Exploring polymer mechanics over multiple scales

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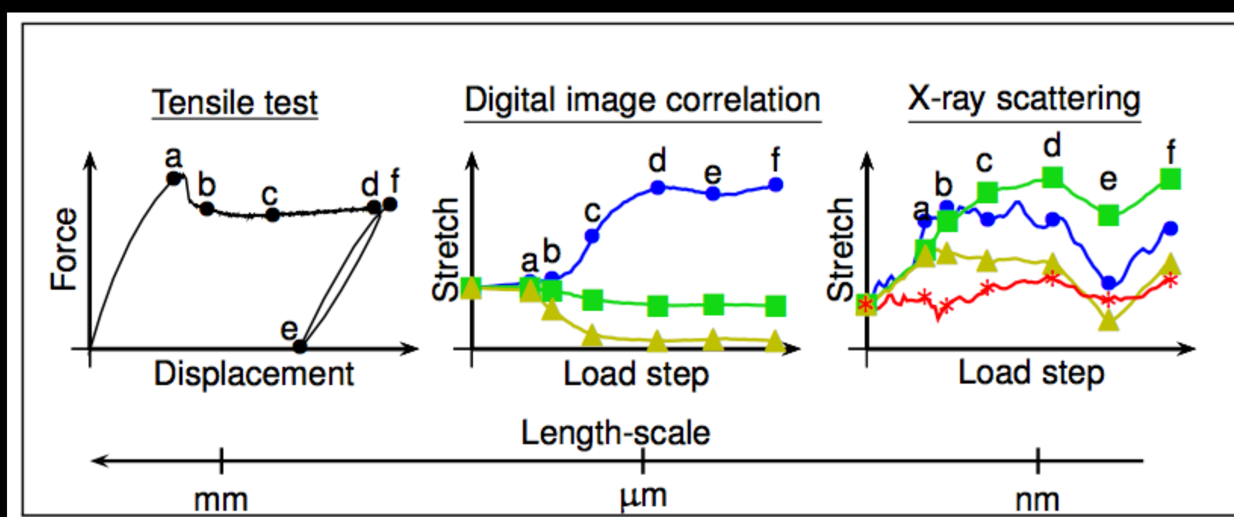
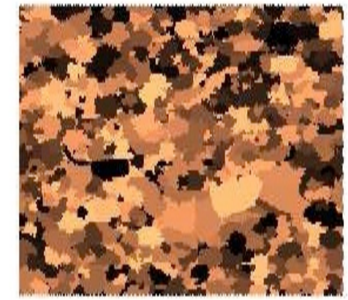
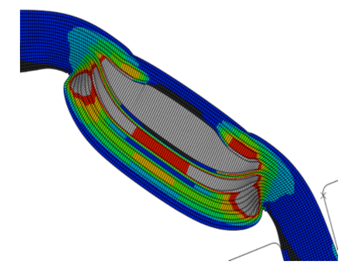


DIVISION OF SOLID MECHANICS @ LTH

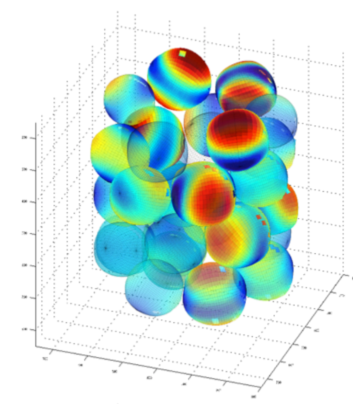


- Research areas: constitutive modeling, computational mechanics and experimental mechanics:

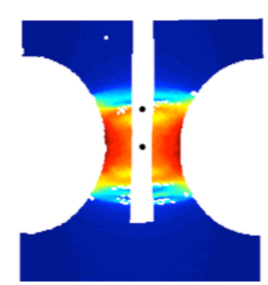
    - microstructure mechanics, recrystallization, phase transformations, large strain plasticity, viscoplasticity, texture development, coupled physical phenomena, smart materials, electroactive polymers, geomaterials, diffusion processes and structural optimization…



- Application areas: polymers, metals, granular materials, fibre materials, bio-materials and more

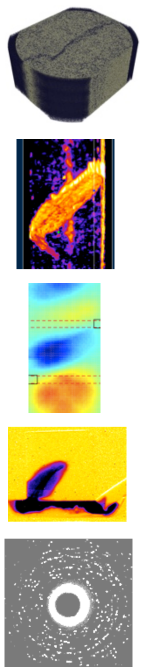


- Experimental mechanics: analysis of mechanical properties including multi-scale and multi-physics couplings and development of full-field measurement methods:
    - DIC, x-ray & neutron imaging & scattering…
    - Close link to model development



General experimental research approach

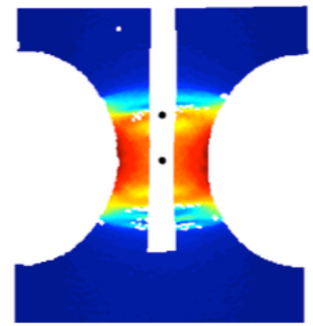
Investigation of the mechanics of (heterogeneous) **deformation and failure in materials** using **full-field methods** with different **sensitivities** to different physical properties, to characterise different aspects of the **mechanical processes**:

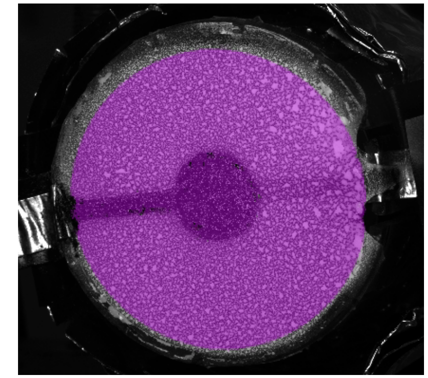


- Digital Image Correlation (DIC)
- X-ray tomography
- Neutron tomography
- 3D Digital image analysis
- Digital Volume Correlation
- Ultrasonic tomography
- Neutron and X-ray Scattering
- Acoustic emissions
- …

- With a view towards defining the characteristics to include in (enriched) modelling

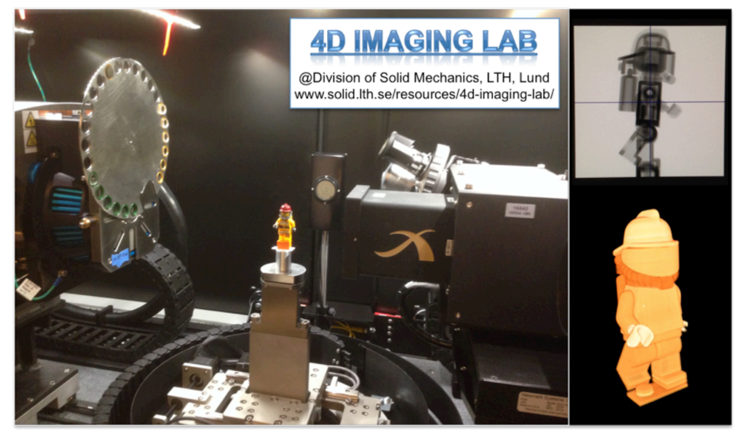
Experimental Mechanics @Division of Solid Mechanics





<u>Surface DIC systems:</u>

- 29 MPx @ 4 Hz
- 1 Mpx @ 500 Hz
- Correlated solutions VIC3D software
- In-house 2D-DIC code

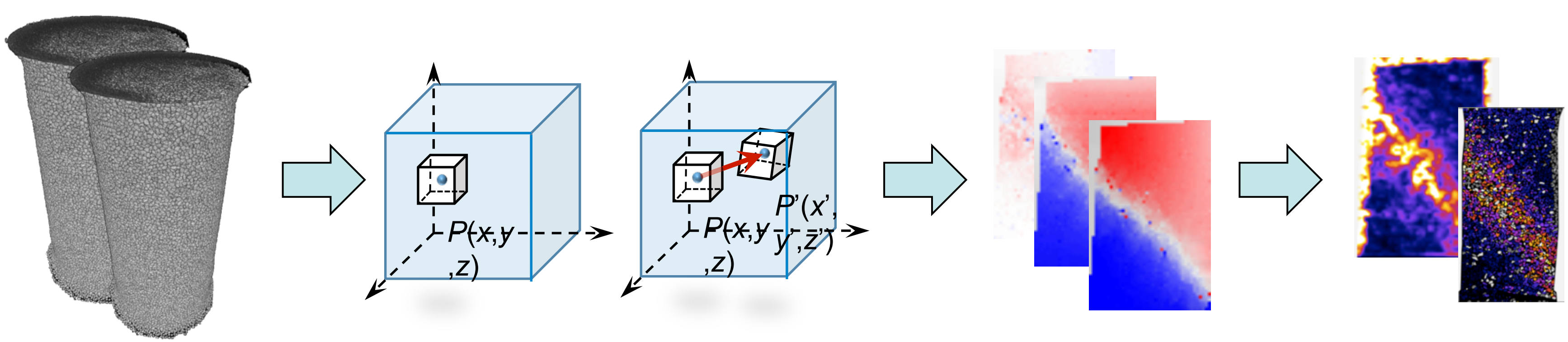


<u>Volume imaging</u>:

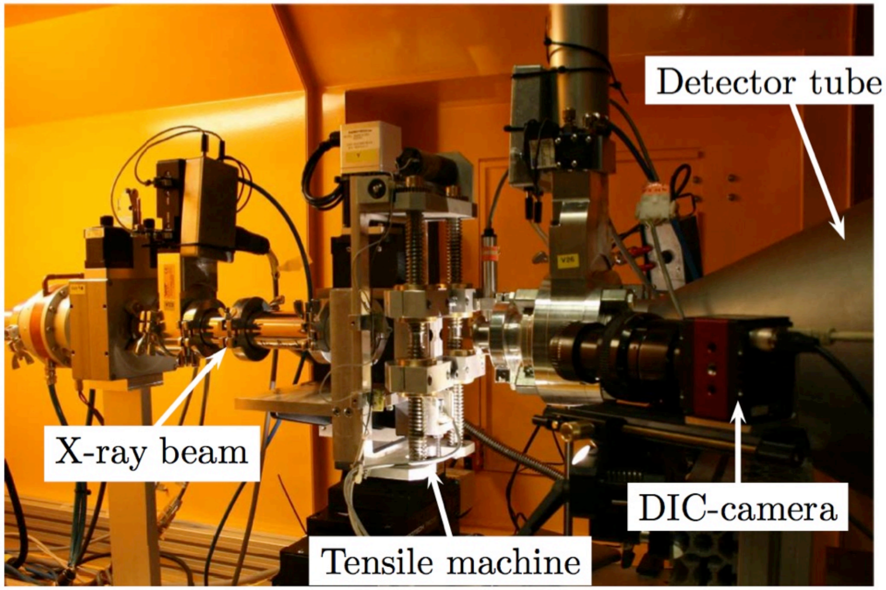
- In-house x-ray tomograph (Zeiss XRM520)
- X-ray and neutron tomography at large-scale facilities

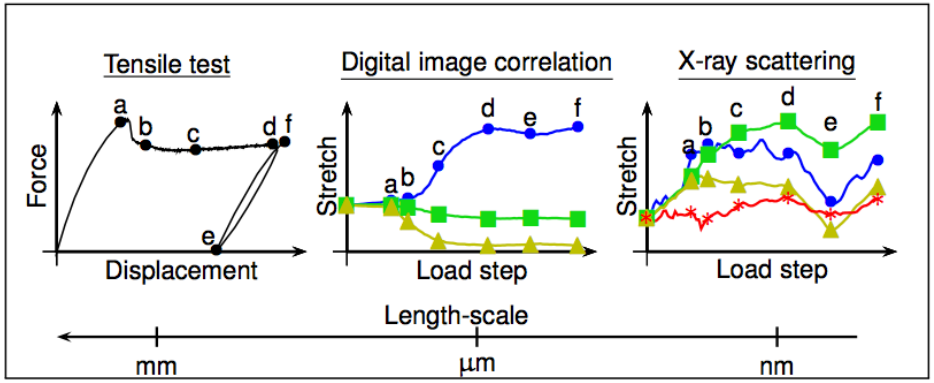
<u>Digital Volume Correlation (DVC)</u>

- In-house DVC code: **TomoWarp2**



EXPLORING POLYMER MECHANICS OVER MULTIPLE SCALES





PhD project of J. Engqvist, Div. Solid Mechanics, Lund University
Engqvist et al., 2014, Exp .Mech. & Engqvist et al., submitted

Exploring polymer mechanics over multiple scales

Objectives

- Investigate the coupling between deformation mechanisms at the molecular-, micro- and macro-scales in polymers

- To develop more accurate, physically-based constitutive models

  - Glassy polycarbonate (PC)
  - Semi-crystalline HDPE
  - Block co-polymers (SEBS)

