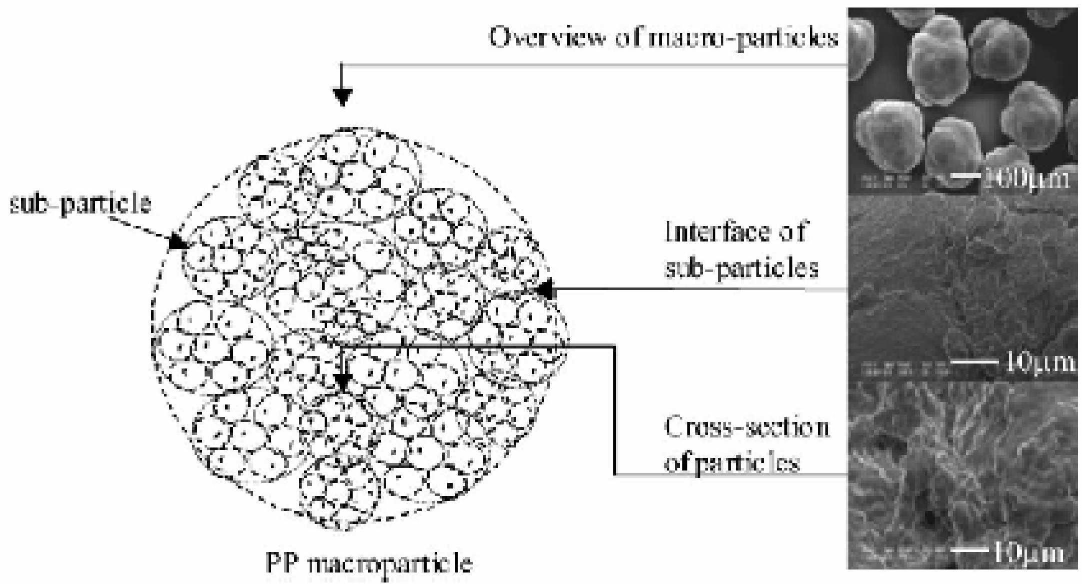
First Scale-Up Results

- In-situ generation with TEOS adsorption and hydrolysis (kg-scale)
- Viscosity reduction in concentration range 0,1-0,5 wt% silica
- Both stiffness & impact slightly improved
- Different results with Aerosil compounds



… but problems in further scale-up

- PP powder morphology has dominant influence on formation of suitable nanoparticles
- Change in surface/volume ratio makes hydrolysis increasingly difficult
- Better understanding of viscosity reduction required for success



Understanding fundamentals of crystallization

- Practically achieved mechanical performance of both PP and PE is far below technical limits
- New polymers often fail because of processing troubles (e.g. SSC-PO)

