Molecular Deformation in High Performance Cellulose Fibres – Influence of Draw Ratio

Nandula D. Wanasekara[1], Stephen J. Eichhorn*[1], Sameer Rahatekar[2], Thomas Welton[3], Alexander Bismarck[4], Herbert Sixta[5], Kevin Potter[2]

[1]College of Engineering, Maths and Physical Sciences, University of Exeter, UK, [2]Faculty of Engineering, University of Bristol, UK [3]Faculty of Natural Sciences, Imperial College of London, [4]Institute of Materials Chemistry & Research, Polymer & Composite Engineering (PaCE), University of Vienna, Austria, [5]Department of Forest Products Technology, Aalto University, Finland

EPSRC
Engineering and Physical Sciences Research Council

UNIVERSITY OF EXETER

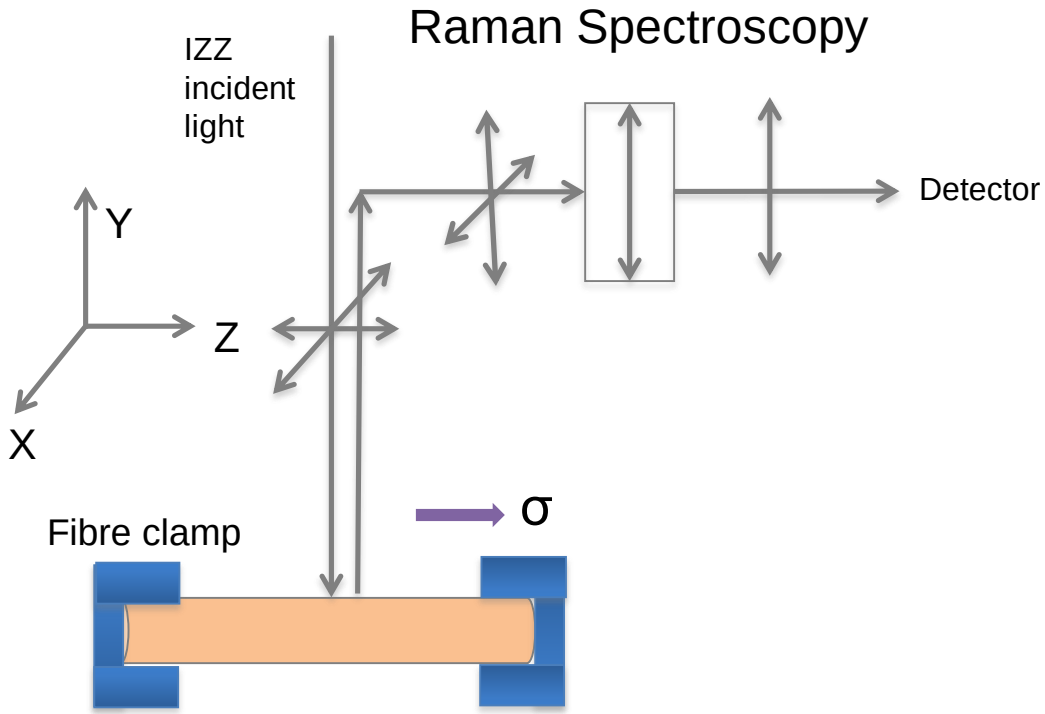
Goals and Materials

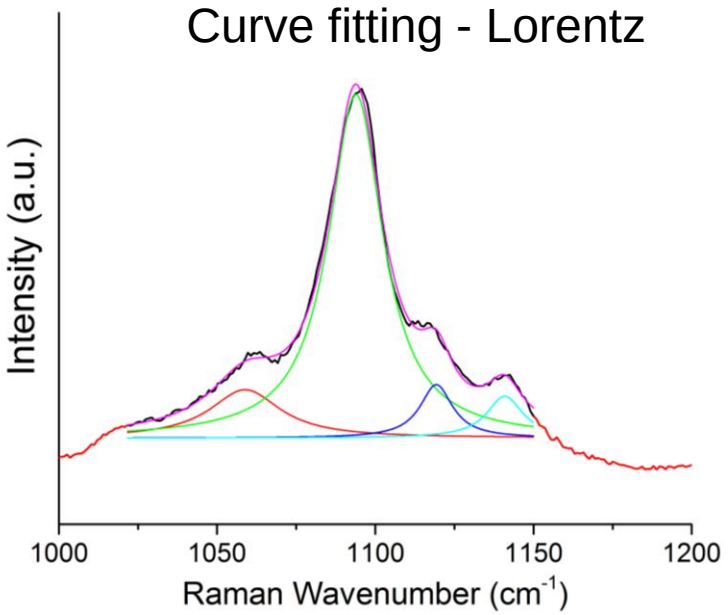
- Investigate the molecular strain in high performance cellulose fibres.
- Study the effect of draw ratio on molecular strain in cellulose fibres spun from liquid crystalline solutions.

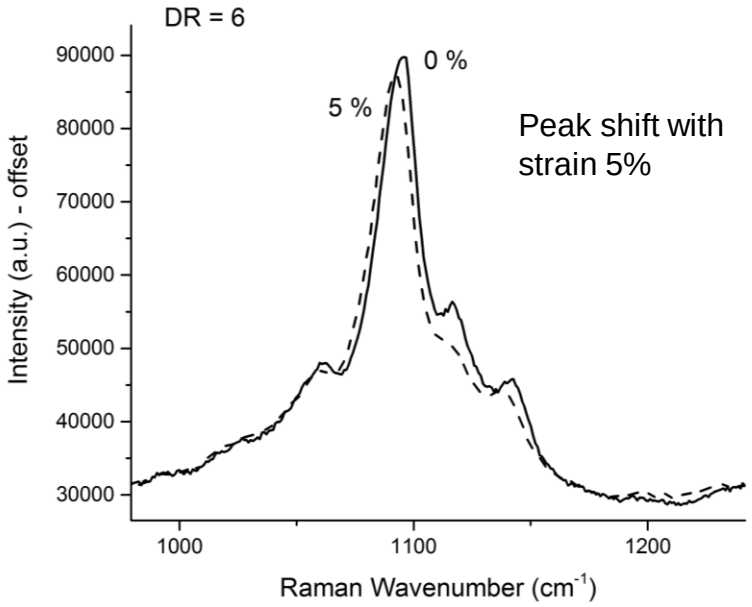
Bocel = A high modulus cellulose fibre spun from anisotropic phosphoric acid solution

Ioncell, Bristol = Fibres produced by dry-jet wet spinning using IL as the solvent.

