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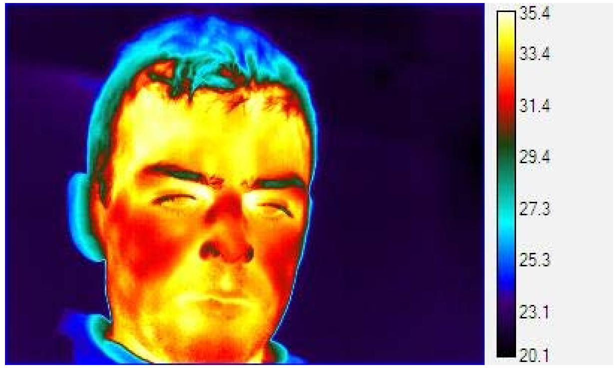
Changes in the thermal properties of polymeric materials induced by molecular orientation: Experimental methods, current understanding and strategies for the application to numerical methods.

David Nieto Simavilla

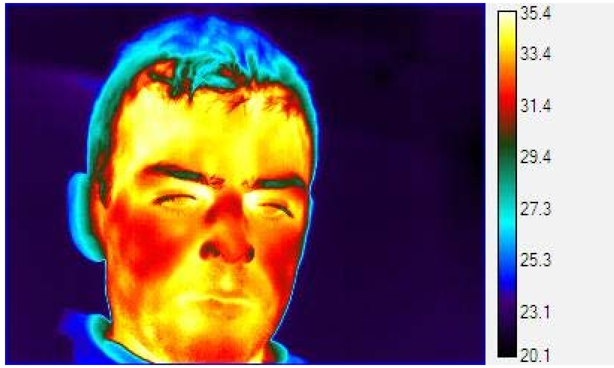
MARIE CURIE ACTIONS

HORIZON 2020

Outline



- Who am I?
- The MCIATTP project
- Anisotropic Thermal Transport: Experiments
- Key findings and open questions
- The road to macroscopic simulations
- Roadmap for the next 6 (5.25) months



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16-17 Postdoc – Université livre de Bruxelles
14-16 Applications Engineer at RheoSense Inc.
09-14 Ph.D & Master in Chemical Engineering – Illinois Institute of Technology
03-09 Industrial Engineering - Madrid Polytechnic University

Deformation & molecular orientation induced phenomena:

- Anisotropy in thermal conductivity
- Heat capacity changes in elastomers

Transport phenomena: Marangoni flow

- Temperature vs. Concentration induced gradients in WT

Microfluidic-based rheological instrumentation development:

- Biopharma applications

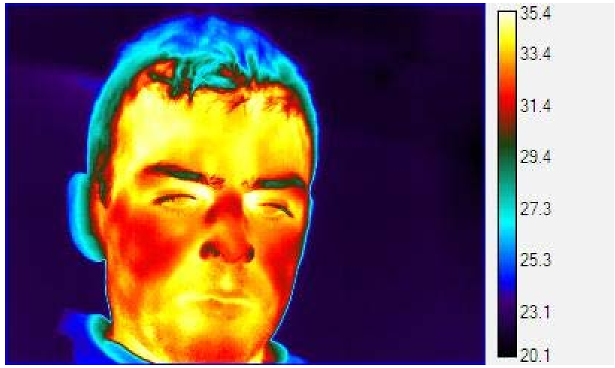
Polymer melt adsorption onto solid substrates:

- Adsorption mechanisms
- Control of the adhesion forces through film thickness
- Control of adsorption kinetics through annealing temperature

Non-isothermal polymer flow simulation:

- Finite volume simulation of industrially relevant flows
- Molecular simulation of transport processes – answer some key experimental questions

POLITÉCNICA



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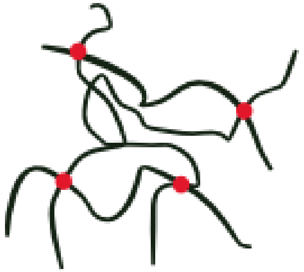
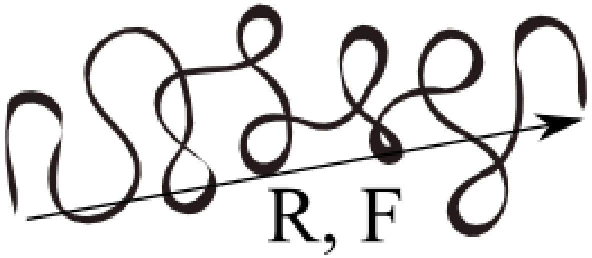
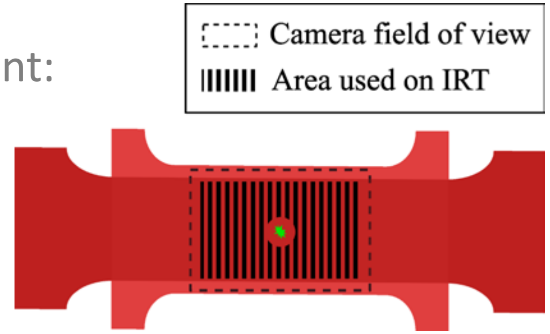
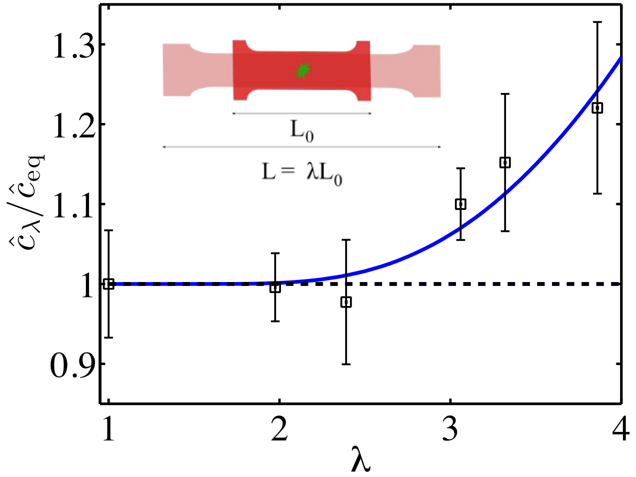
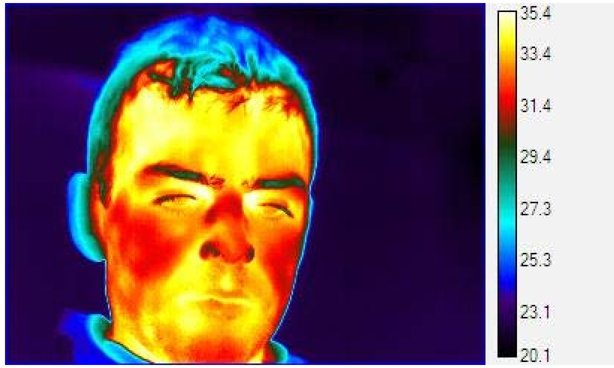