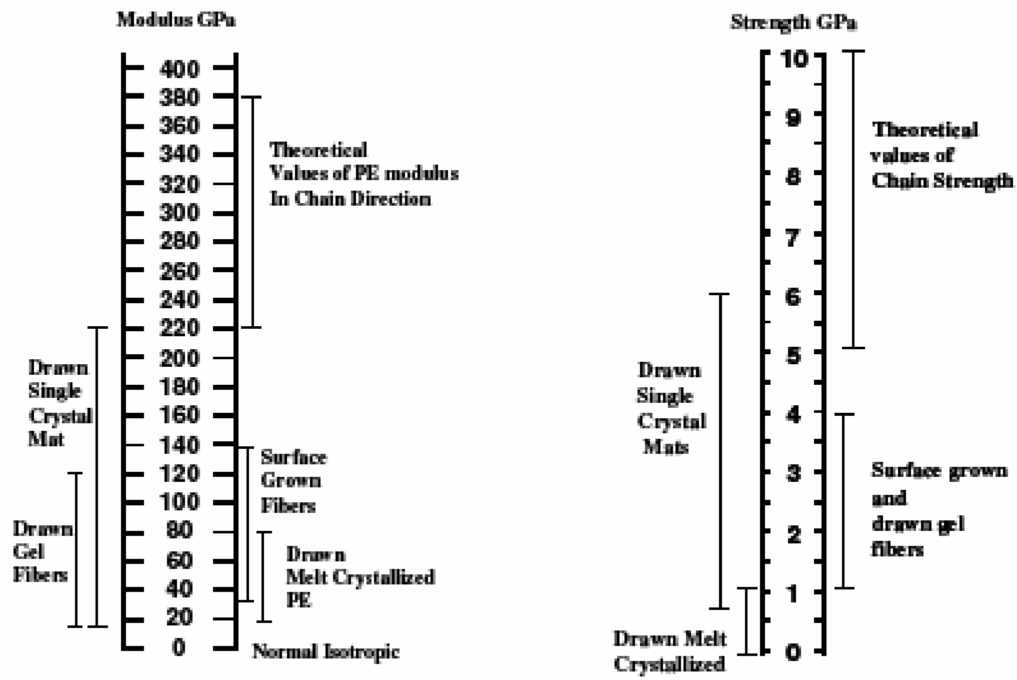
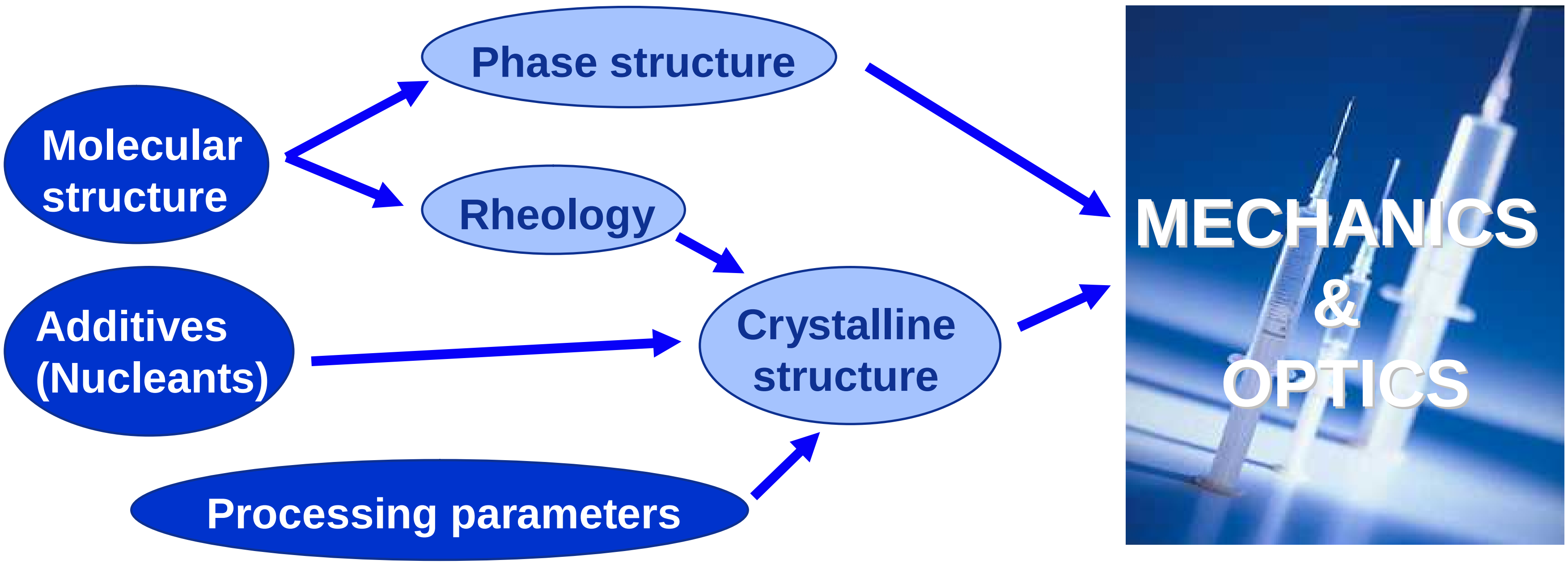


Figure 1.10 Scales showing tensile strength and modulus for polyethylene. (Reproduced from Barham, P. J.; Keller, A. *J. Mat. Sci.* **1985**, 20, 2281).