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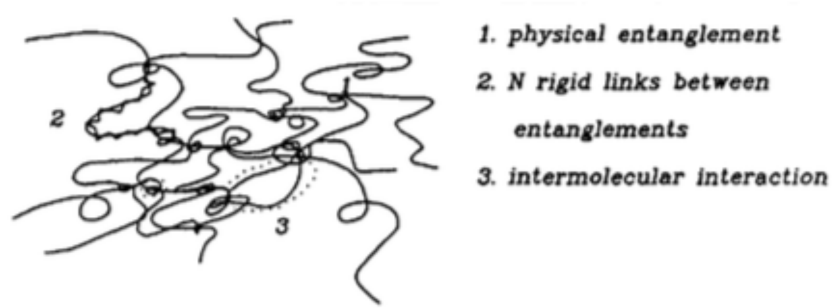
EXPLORING POLYMER MECHANICS OVER MULTIPLE SCALES

Glassy polycarbonate (PC)

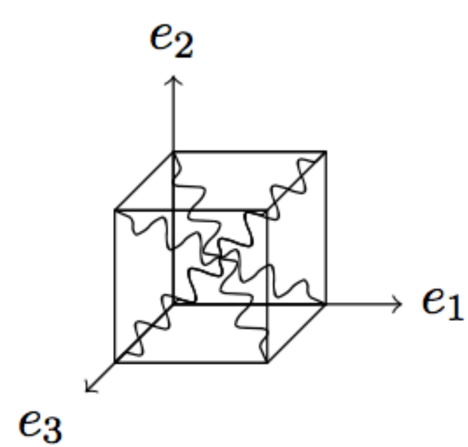
- Amorphous, glassy polymer
- Initially isotropic and homogeneous
- Development of significant heterogeneity (localised deformation) with loading
- Evolving anisotropy
- Multi-scale processes



Boyce et al. Mech. of Materials (1988)

The BPA model

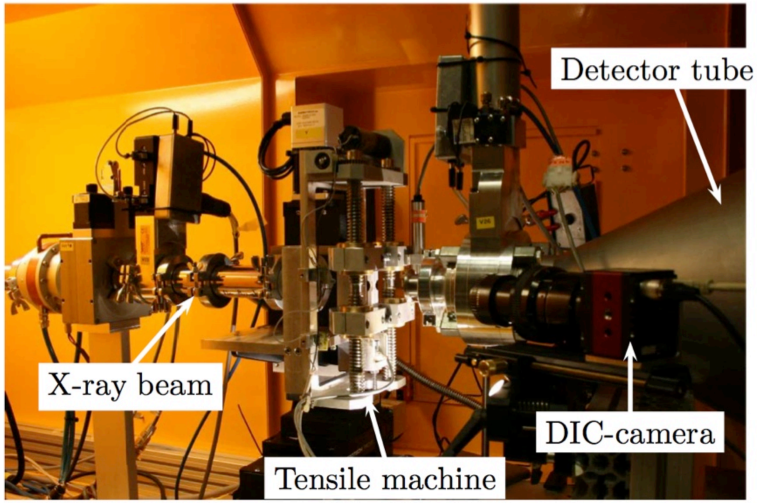
- Polymer model
- Proposed by Boyce, Parks and Argon (1988)
- Idealised chain network consisting of eight chains

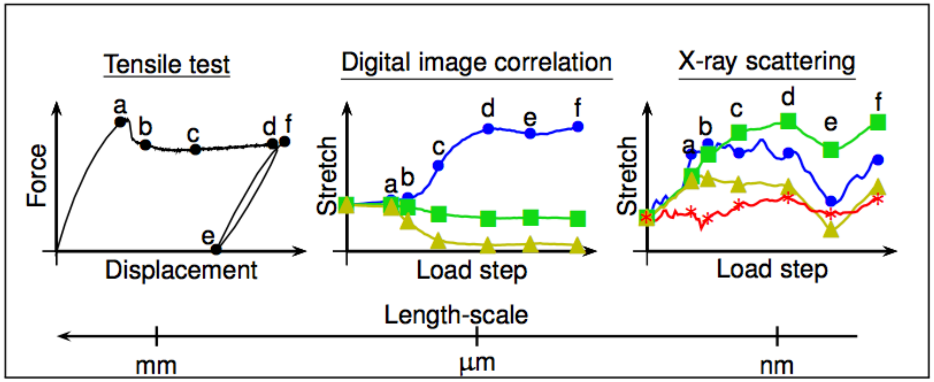


Exploring polymer mechanics over multiple scales

Methods

- **<u>Tensile loading</u>**: “averaged” stress-strain response of the sample
- **<u>3D-surface DIC</u>**: local “macroscopic” strain field and sample thickness evolution
- **<u>Small- and Wide-angle scattering</u>** (SAXS/WAXS: structures from about 100 nm down to a few Ångström (with spatial resolution)
- **<u>Simultaneous measurements</u>** to relate measurements across scales (DIC triggered with SAXS/WAXS)
- **<u>Spatial resolution</u>** to capture heterogeneity

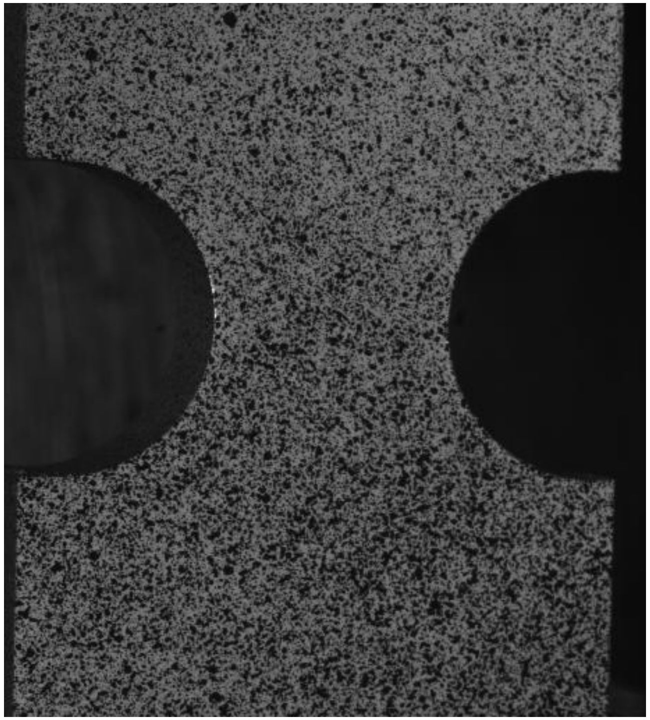




EXPLORING POLYMER MECHANICS OVER MULTIPLE SCALES

3D-surface Digital Image Correlation

- Measurement of surface displacement fields
  - In-plane and out of plane displacements
    - Strain fields → strain heterogeneity
      - Local measures of strain to relate to x-ray scattering measurements (macroscopic strain is at best a global average measure)
      - Understanding of meso-scale failure mechanisms (strain localisation)
    - Thickness changes of sample to correct scattering measurements (accounting for varying sample attenuation with change in sample thickness)



X-ray scattering

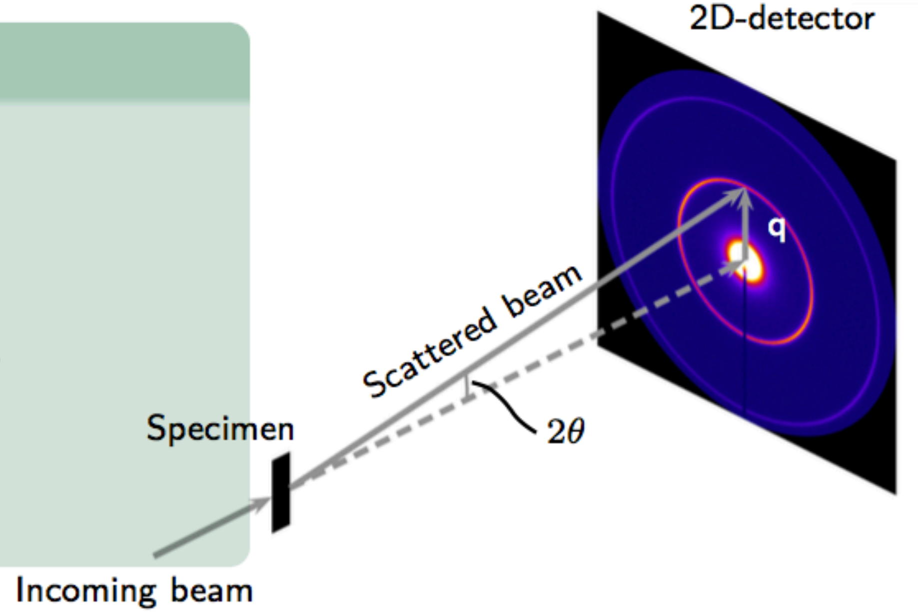
X-ray scattering

Bragg's law

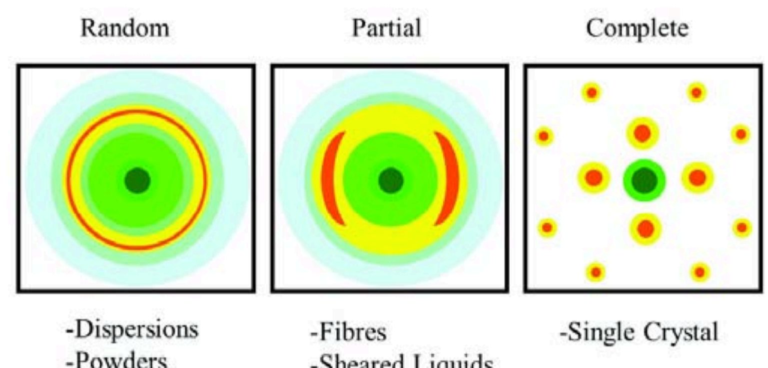
$$n\lambda = 2d \sin\theta$$

Length of the scattering vector

$$q = \frac{2\pi}{d}$$

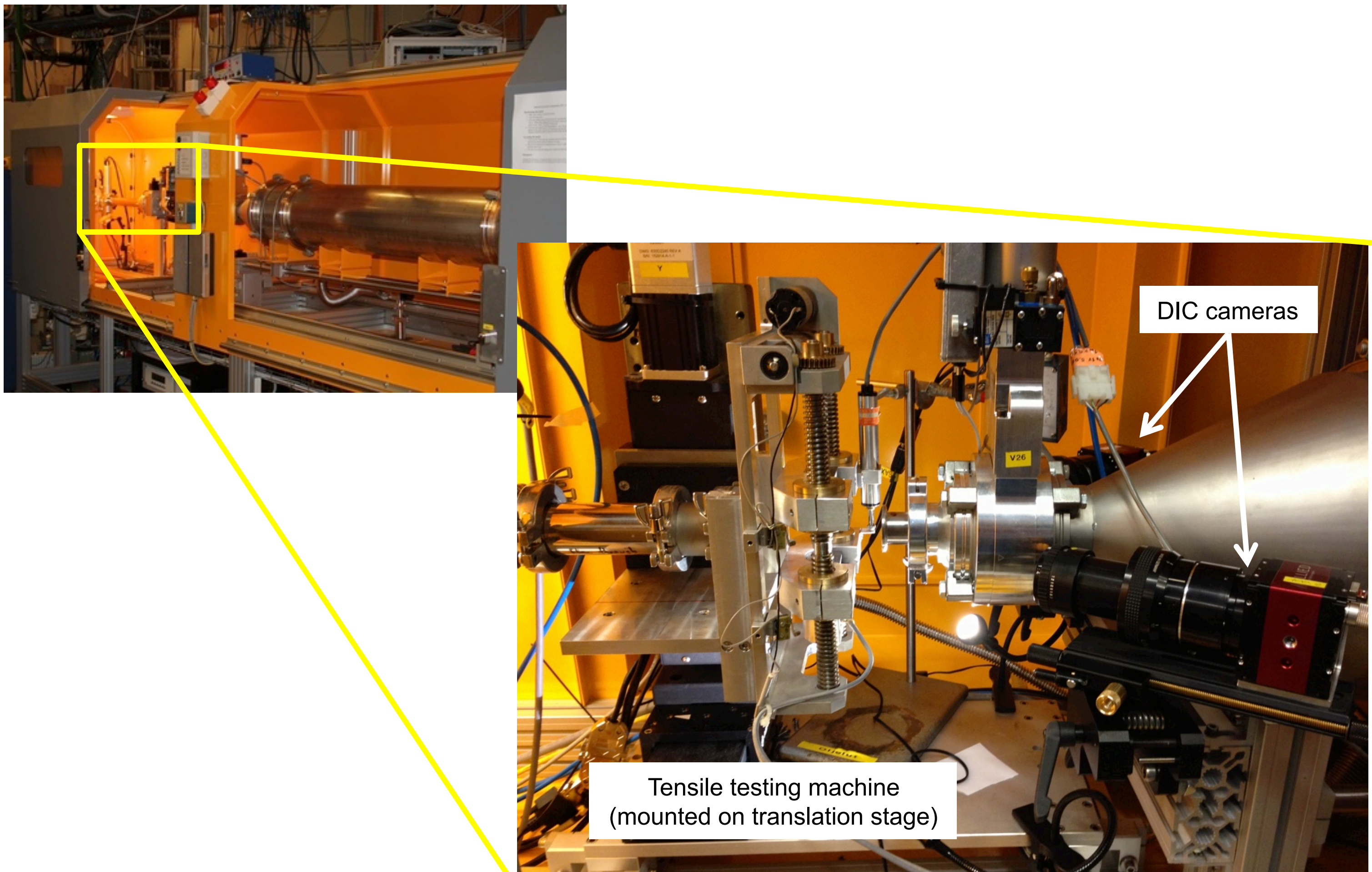


- information about the shape and size of macromolecules, characteristic distances of partially ordered materials, pore sizes, and other data.
- structural information of macromolecules between <1 nm and 25 nm, of repeat distances in partially ordered systems of up to 150 nm