Nieto Simavilla et al. J. Pol. Sci. B 2012
Nieto Simavilla et al. J. of Heat Tranf. 2014
Nieto Simavilla et al. Macromolecules 2018



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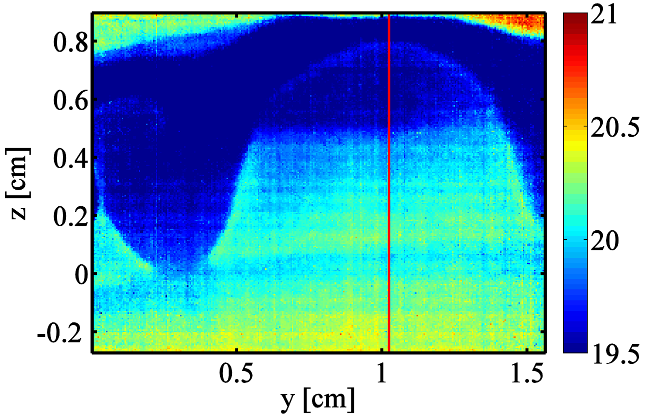
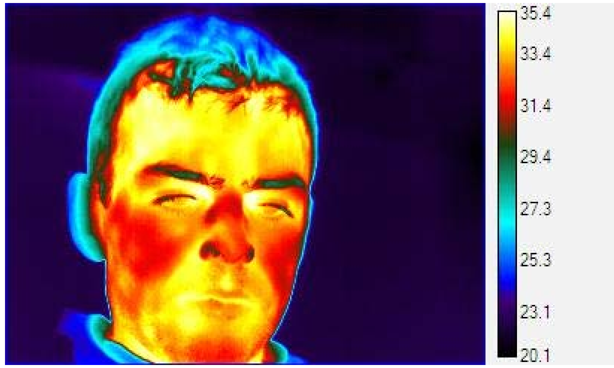


Venerus et al. Scientific Reports 2015



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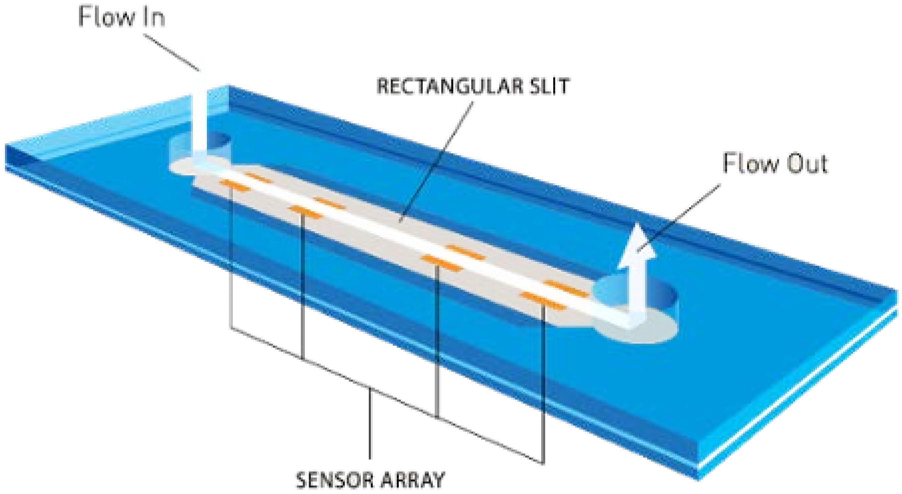