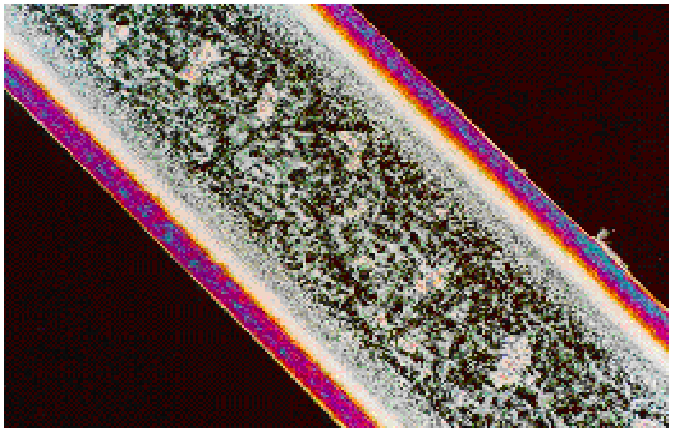
Processing effects – Rheology & crystallisation

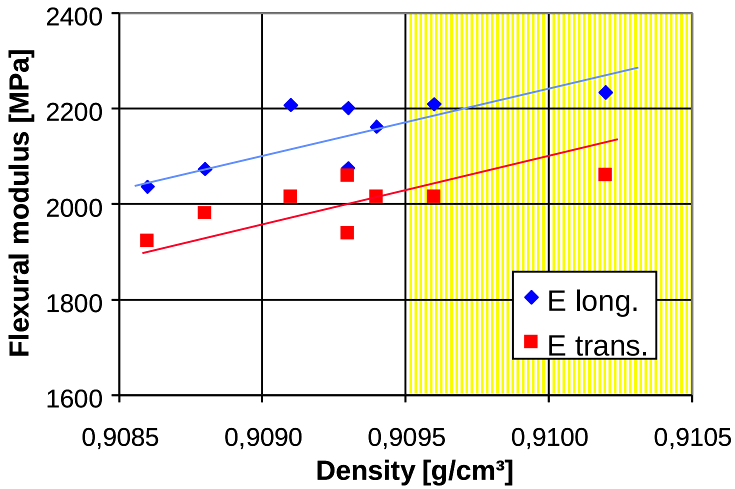


Models, Parameters & Targets

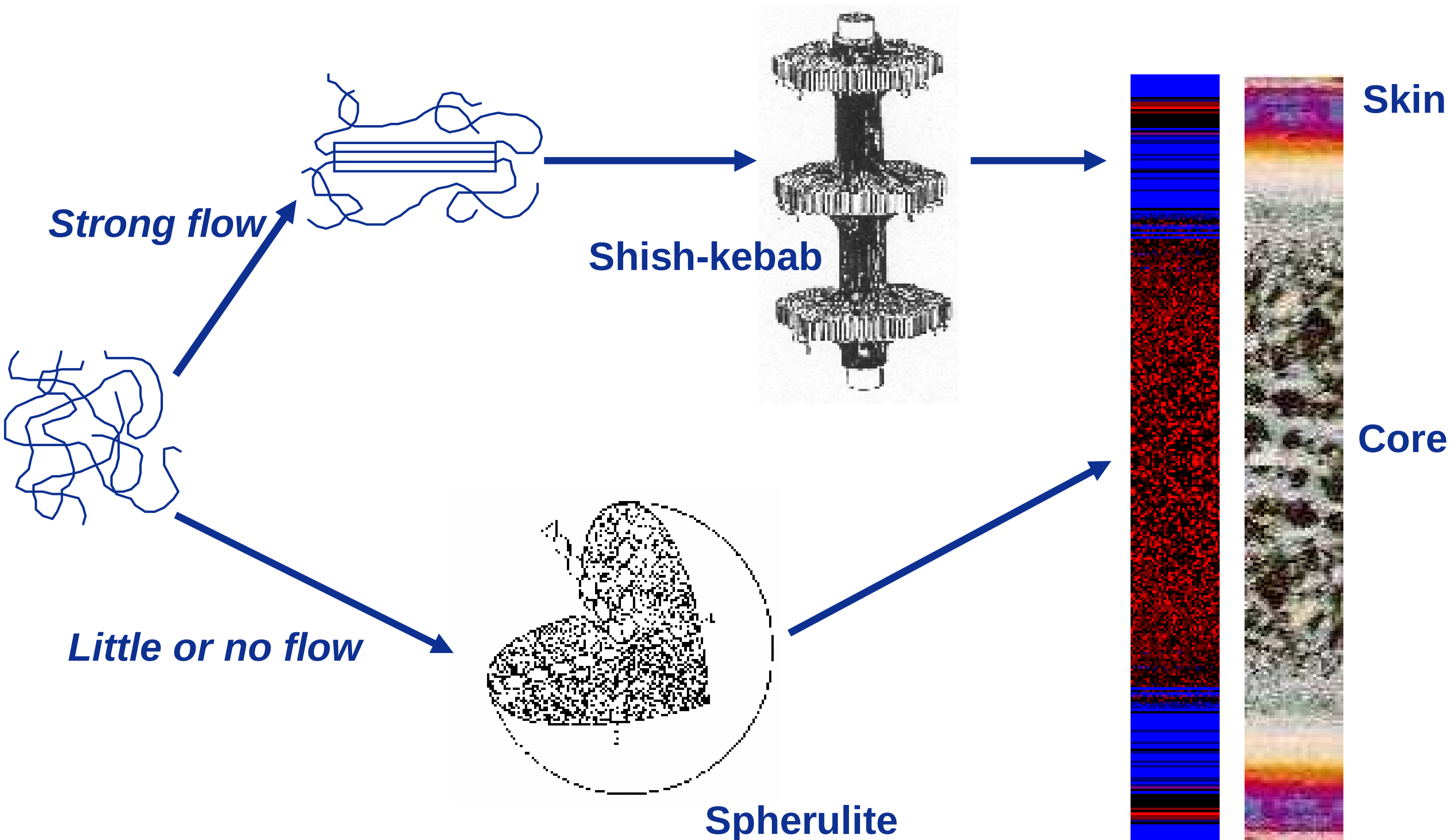
To be widely applicable, a **crystallization model** must:

- … be compatible with existing CAE(D) software
- … have a limited number of parameters with possible corerelation to structural features of the polymer
- … be capable of predicting mechanics and dimensional stability