Raman Band Shift with strain – cellulose fibres

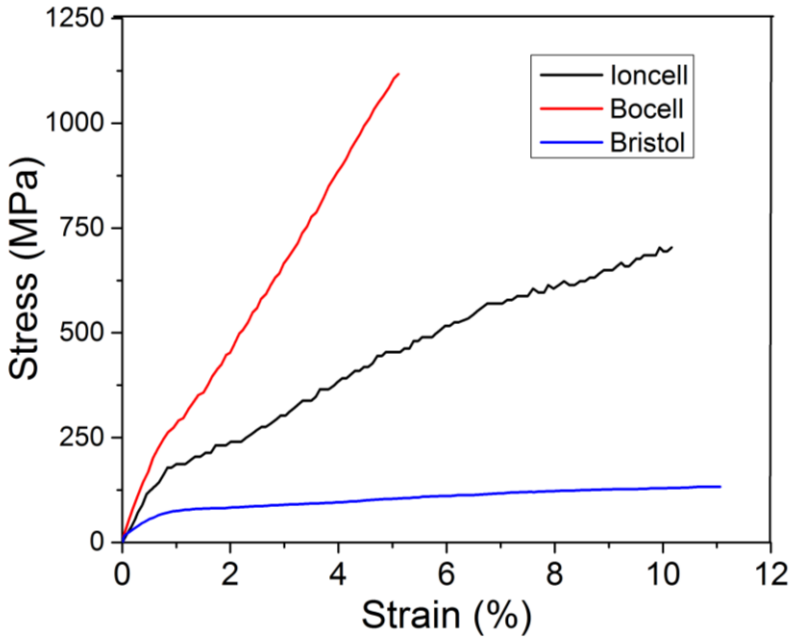


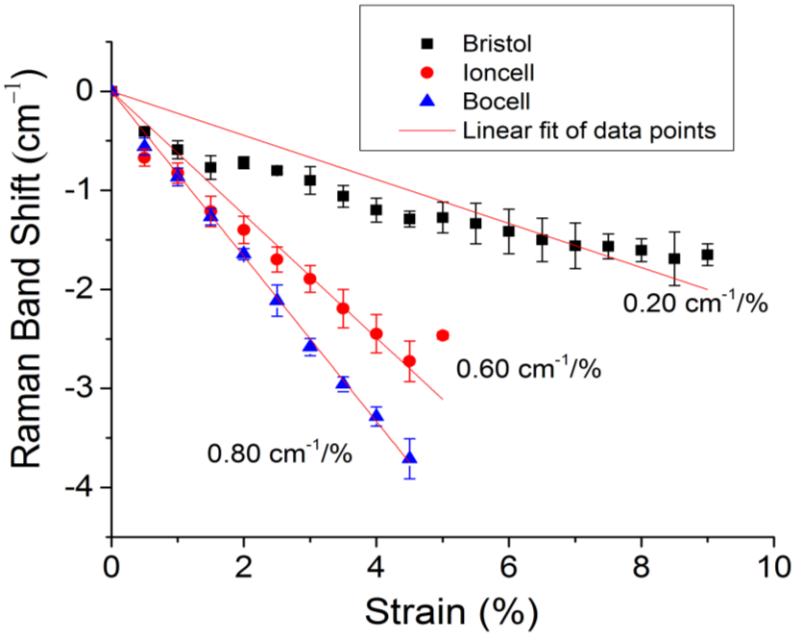




- The single fibres are stretched using a Deben Rig instrument.
- A Raman spectra is collected at every 0.5% increments of strain until failure.
- The peak position at 1095 cm^{-1} is analyzed for shift with strain and Raman shift rate with strain is calculated.