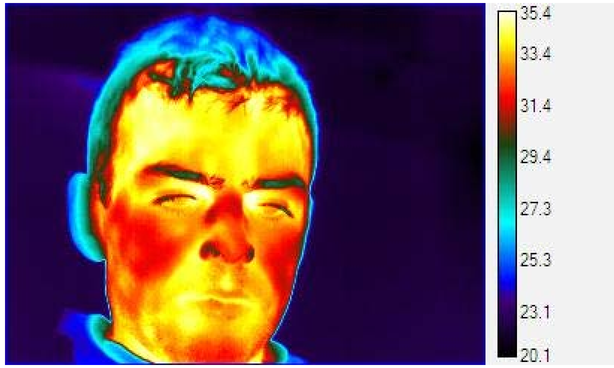

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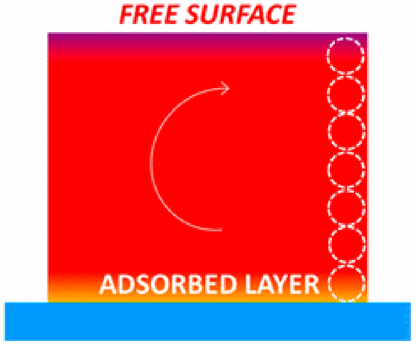
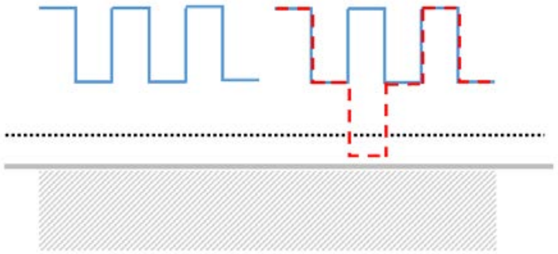
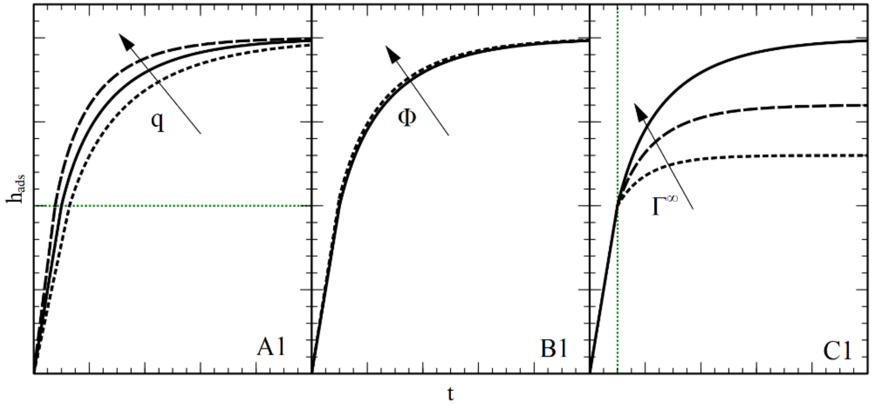
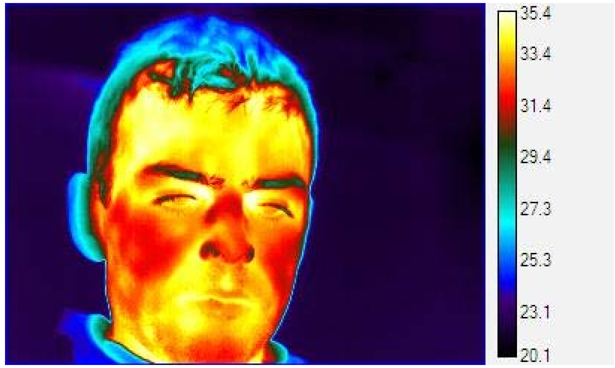






Nieto Simavilla et al. Macro. Chem. & Phys. 2017
Nieto Simavilla et al. ACS Macro Letters 2017
Nieto Simavilla et al. ACS Central Science. Under Review



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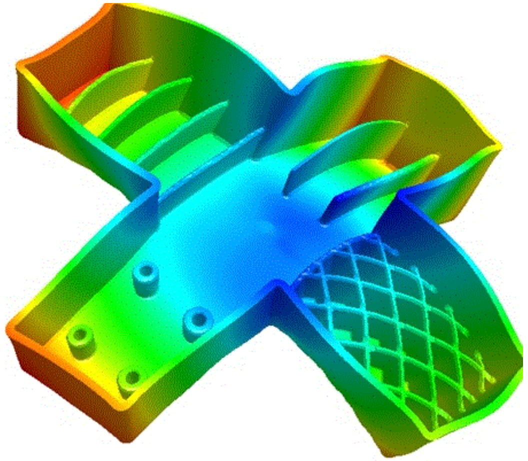
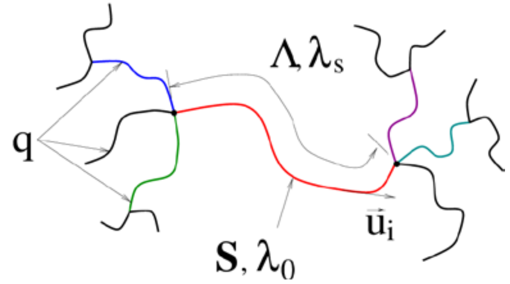
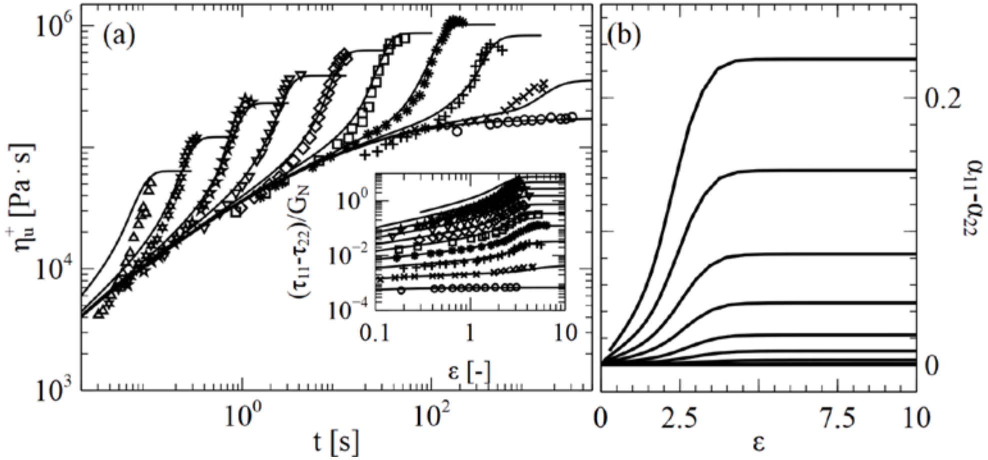