Experiments:

- I911-SAXS beamline at MAX IV Laboratory, Lund University
- Custom built uniaxial tensile test machine
- 29 MPx stereo DIC system



Engqvist et al., 2014

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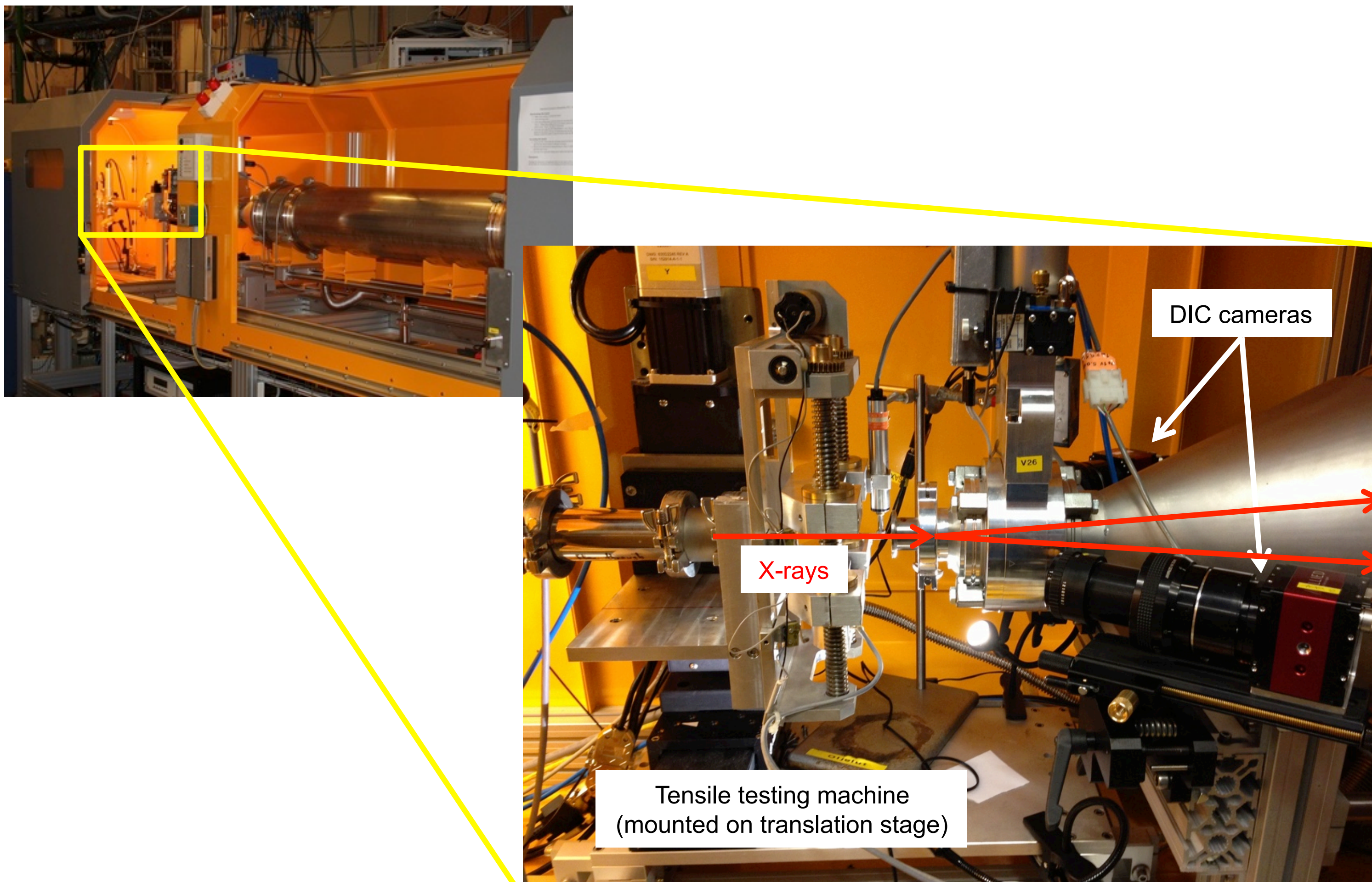
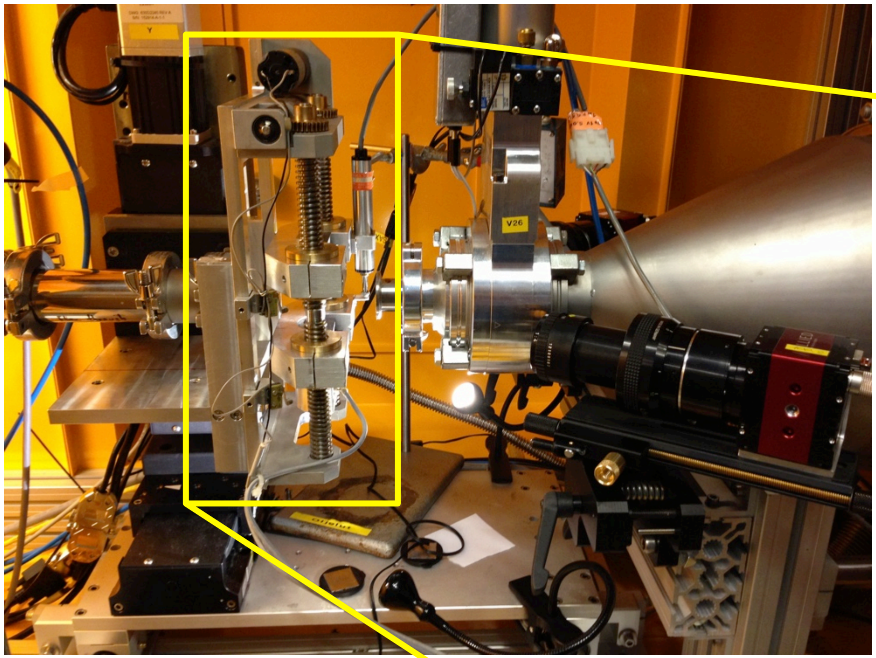
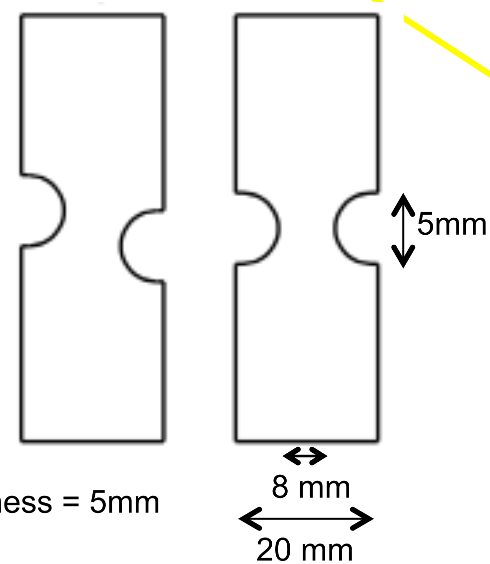