Raman Band Shift with strain



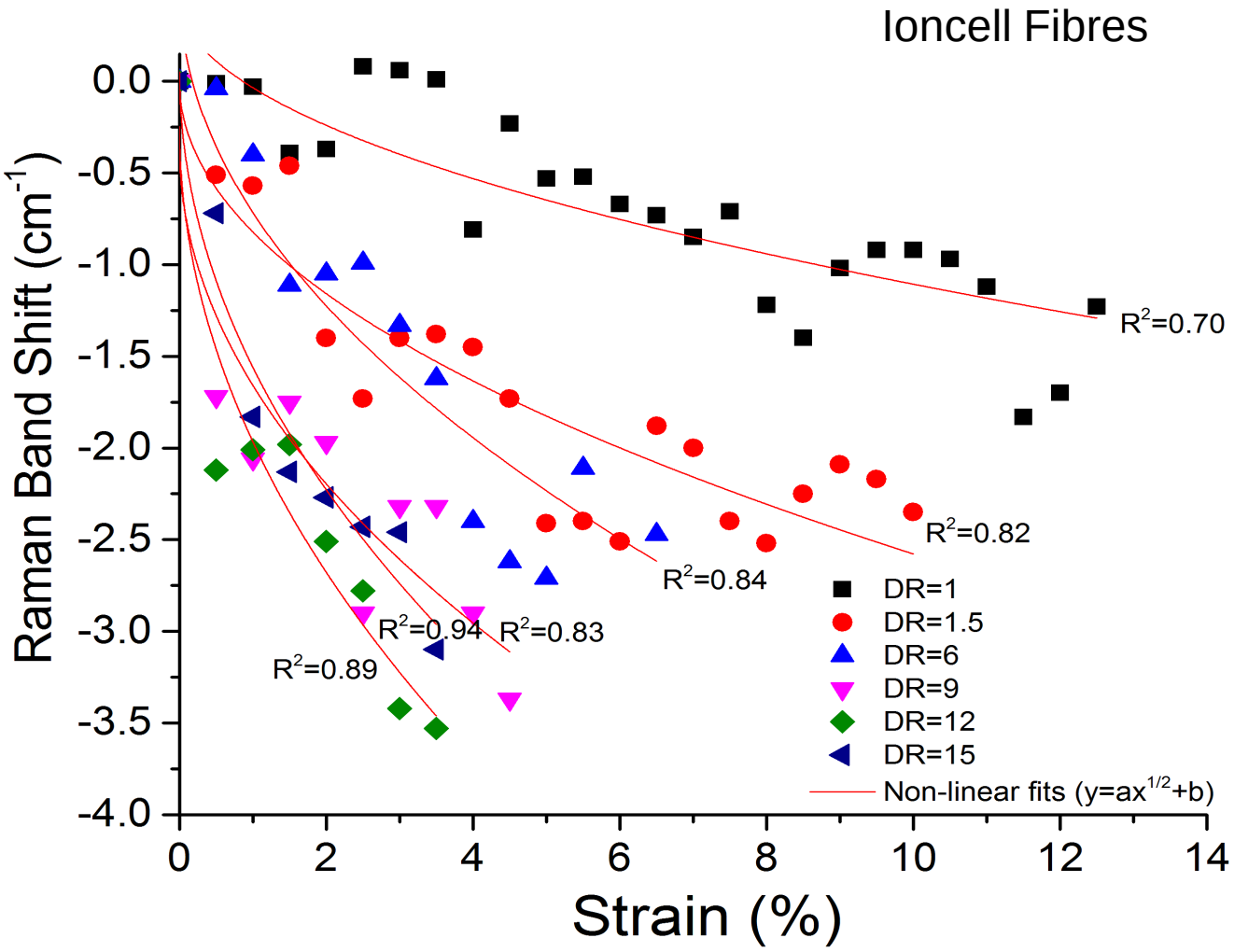


	Young's Modulus (GPa)	Tensile Strength (MPa)	Strain-at-break (%)
Ioncell	28 ± 1.2	724 ± 23	7.5 ± 0.4
Bocel	43 ± 2.4	1187 ± 58	5.2 ± 0.1
Bristol	22 ± 1.3	158 ± 6.2	14 ± 0.6

- Bocel fibres exhibited higher modulus and lowest strain-at-break.
- Bocel fibres exhibited the highest Raman band shift rate with strain showing higher molecular strain on cellulose chains upon deformation