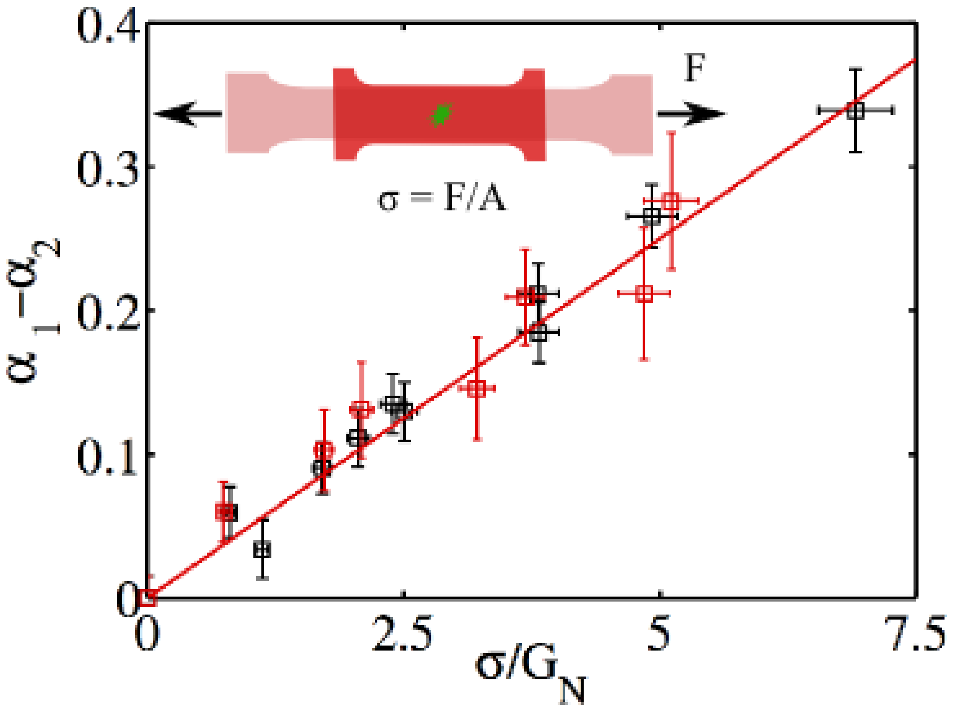
The MCIATTP project

A. Experimental investigation of thermal transport in polymers
- Anisotropy in thermal conductivity
- Stress-Thermal Rule
- Heat capacity vs. Deformation

B. Implementation of constitutive models
- Branched: eXtended Pom-Pom
- Linear: Rolie Poly
- Compare predictions with available experimental data PE, PS, PMMA…

C. Develop a deeper molecular understanding
- MD Simulations
- Why universal?
- Why beyond finite extensibility?

D. Implementation of non-homogeneous non-Isothermal flow simulations



Nieto et al. J. Heat Transfer 2014

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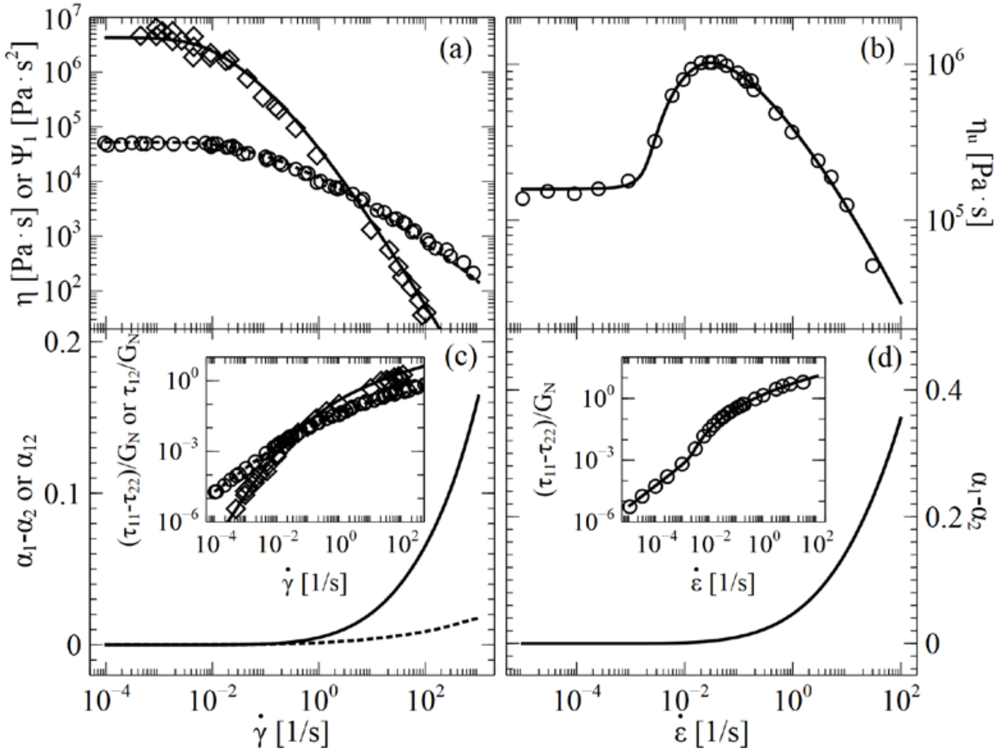

Nieto et al. Polymer Processing Society 33, 2017

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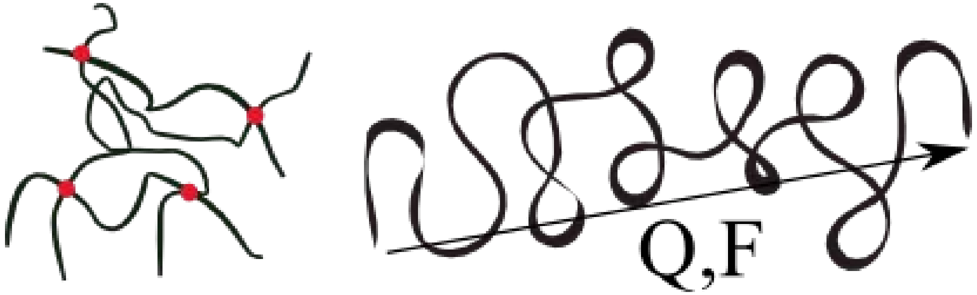

$$\boldsymbol{k} - \frac{1}{3}\mathrm{tr}(\boldsymbol{k})\boldsymbol{\delta} \propto n_i \langle \boldsymbol{RR} \rangle_i$$