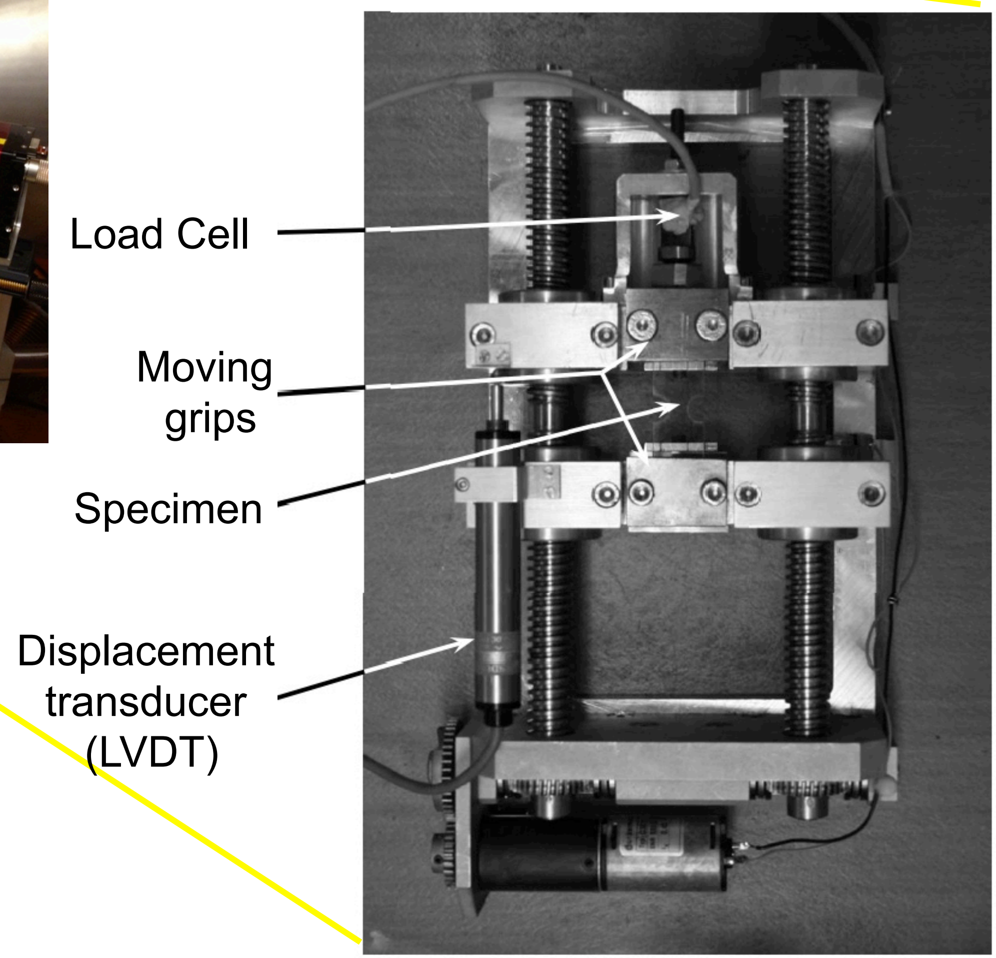
Engqvist et al., 2014

Experiments: set-up





Thickness = 5mm



Engqvist et al., 2014

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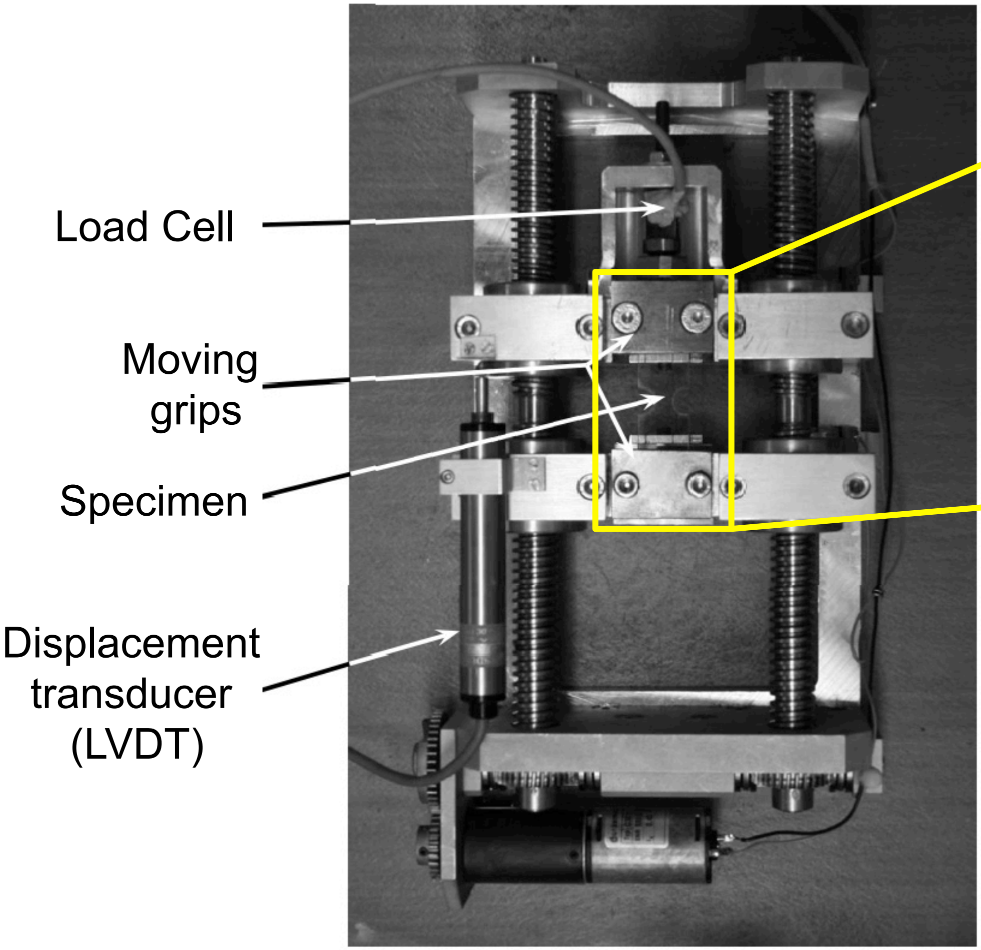
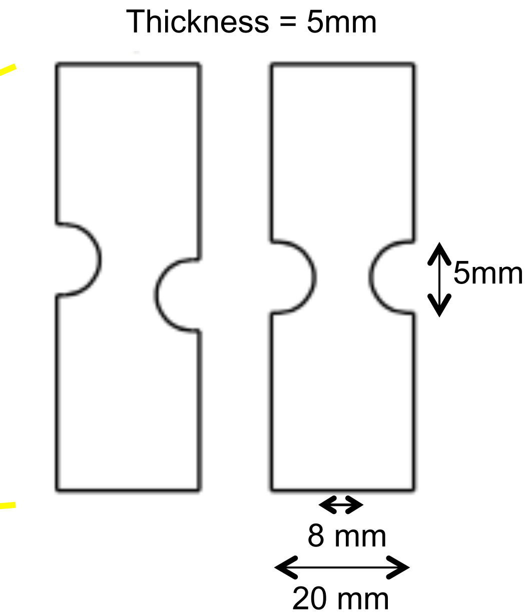
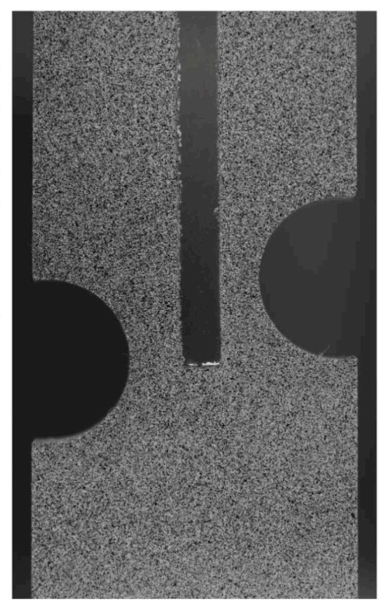


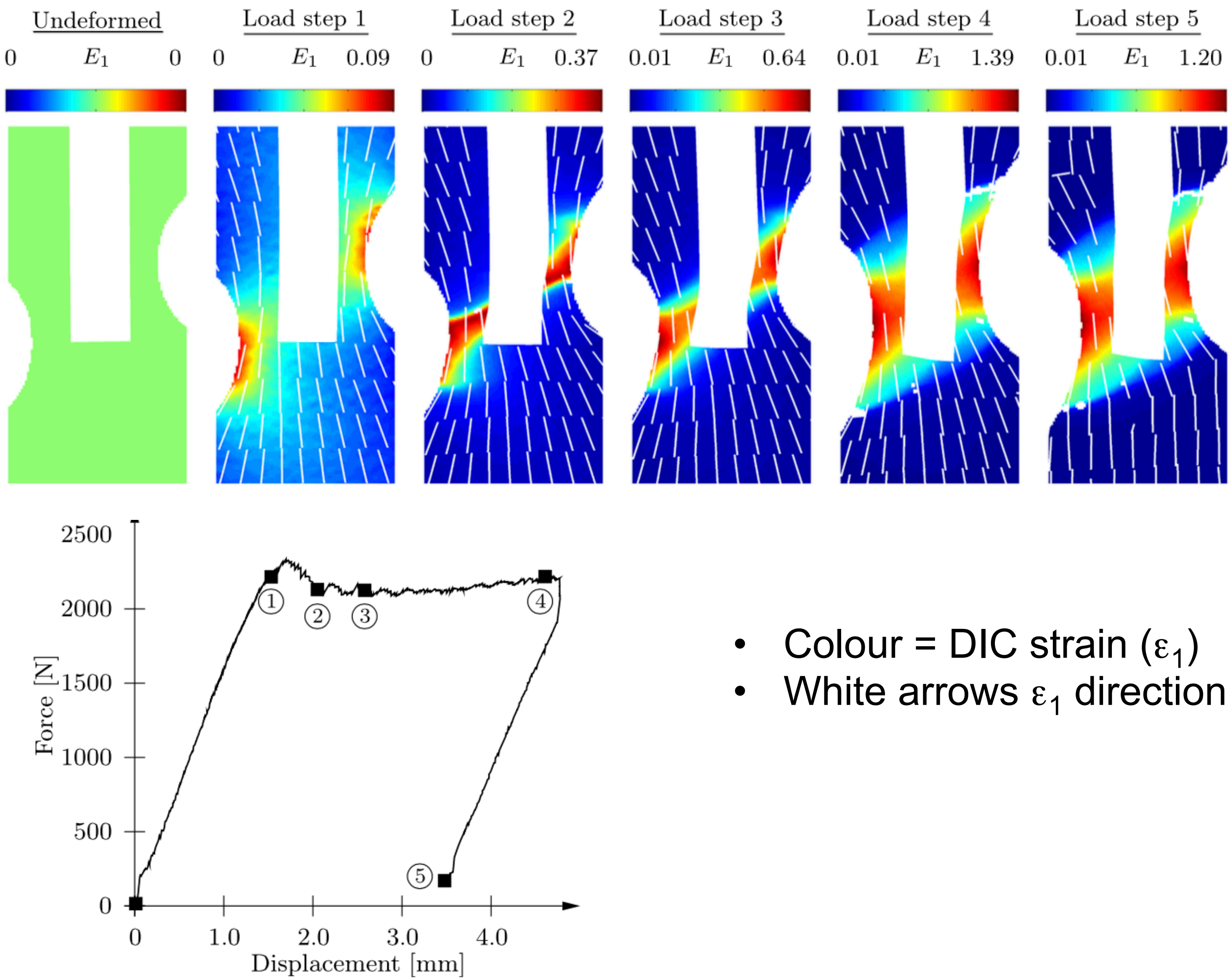




- Speckle applied with water-based paint (white then black speckle)
- Gap left for SAXS/WAXS to avoid scattering from paint

Engqvist et al., 2014

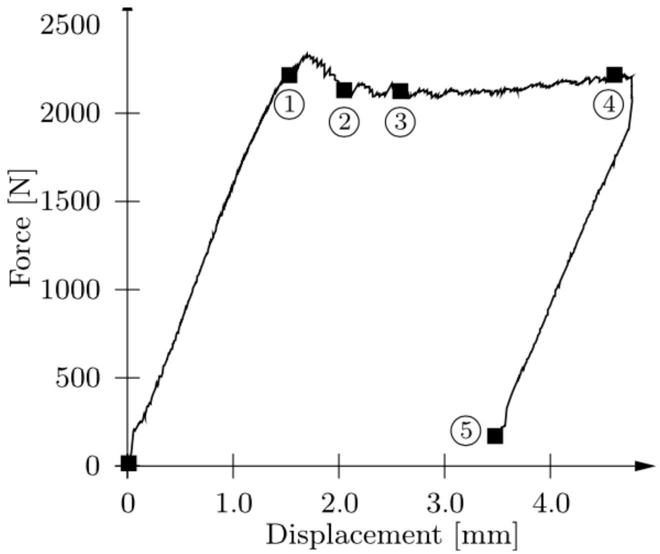
Experiments: DIC + in-situ loading

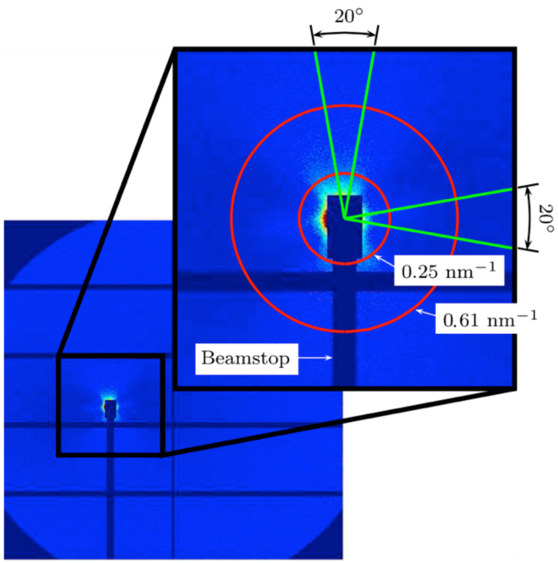


- Colour = DIC strain (ε_1)
- White arrows ε_1 direction

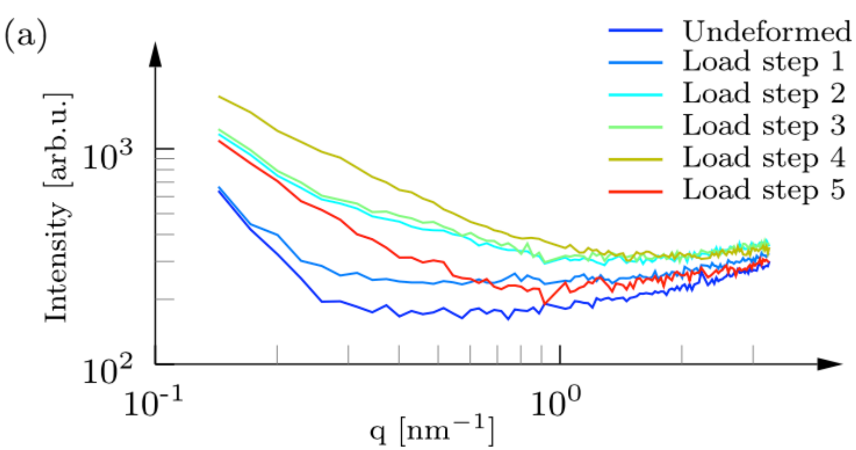
Engqvist et al., 2014

Experiments: SAXS + DIC + in-situ loading

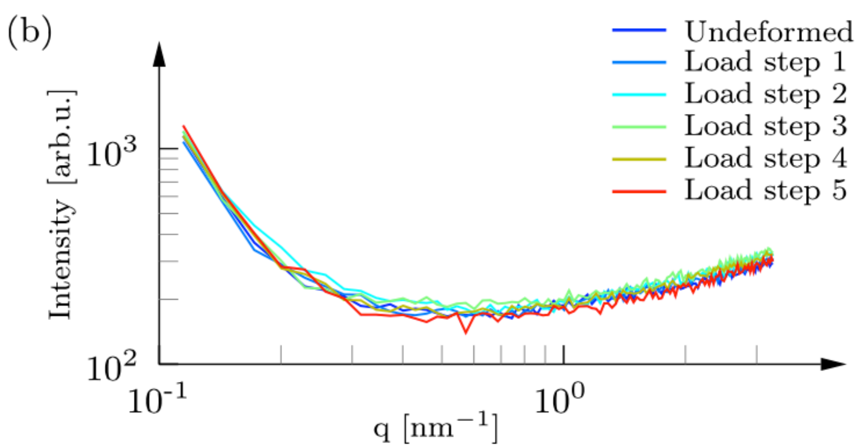




SAXS parallel to loading

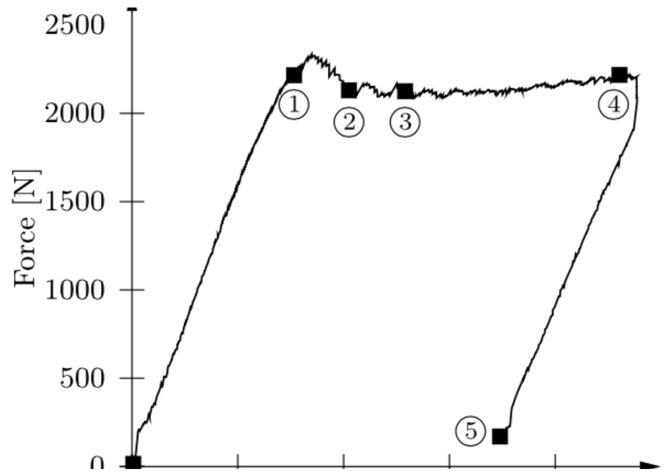


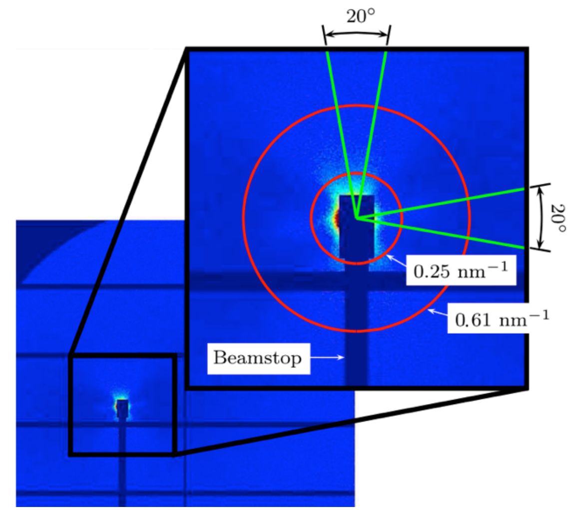
SAXS perpendicular to loading



Engqvist et al., 2014

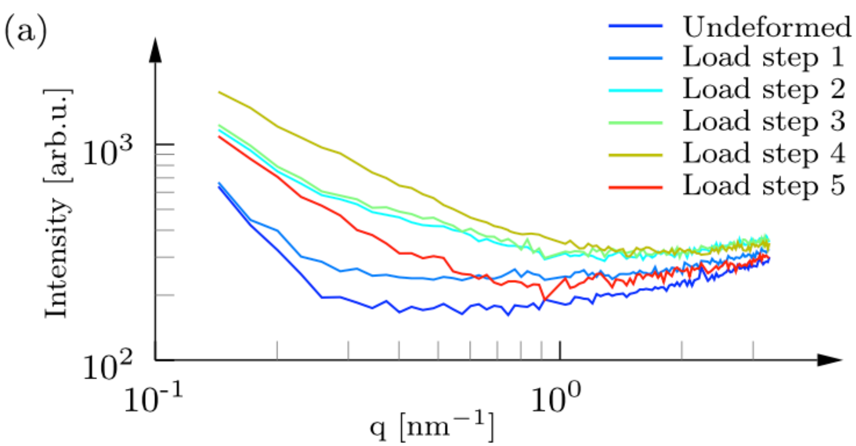
Experiments: SAXS + DIC + in-situ loading