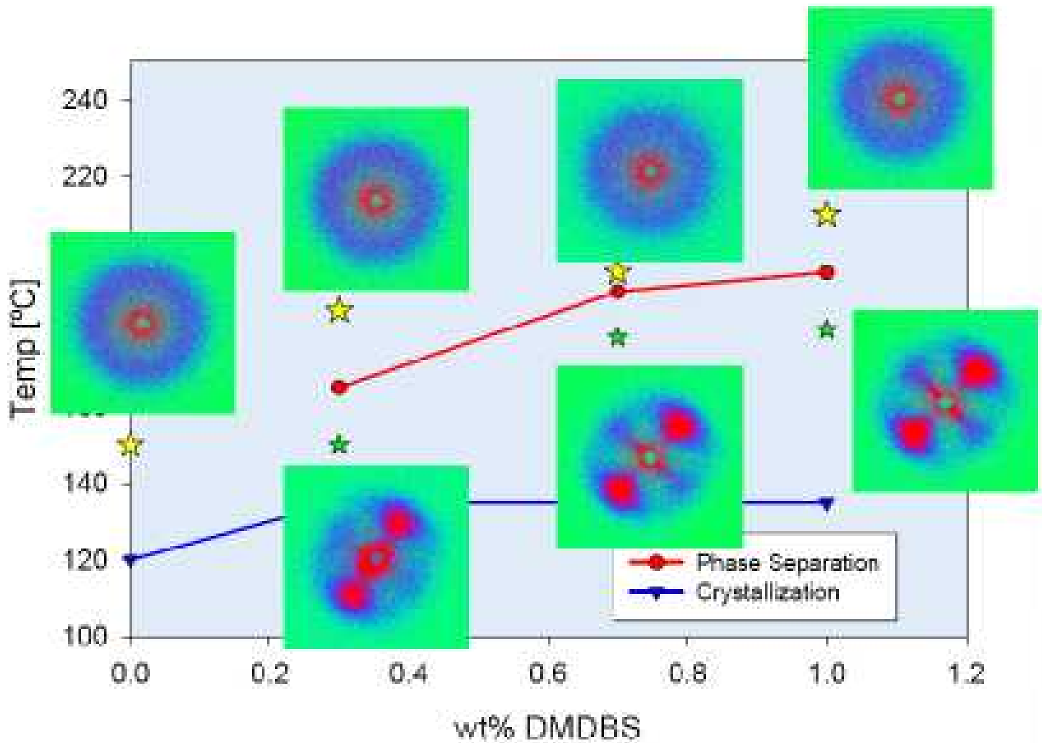
From molecules to crystals



Understanding materials …

Example: Polymer/nucleation interaction

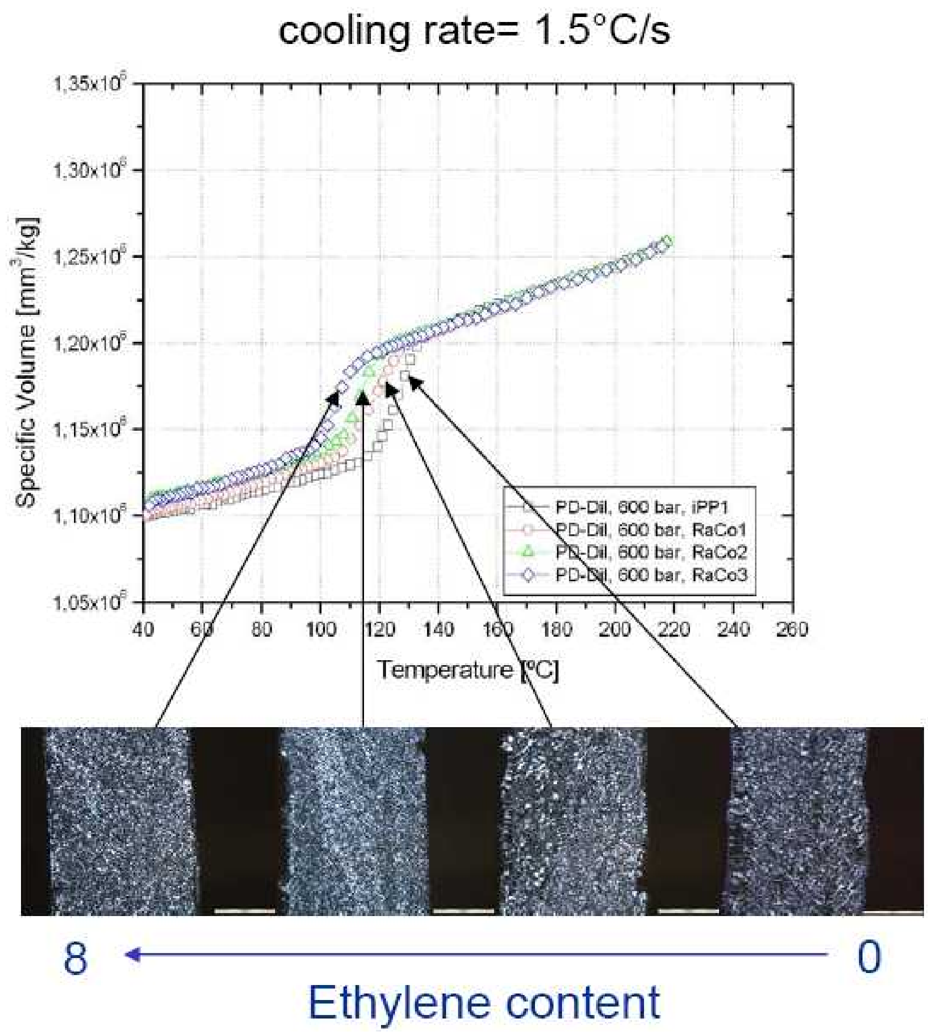
- Similarities in high molecular weight & nucleant effects on flow-induced crystallization
- Enables process-related material design