B.H.A.A. van den Brule. Rheol. Acta 1989

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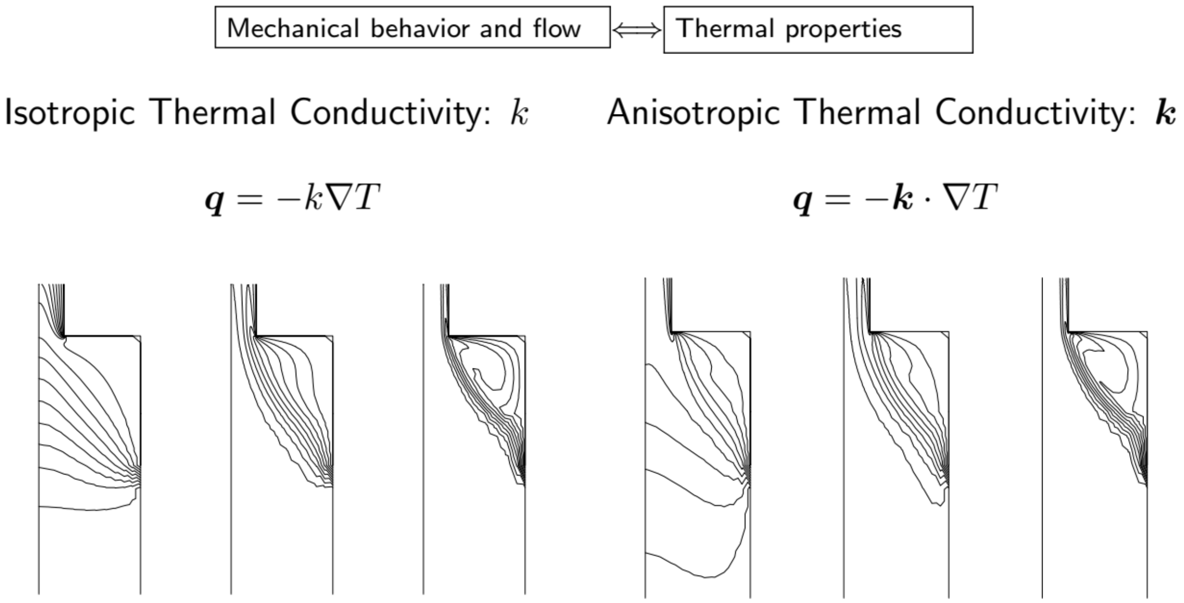


Isotropic Thermal Conductivity: k

$$\boldsymbol{q} = -k\nabla T$$

Anisotropic Thermal Conductivity: $\boldsymbol{k}$

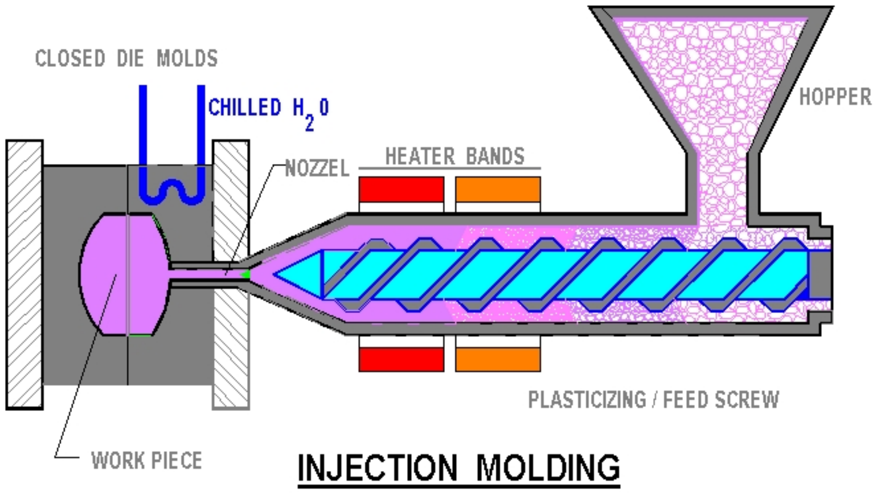
$$\boldsymbol{q} = -\boldsymbol{k}\cdot\nabla T$$

Isotherms for Pe = 10, Pe = 100 and Pe = 1000.

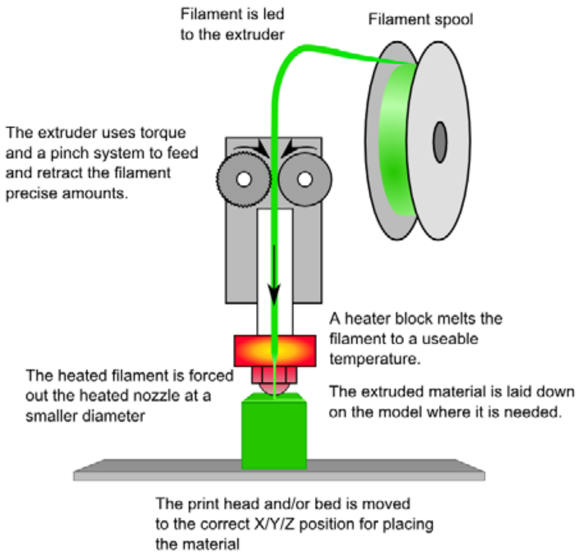
Isotherms for Pe = 10, Pe = 100 and Pe = 1000.