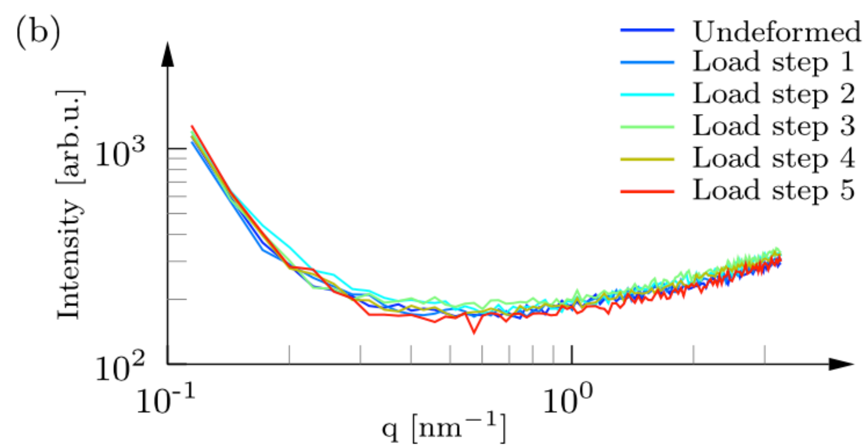


Note: SAXS data corrected for thickness change based on DIC

SAXS parallel to loading

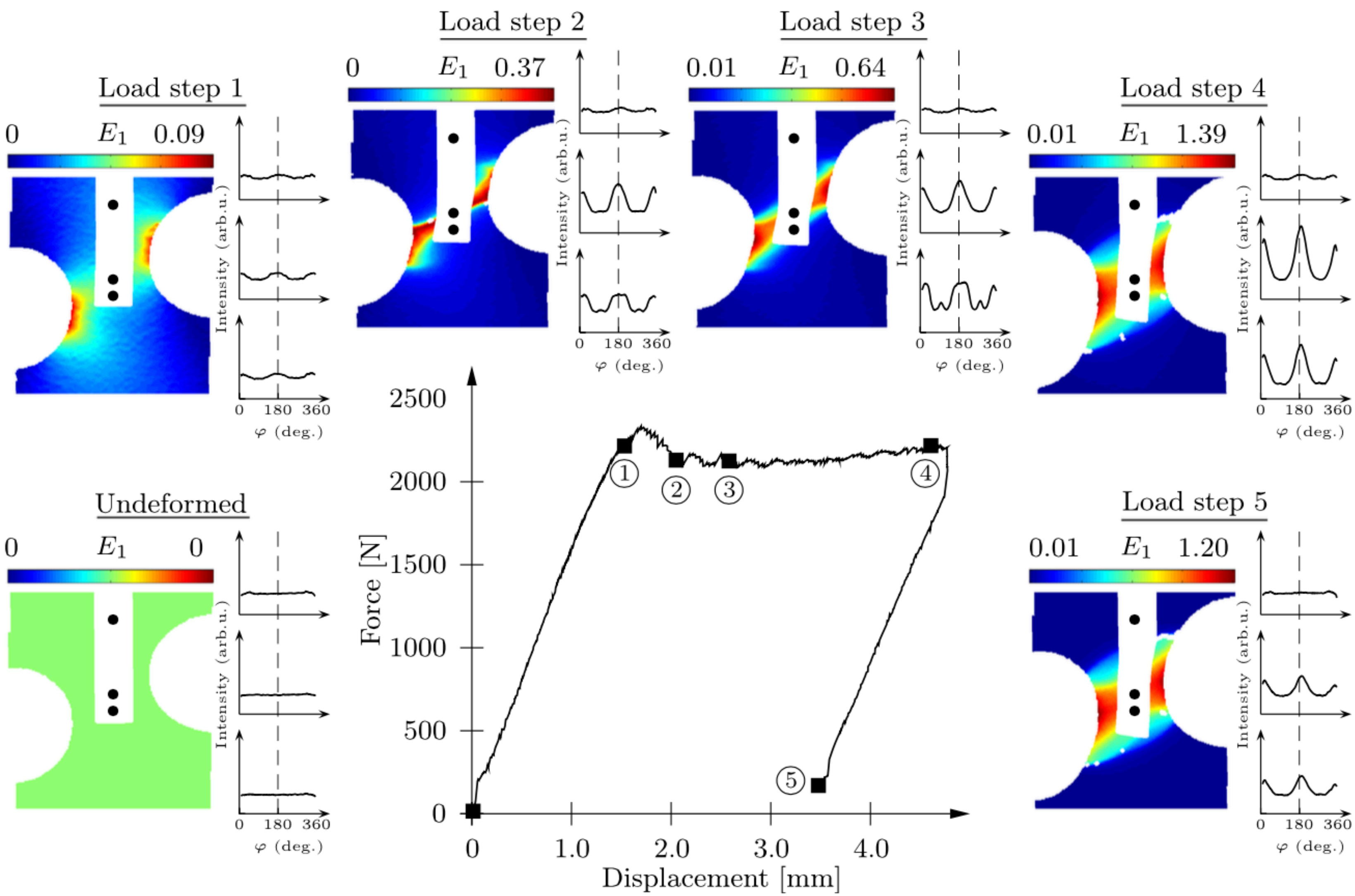


SAXS perpendicular to loading



Engqvist et al., 2014

Experiments: SAXS + DIC + in-situ loading

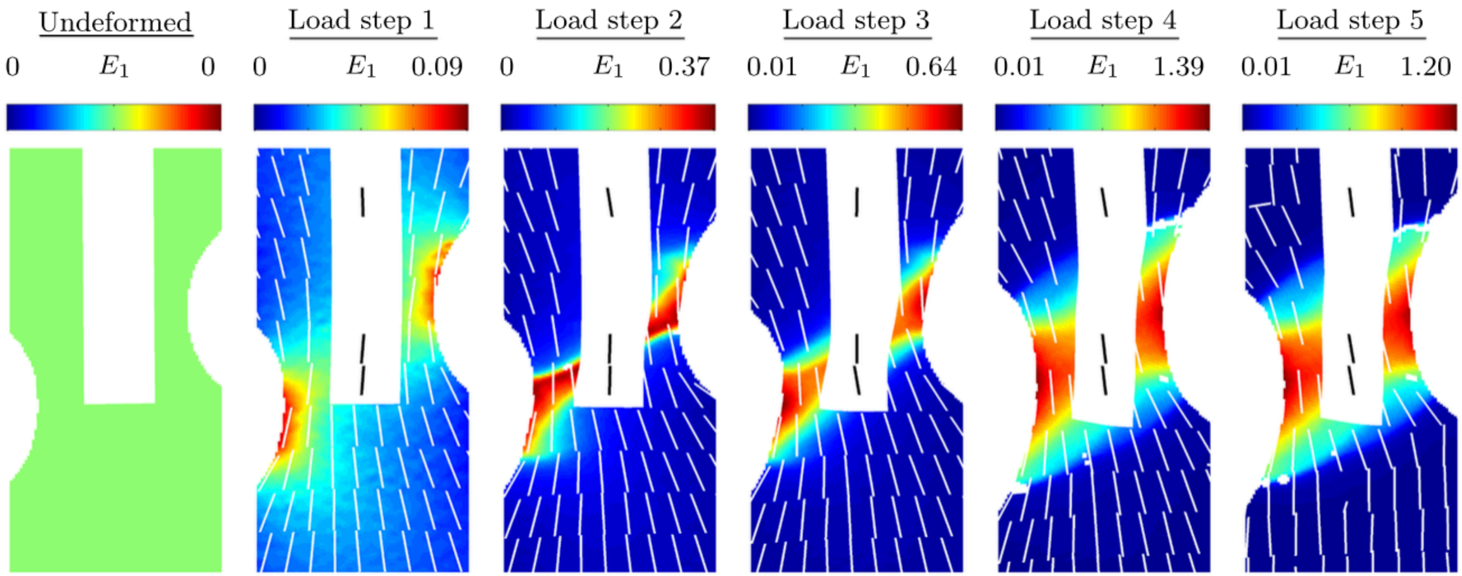


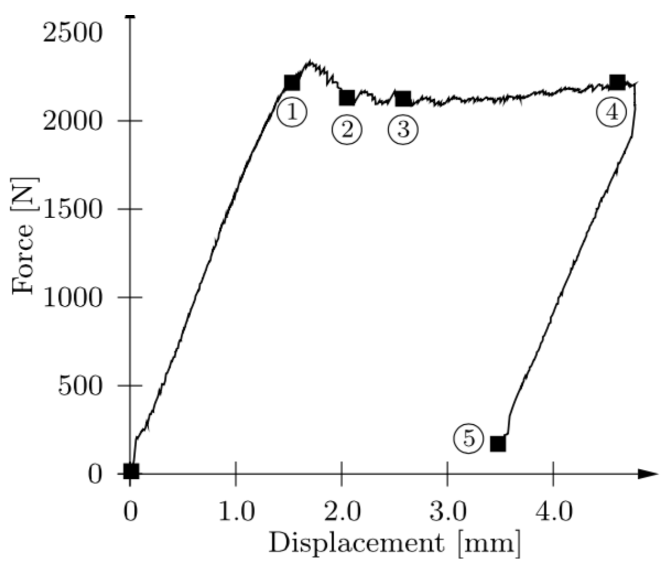
Colour maps = DIC strain (ε_1), azimuthal SAXS profiles to right of each plot

Engqvist et al., 2014

Experiments: SAXS + DIC + in-situ loading

- Strain Anisotropy vs SAXS anisotropy



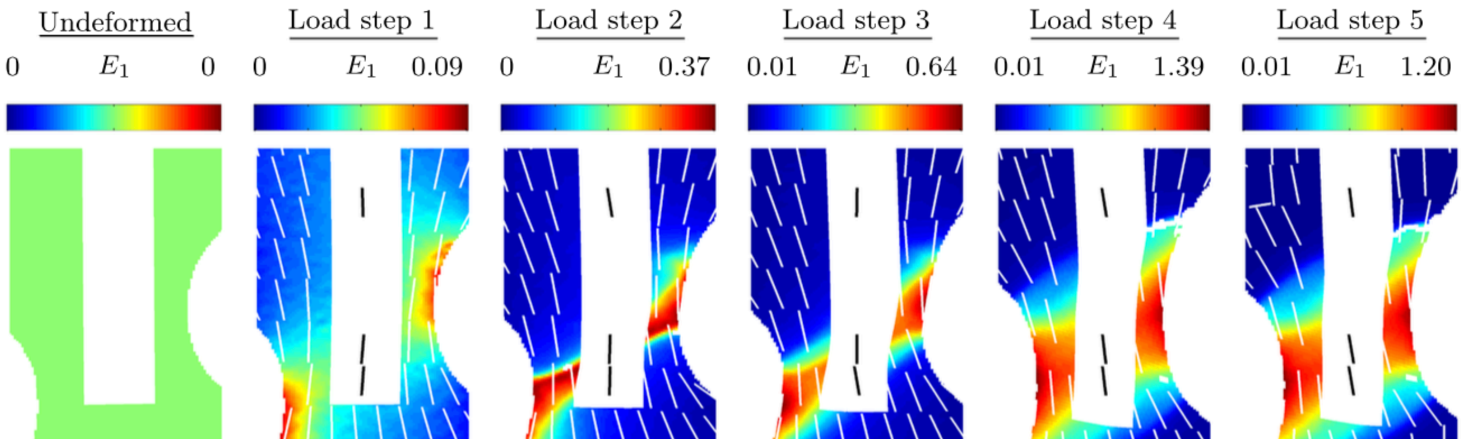


- Colour = DIC strain (ε_1)
- White arrows ε_1 direction
- Black arrows SAXS principle direction