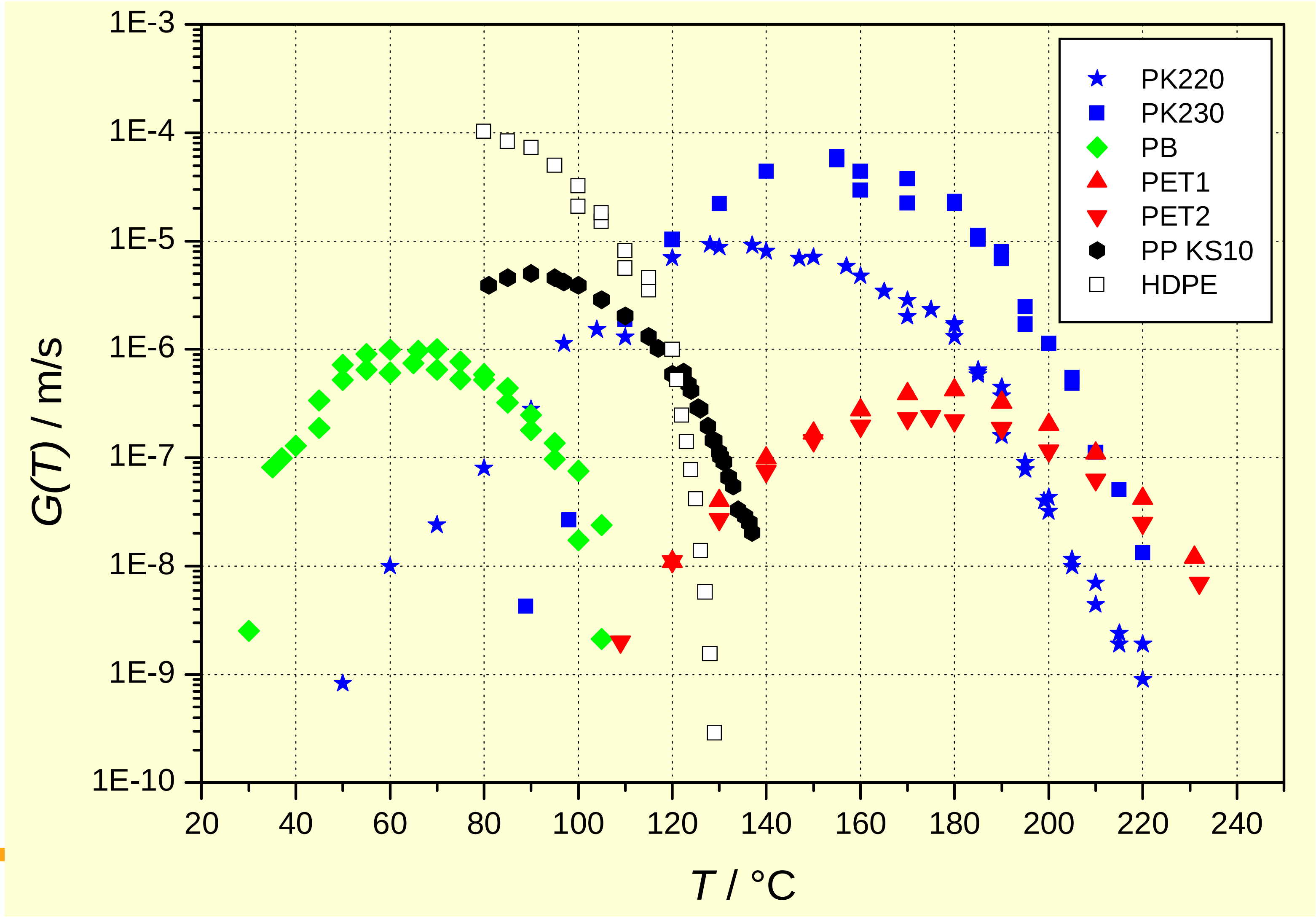
… and understanding processes

Example: *pVTα* setup

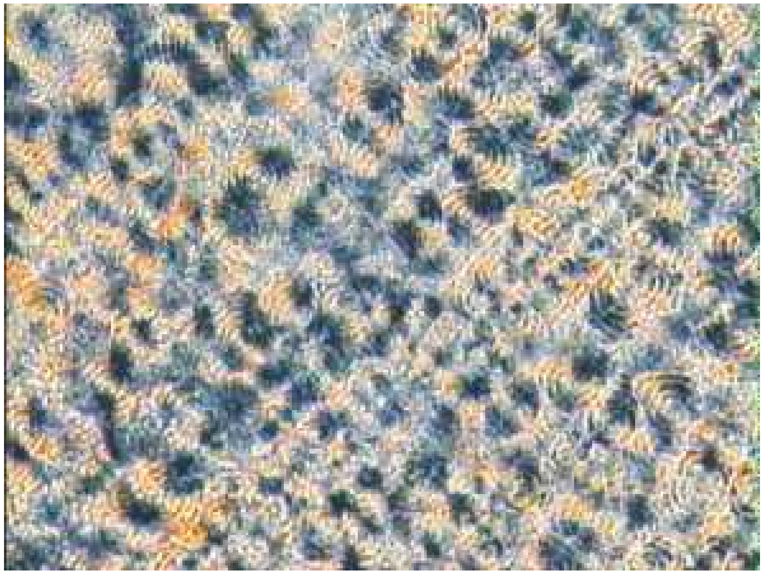
- Allows rapid characterization of a semicrystalline polymer in wide range of solidification conditions
- Can deliver parameters for tomorrow‘s processing simulations