Wapperon et al. Fluid Mech. and App. 1995

Motivation: Polymer Processing



Global plastics market is expected to reach 654 billion USD by 2020



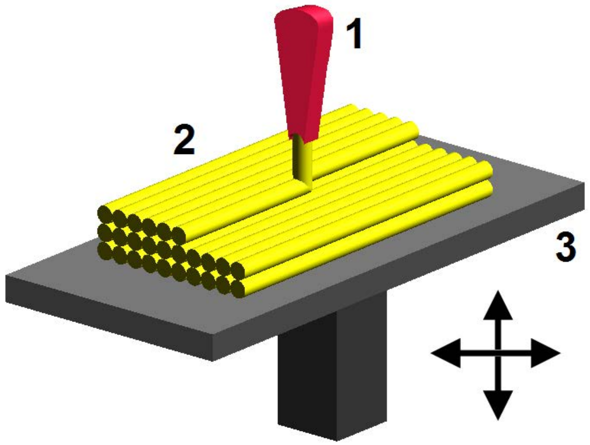
The extruder uses torque and a pinch system to feed and retract the filament precise amounts.

A heater block melts the filament to a useable temperature.

The heated filament is forced out the heated nozzle at a smaller diameter

The extruded material is laid down on the model where it is needed.

The print head and/or bed is moved to the correct X/Y/Z position for placing the material



Thermal Transport Affects:

- Injection Pressure
- Cavity Flow
- Residual Stress
- Part Shrinkage

www.astra-polymers.com

Non-Isothermal Transport Phenomena

Balance Equations:

$$\begin{aligned}
\text{Mass: } \quad & \frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}) \\
\text{Momentum: } \quad & \frac{\partial \rho \boldsymbol{v}}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v} + \boldsymbol{\pi}) \\
\text{Internal Energy: } \quad & \frac{\partial \rho \hat{u}}{\partial t} = -\nabla \cdot (\rho \hat{u} \boldsymbol{v} + \boldsymbol{q}) - \boldsymbol{\pi} : \nabla \boldsymbol{v}
\end{aligned}$$

Constitutive equations:

$$\boxed{\boldsymbol{q} = -k \nabla T} \qquad \boxed{\hat{c}_v = \hat{c}_v(T)} \qquad \boldsymbol{\tau} = \eta(T)\left[\nabla v + \nabla v^{\intercal}\right]$$

- High stresses & Low thermal conductivity.

$$\boxed{\text{Mechanical behavior and flow}} \Longleftrightarrow \boxed{\text{Thermal properties}}$$

Anisotropic Thermal Conduction

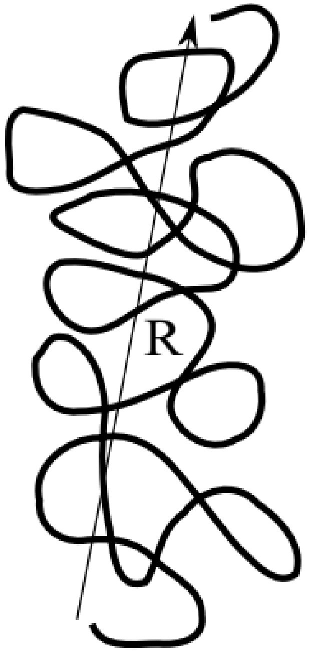
Fourier's Law: Thermal transport in deformed polymers is diffusive and anisotropic.

$$\boxed{\boldsymbol{q} = -\boldsymbol{k} \cdot \nabla T}$$

$\boldsymbol{k}$ is a tensor!

Observation: k_{eq} increases with molecular weight.

Ueberreiter & Otto-Laupenmühlen, Kolloid Z. 1953



Hypothesis: *Energy transport along the backbone of a polymer chain is more efficient than between chains.*

Simple molecular arguments:

$$\boldsymbol{k} \propto \langle \boldsymbol{RR} \rangle \qquad + \qquad \boldsymbol{\tau} \propto \langle \boldsymbol{RR} \rangle$$

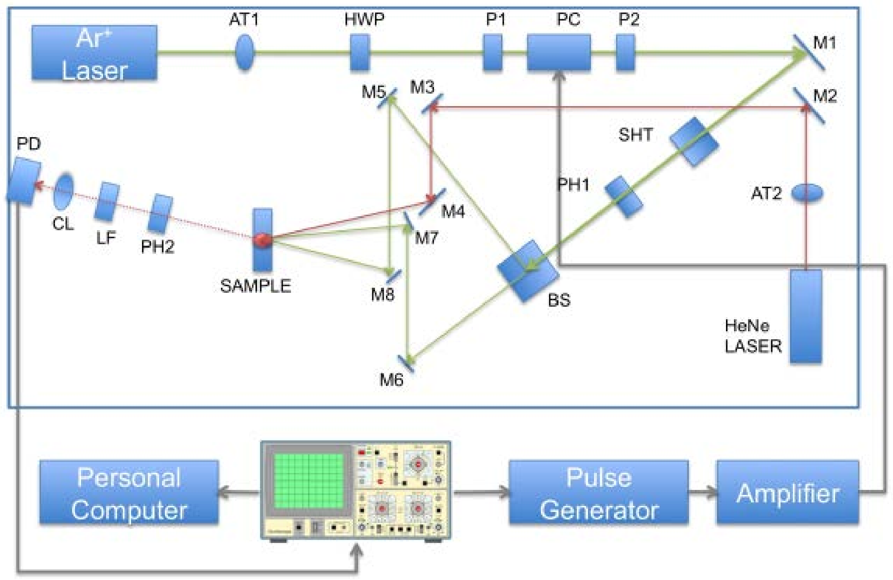
$$\boxed{\boldsymbol{k} - \tfrac{1}{3}\mathrm{tr}(\boldsymbol{k})\boldsymbol{\delta} = k_{\mathrm{eq}} C_{\mathrm{t}} \left[\boldsymbol{\tau} - \tfrac{1}{3}\mathrm{tr}(\boldsymbol{\tau})\boldsymbol{\delta} \right]}$$