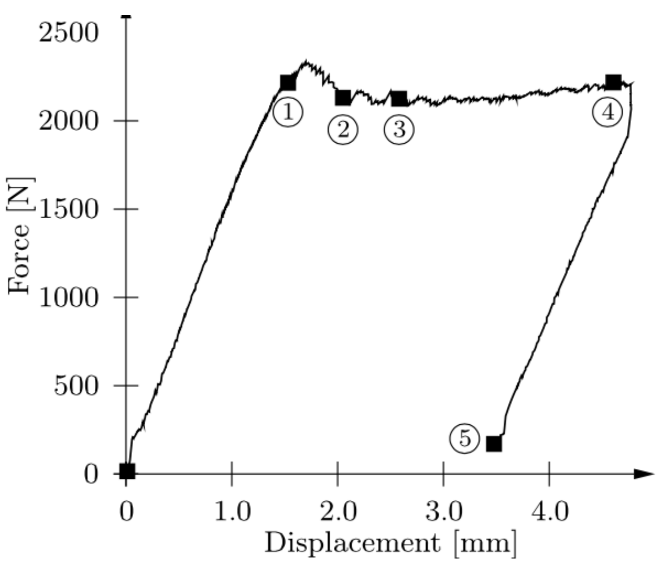
Engqvist et al., 2014

Experiments: SAXS + DIC + in-situ loading

- Strain Anisotropy vs SAXS anisotropy



Correlation between micro- and meso-scale anisotropies



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Engqvist et al., 2014

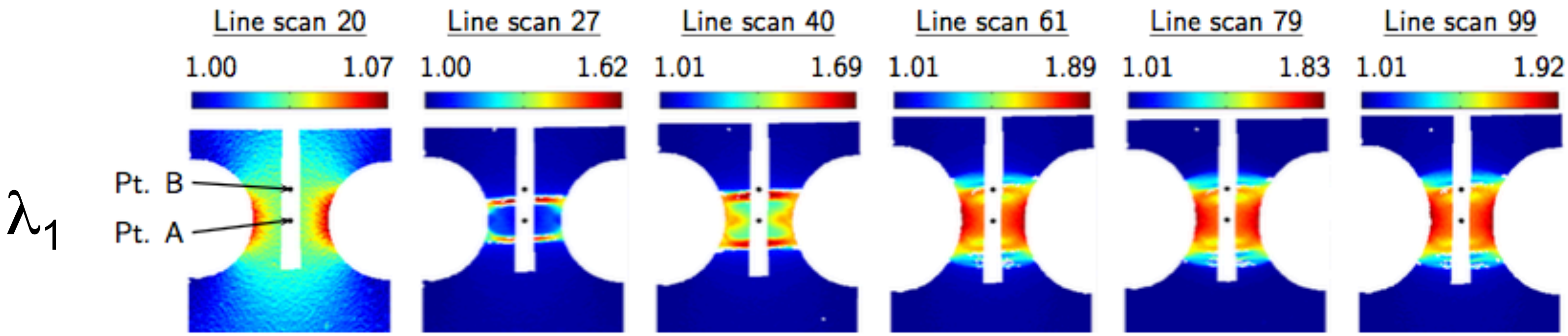
Experiments: WAXS + DIC + in-situ loading

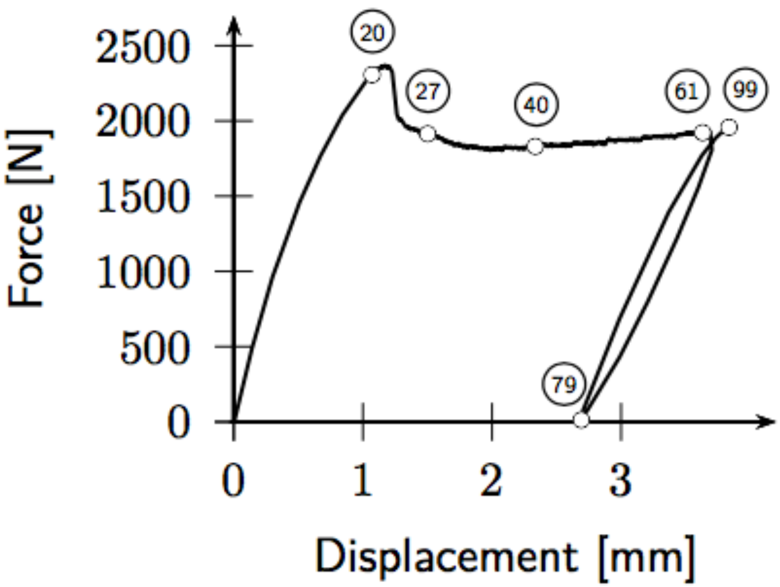
Engqvist et al., 2015, submitted

Experiments: DIC + in-situ loading

Engqvist et al., 2015, submitted

<u>Principal stretches</u>



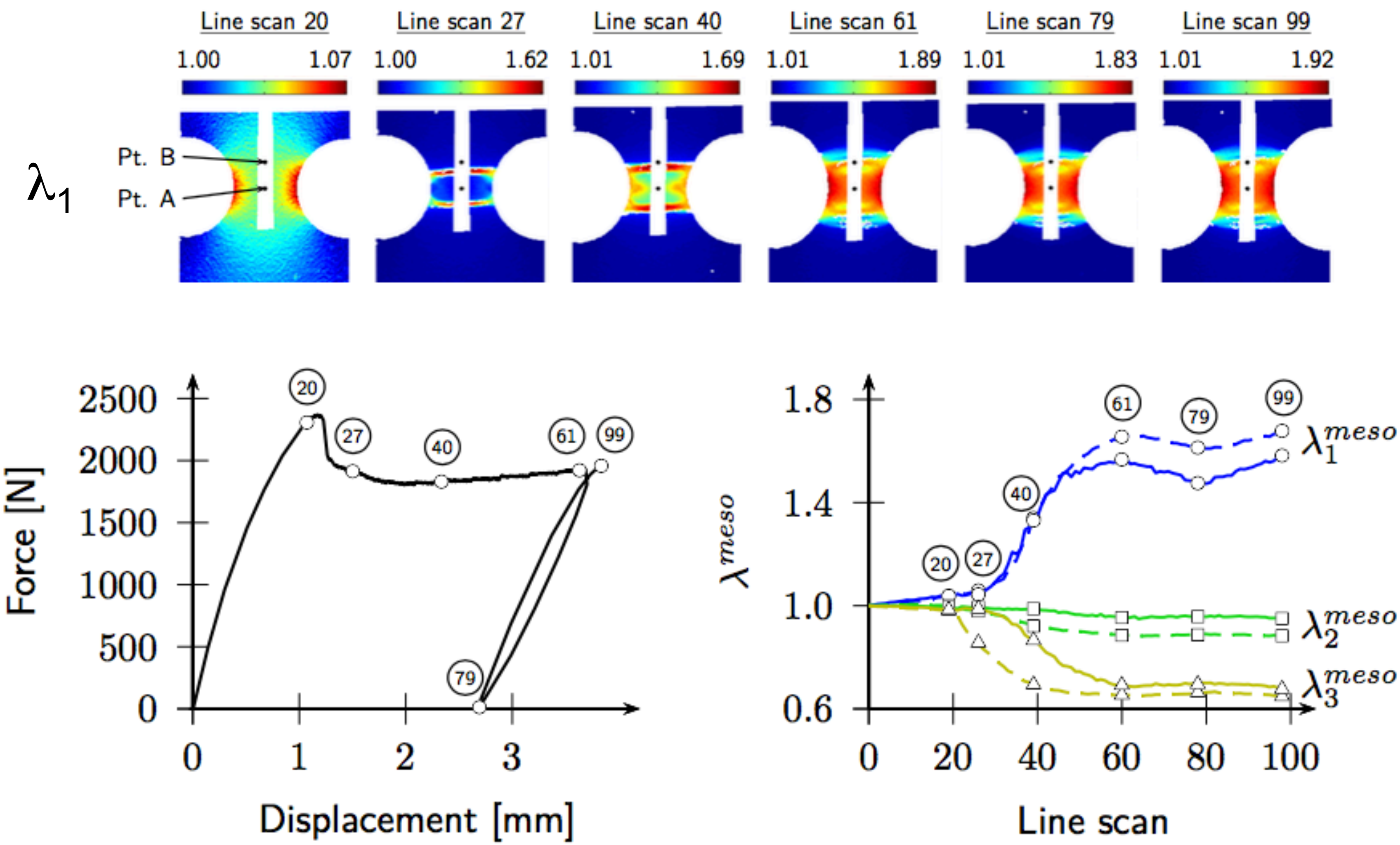


λ_{1meso} is dominated by longitudinal in-plane deformation,
λ_{2meso}meso - transverse in-plane deformation,
λ_{3meso} - out-of-plane deformation

Experiments: DIC + in-situ loading

Engqvist et al., 2015, submitted

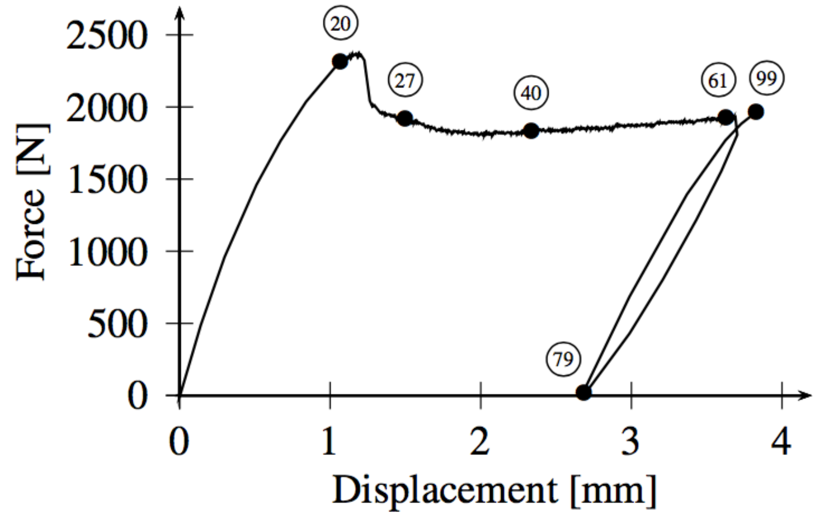
Principal stretches



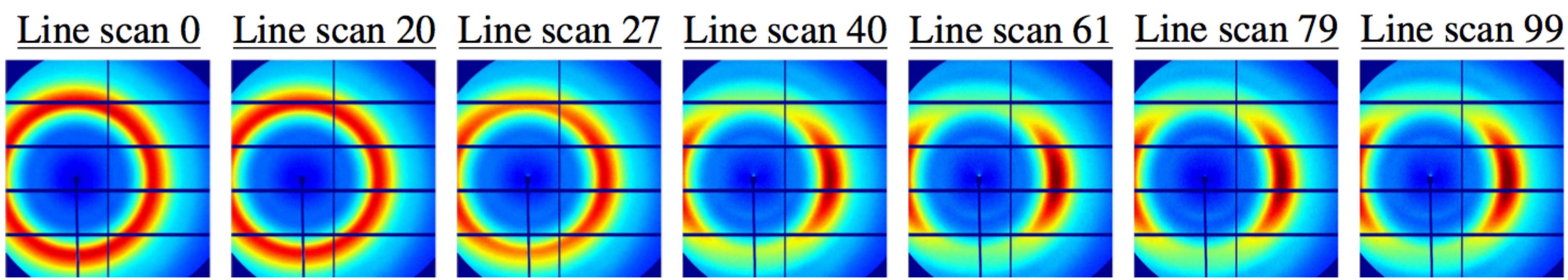
- Dashed lines – point A
- Solid lines – point B

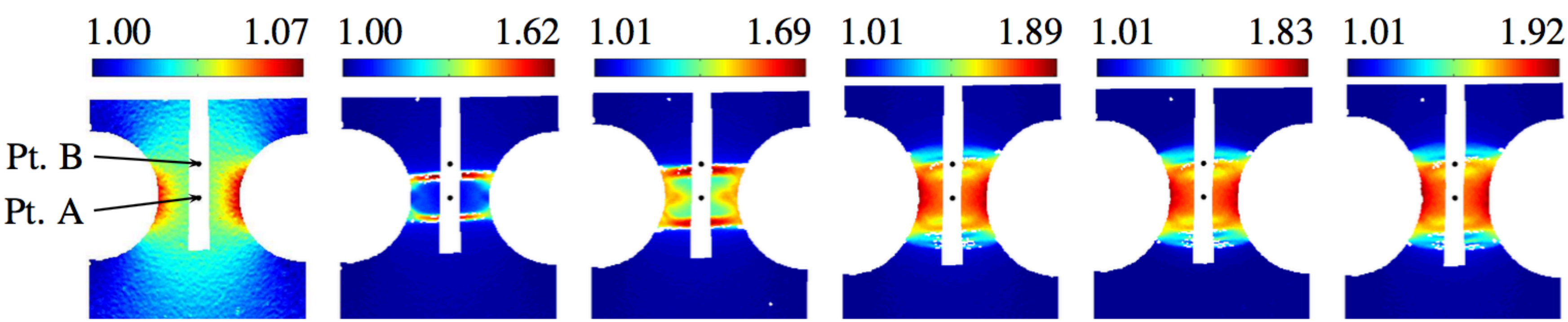
Experiments: WAXS + DIC + in-situ loading