Unpublished Data

Non-linear behavior – Raman Spectroscopy

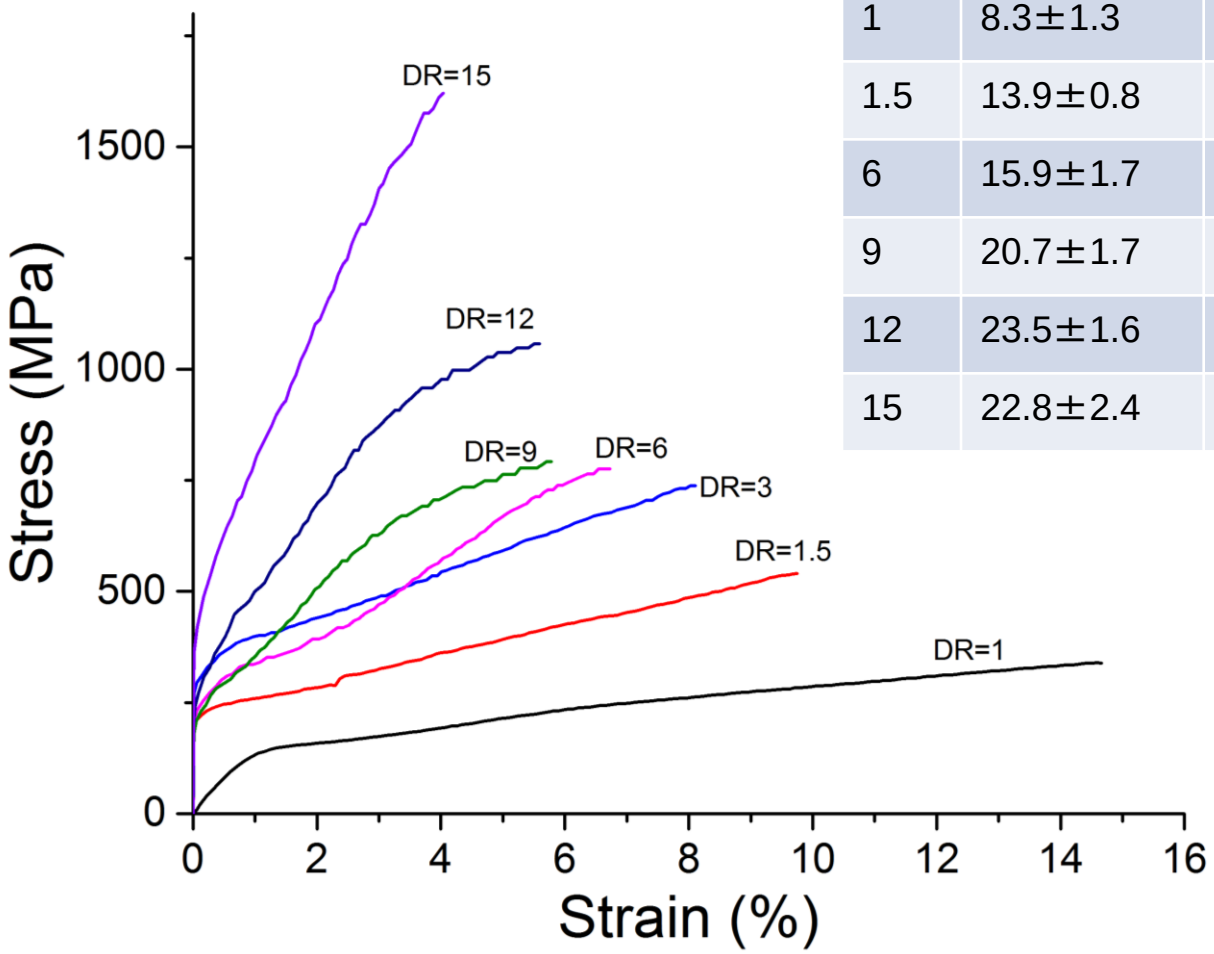


Draw Ratio	Raman shift per strain (cm-1/%) at 1% strain
1	-0.25
1.5	-0.40
6	-0.61
9	-0.65
12	-0.85
15	-0.80

Unpublished Data

Tensile testing of loncell fibres

Draw Ratio	Young's Modulus (GPa)	Breaking Stress (MPa)	Strain-at-break (%)
1	8.3±1.3	390.7±+24.7	14.6±0.3
1.5	13.9±0.8	512.4±15.4	9.7±0.4
6	15.9±1.7	698.5±+50.3	6.1±0.5
9	20.7±1.7	806.5±38.7	5.6±0.1
12	23.5±1.6	1097.4±86.2	4.5±0.4
15	22.8±2.4	1343.5±149.5	5.1±0.3



Unpublished Data

Conclusions

- For a high draw-ratio, c-o-c bond is mostly parallel to the fibre axis, and **chain stretching** is the most dominant deformation mechanism.

- For low draw ratio, **rotation of molecules** dominates the deformation mechanism.