- Could become standard equipment for processing laboratories



Next steps: From PP to PE

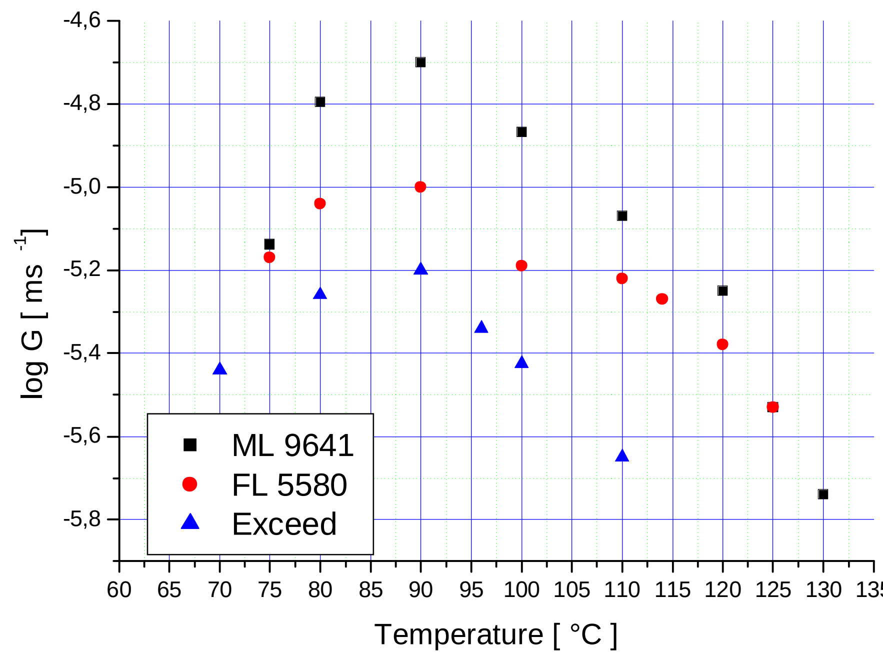


PE: a similar picture …
chain regularity & MWD effects



Shish-kebab structures in bimodal LLDPE

Density effects on quiescent crystallization of HDPE / LLDPE



Stepping into the 21st century

The vision:

- Interdisciplinary university education is standard
- Industrial and academic research are complementary
- Nanotechnology has become efficent & economic
- Sustainability is becoming reality
- Polyolefins are widely accepted performance materials

Borealis Innovation Centre Linz 2009

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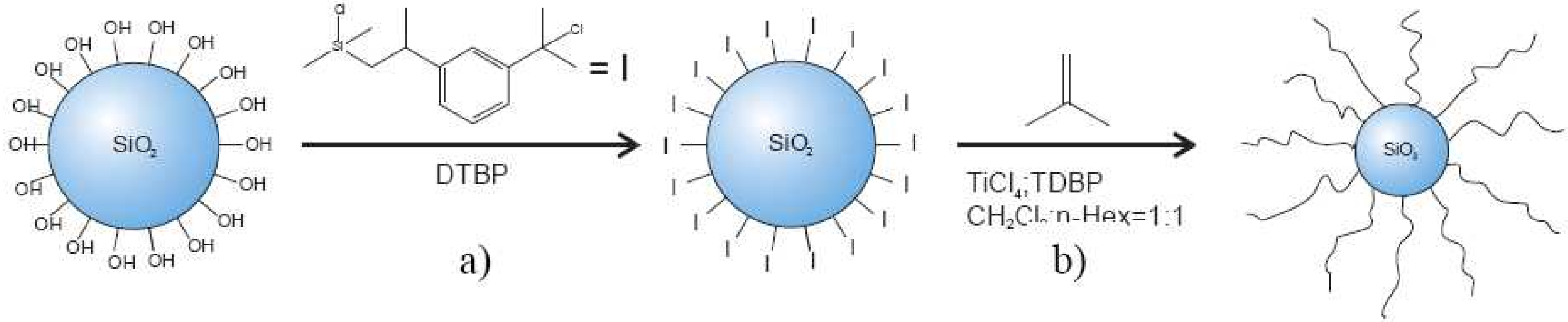
We are taking steps …

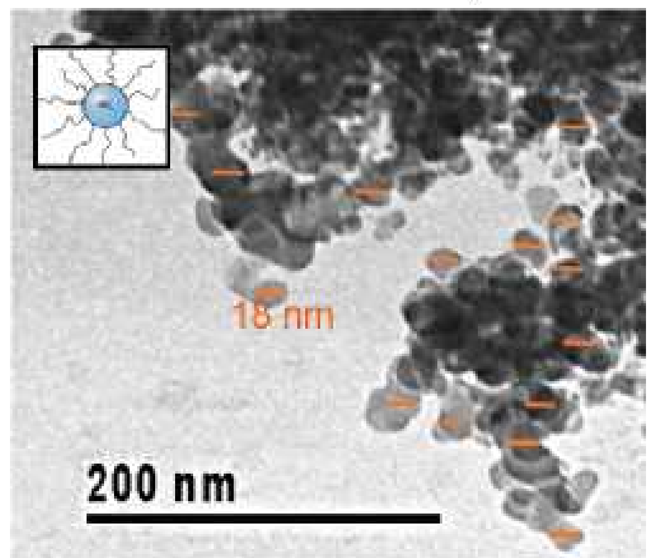
- In 2007-2009 more than 80 scientists, engineers & technicians will be hired for IC Linz
- The equipment in the areas of analytics, characterization, testing and processing is being expanded (WAXS, ^{13}C-NMR, AFM, multilayer extrusion, meltblown fibers, …)
- Cooperation with Austrian & International universities is being intensified

A glimpse into the future: Core-shell nanoparticles



Mineral core + chemically coupled polymer shell – possibly the next generation of impact modification with controlled nanostructure

(patent application filed)



Mn~5000

Thanks to ...

Dr. Elisabeth Ingolic (ZFE Graz, Austria) for the excellent TEM images

Gerhard Eder & Ewa Ratajski (JKU Linz) for PE crystallization data

Wolfgang Binder & Ronald Zirbs (MLU Halle) for the nano-core-shell results

... and thanks for your attention!

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