Engqvist et al., 2015, submitted

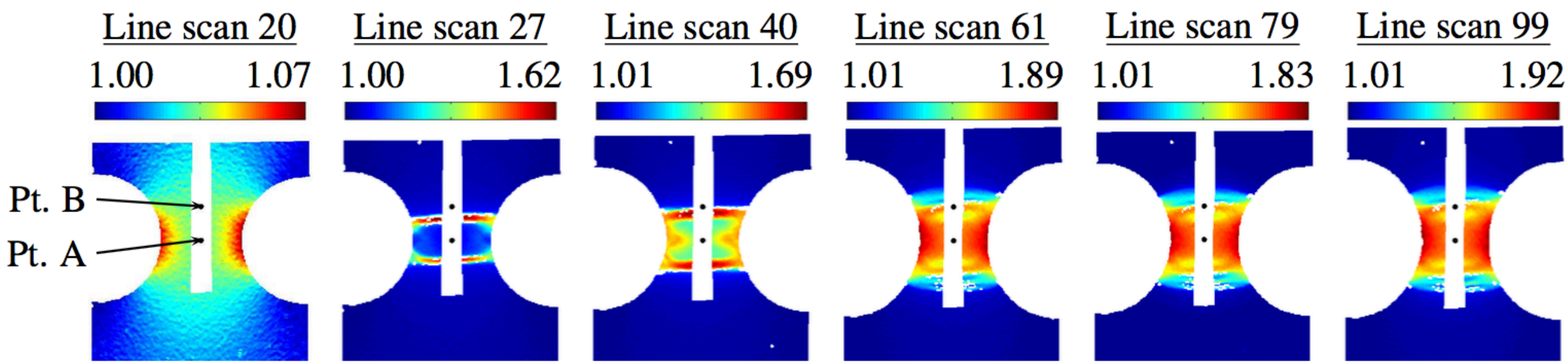


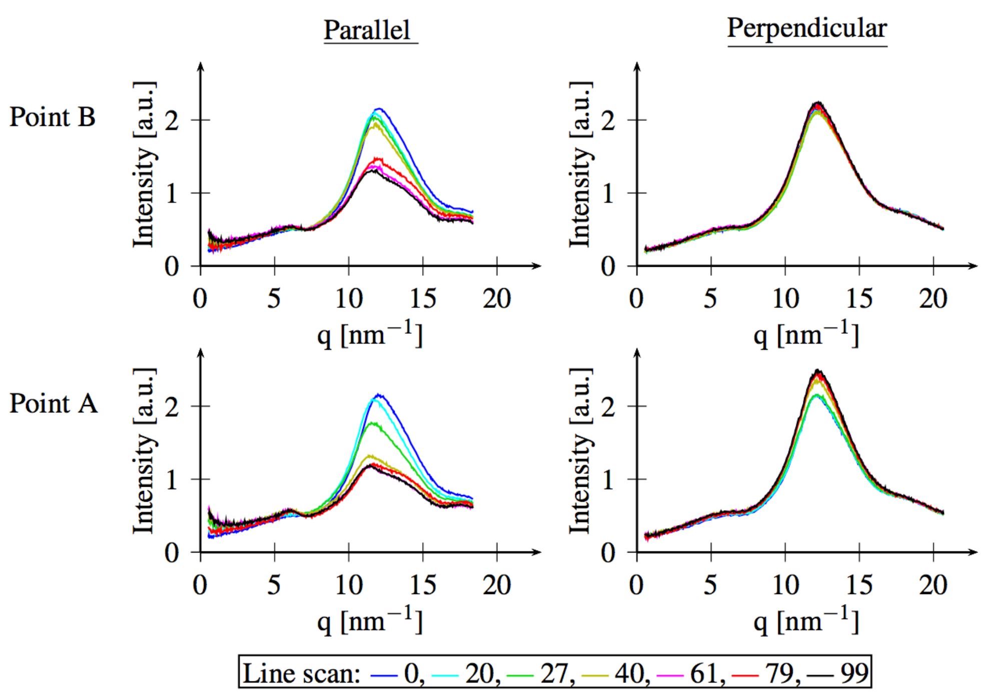
WAXS: point A





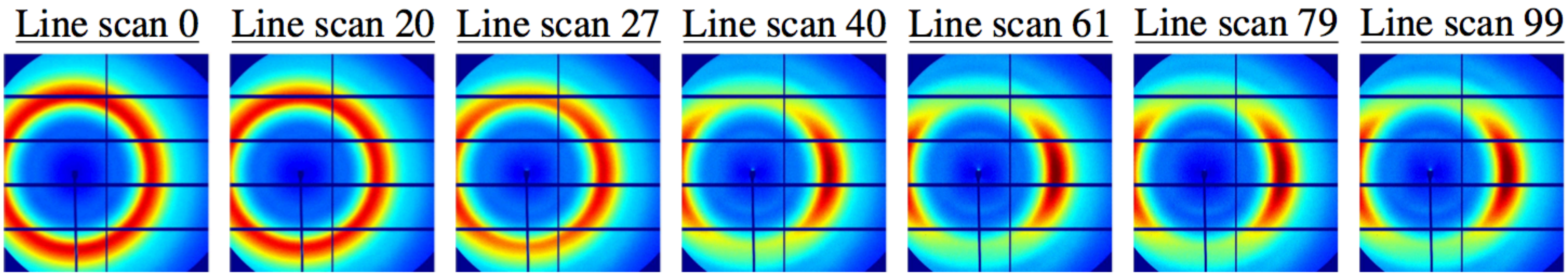
Experiments: WAXS + DIC + in-situ loading



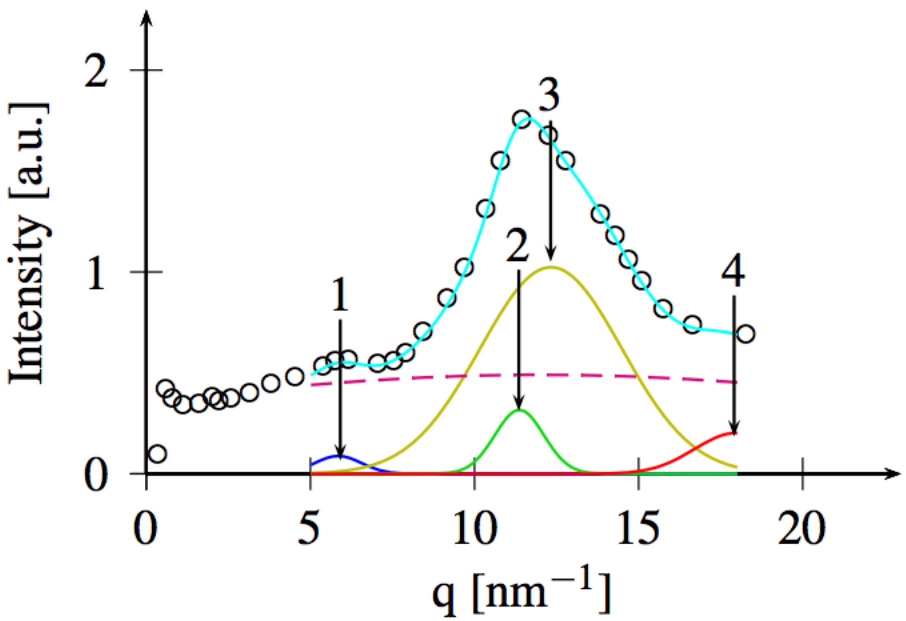


Experiments: WAXS + DIC + in-situ loading

WAXS: point A



Peak fitting



Peak 1: correlations between consecutive carbonate groups along the chain

- (q = 6.2 nm−1, d = 1.0 nm);

Peak 2: correlations between neighbour chains

- (q = 11.8 nm−1, d = 0.53 nm);

Peak 3: correlations between closely positioned entities along the chain

- (q = 12.7 nm−1, d = 0.49 nm);

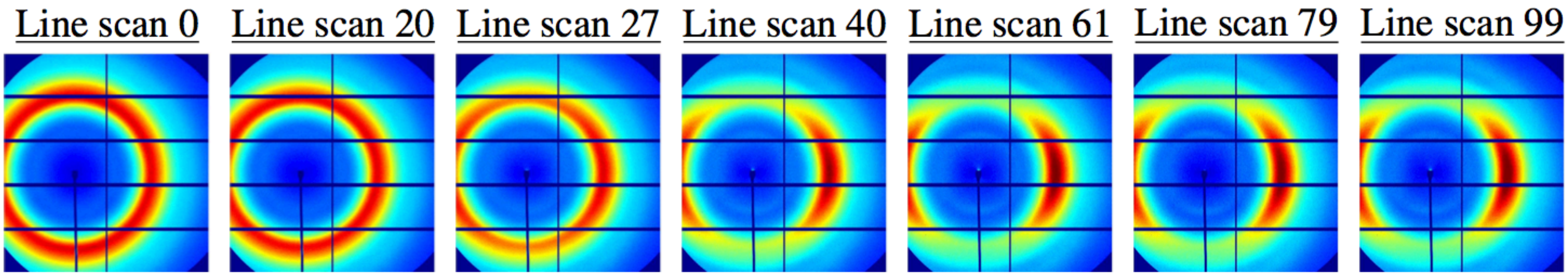
Peak 4: a mixture of inter- and intramolecular correlations

- (q = 18 nm−1, d = 0.35 nm).

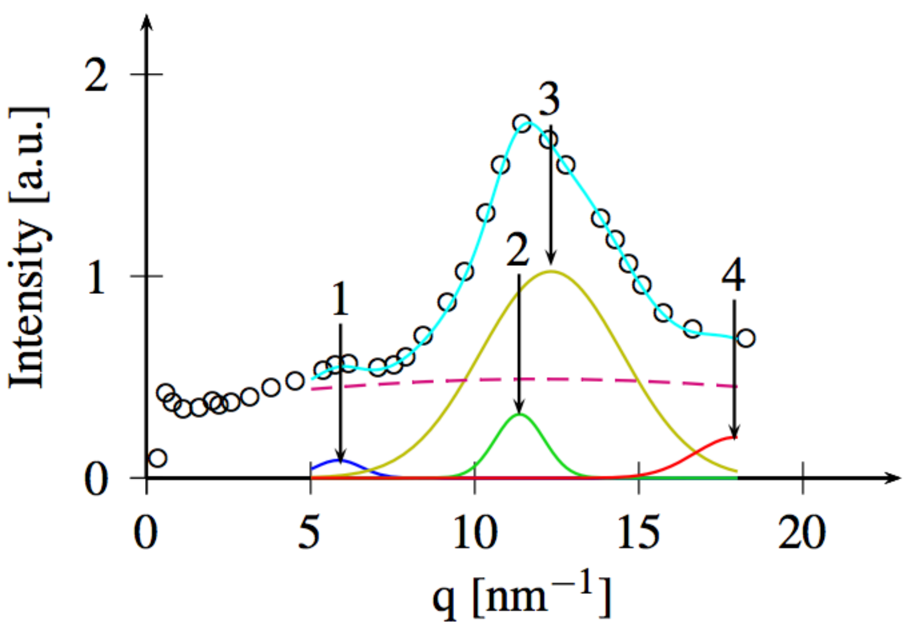
Engqvist et al., 2015, submitted

Experiments: WAXS + DIC + in-situ loading

WAXS: point A



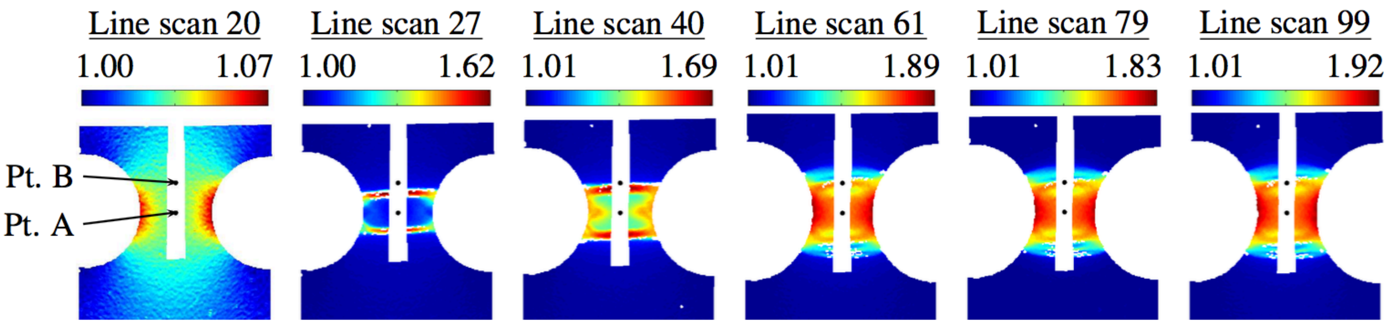
Peak fitting

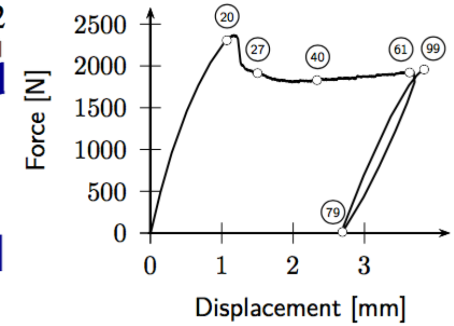


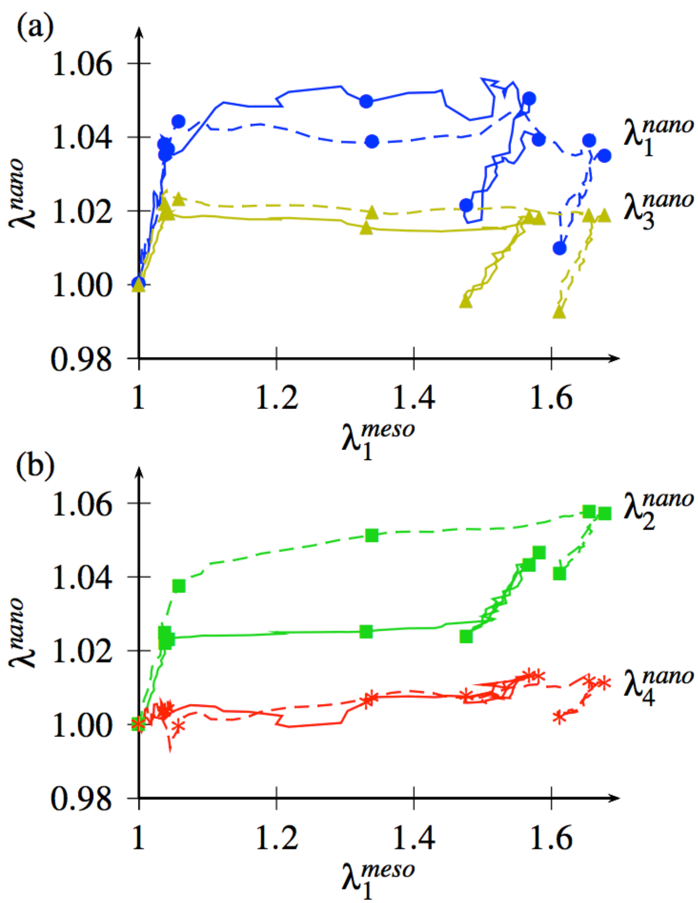
- Peak positions → strain
- Peak intensities → number of scatterers, anisotropy
- Peak width → spread of q values

Engqvist et al., 2015, submitted

Multi-scale strain measurements: WAXS + DIC







λ_{meso} “meso-scopic” (local) strain from DIC

Peak 1: correlations between consecutive carbonate groups along the chain

Peak 3: correlations between closely positioned entities along the chain

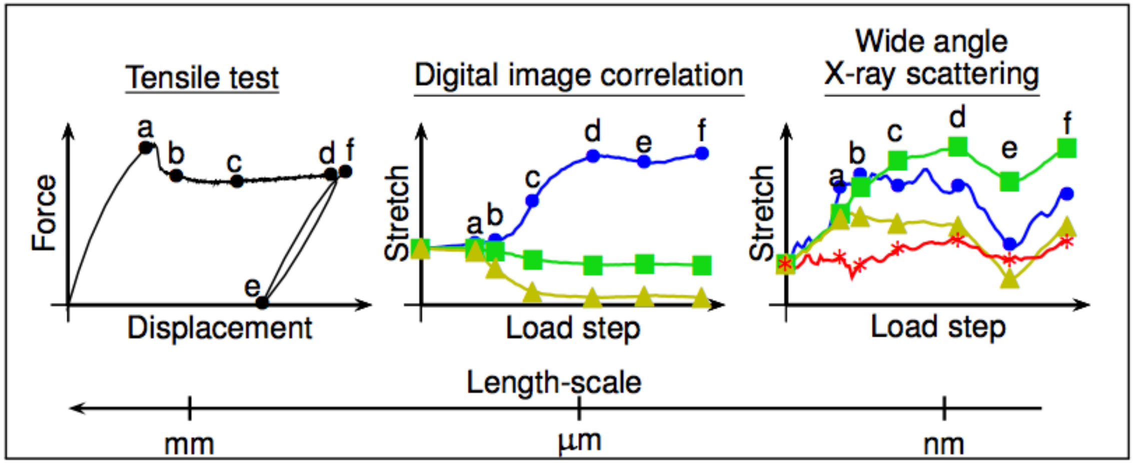
Peak 2: correlations between neighbouring chains

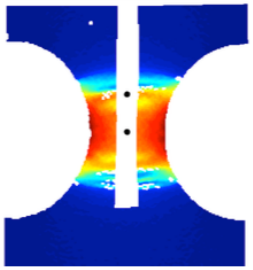
Peak 4: a mixture of inter- and intramolecular correlations

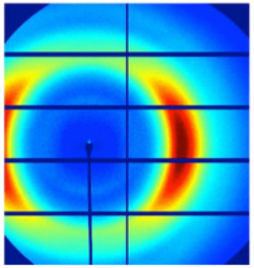
- Dashed lines – point A
- Solid lines – point B

Engqvist et al., 2015, submitted

Multi-scale Deformation of Polycarbonate Using X-ray Scattering with In-situ Loading and Digital Image Correlation







- Tensile loading: “averaged” stress-strain response of the sample
- DIC: local “macroscopic” strain field
- SAXS and WAXS: structures from about 100 nm to a few Ångström
  - Scanning to get spatial resolution

Engqvist et al., 2015, submitted

New model for amorphous polymers

- Elasto-plastic model with inclusion of evolving orientation-distribution function
- Developed independently from experiments, but calibrated to “homogeneous” test data (macroscopic)

Engqvist et al., 2016, in preparation

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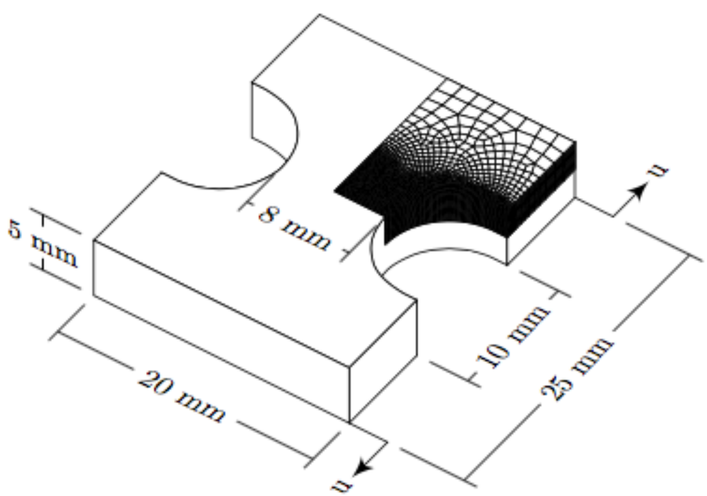

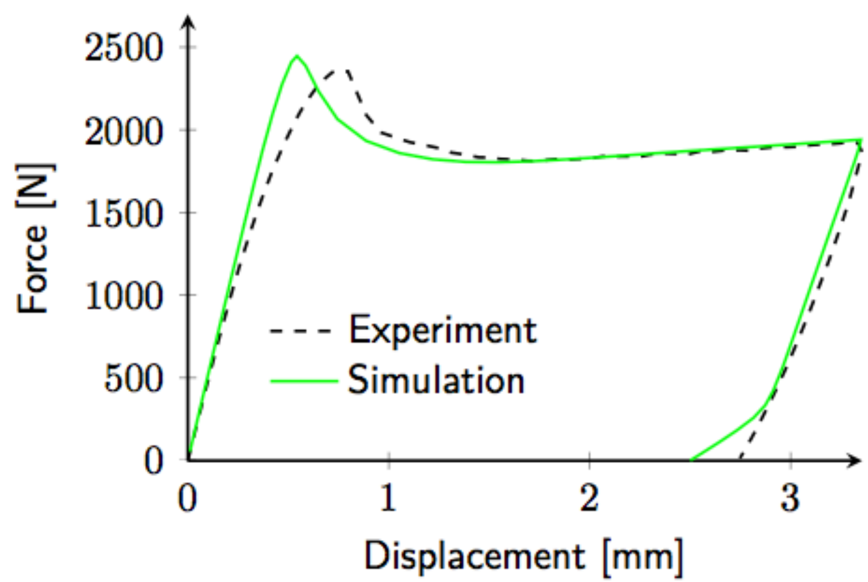

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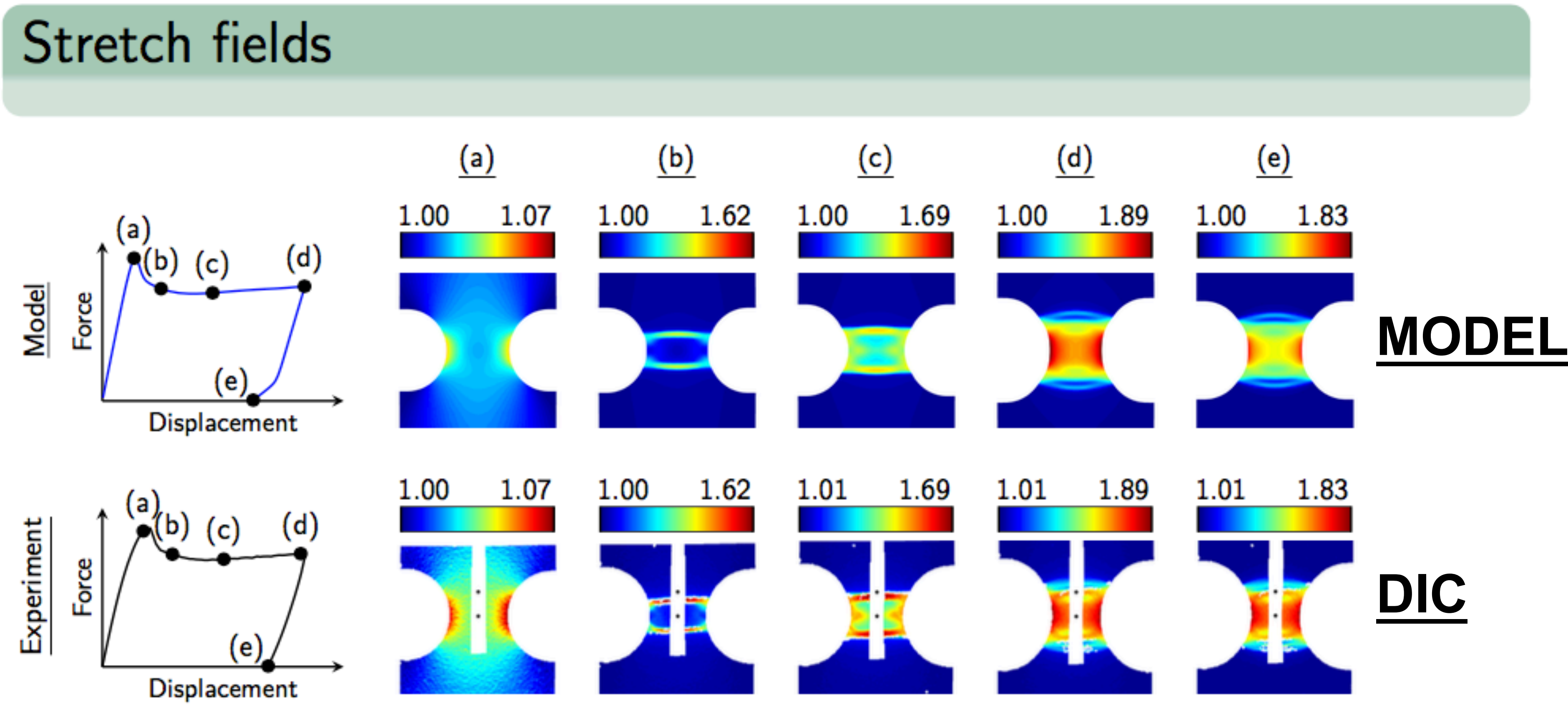

Engqvist et al., 2016, in preparation

SUMMARY

- Spatially-resolved measurements are essential to capture material and process heterogeneity
- Different measurement approaches can provide different details on the material behaviour
- In this case
  - DIC has been used to characterise local strains and strain heterogeneity)
  - Also provides essential information on sample thickness changes
  - X-ray scattering allows nano/micro-structural length scale evolution to be captured
    - Essential to have spatial resolution
    - Essential to also have appropriate <u>local</u> strain measures

- Next steps include enhancing link to modelling (beyond qualitative verification)