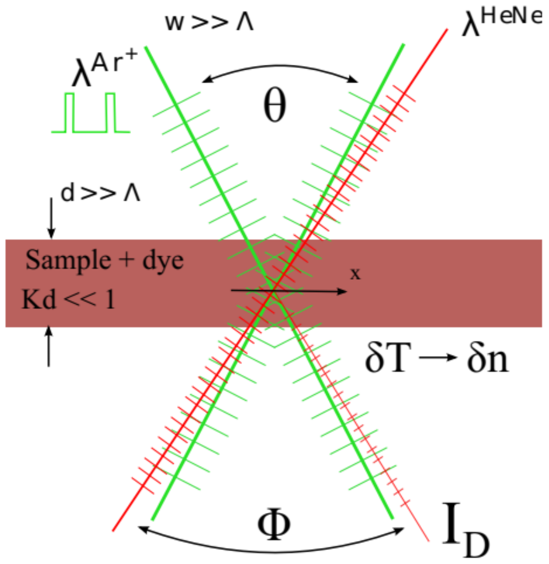
The Stress-Thermal Rule

B.H.A.A. van den Brule, Rheol Acta 1989.
Öttinger and Petrillo, J. Rheol. 40 (5) 1996.
Curtiss and Bird, J. Chem. Phys. 107 (13) 1997.

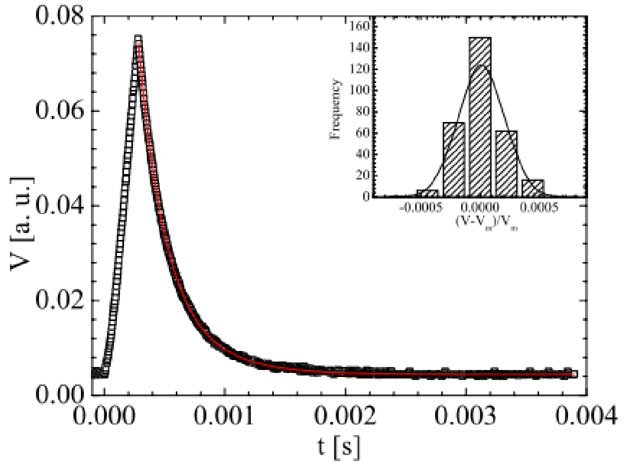
$$C_t \propto \frac{n k_B^2 T}{\zeta}$$

Experiments: Forced Rayleigh Scattering (FRS)

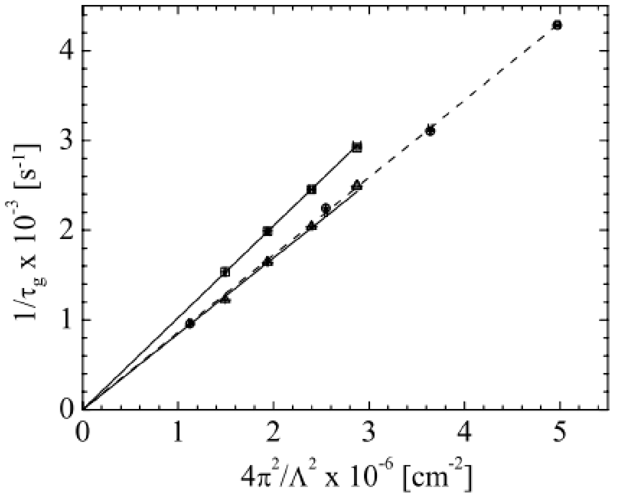




100 waveforms for each grating size



4 grating sizes for each elongation



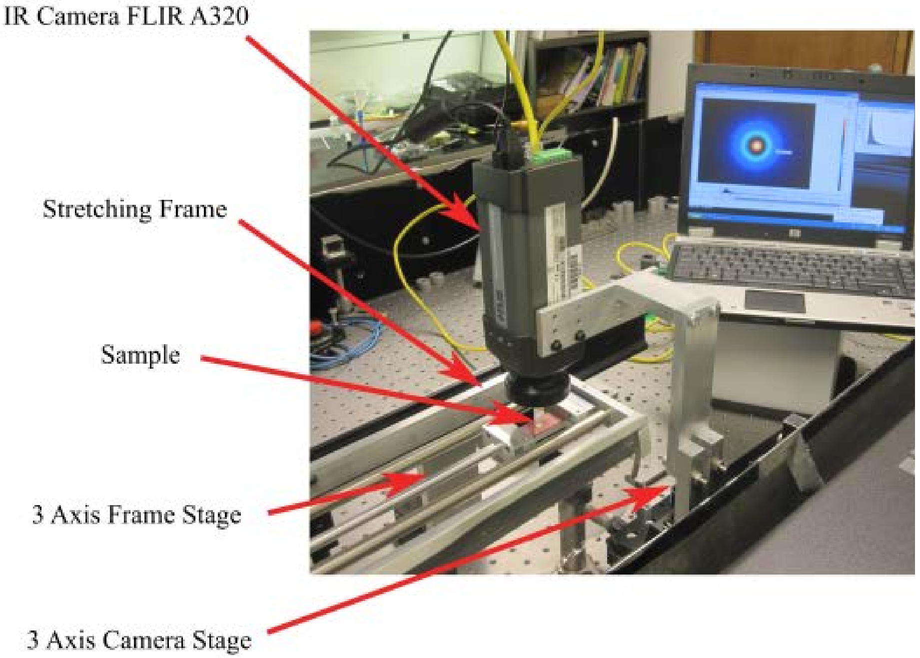
Intensity/Voltage at the photodetector:

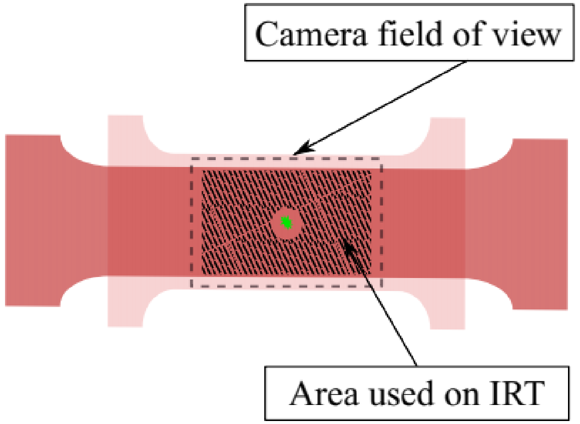
$$V(t) = \mathrm{A}\exp\left(-2\frac{t}{\tau_{\mathrm{g}}}\right) + \mathrm{B}\exp\left(-\frac{t}{\tau_{\mathrm{g}}}\right) + \mathrm{C}$$

$$\frac{1}{\tau_{\mathrm{g}}} = \boxed{D_{\mathrm{th}}}\frac{4\pi^2}{\Lambda^2} \qquad D_{\mathrm{th}} = \frac{k}{\rho\hat{c}_p}$$

Nieto Simavilla et al. J. Pol. Sci. B 2012

Experiments: Infrared Thermography (IRT)

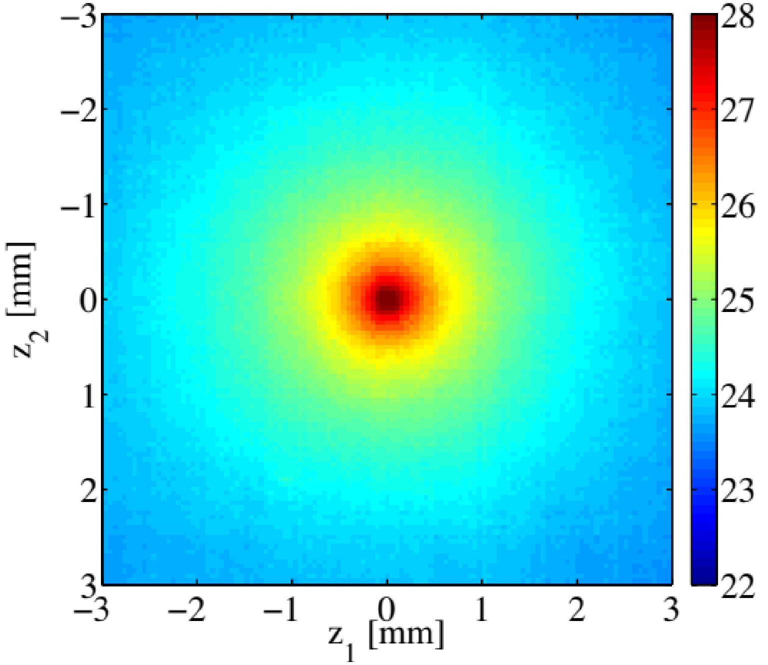




$$\theta(x_1, x_2) = \frac{1}{4\sqrt{\alpha_1 \alpha_2}} K_0\left(\sqrt{2\mathrm{Bi}({x_1}^2/\alpha_1 + {x_2}^2/\alpha_2)}\right)$$

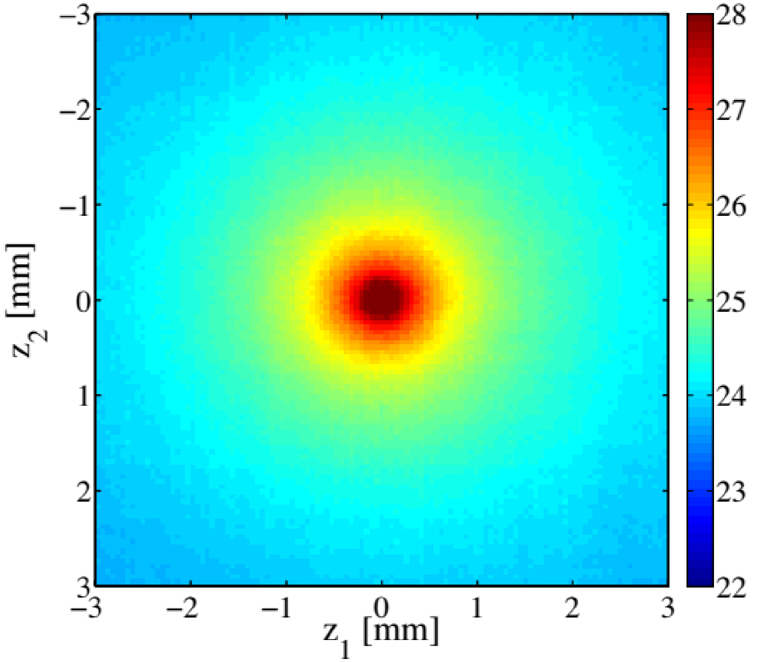
$KI_0 w^2/k_{\mathrm{eq}}$, $\mathrm{Bi} = hd/k_{\mathrm{eq}}$

$\alpha_1 = k_{11}/k_{\mathrm{eq}}$, $\alpha_2 = k_{22}/k_{\mathrm{eq}}$



Un-stretched sample, $\lambda = 1$

and $\mathrm{Bi}_0 = 0.029 \pm 0.001$

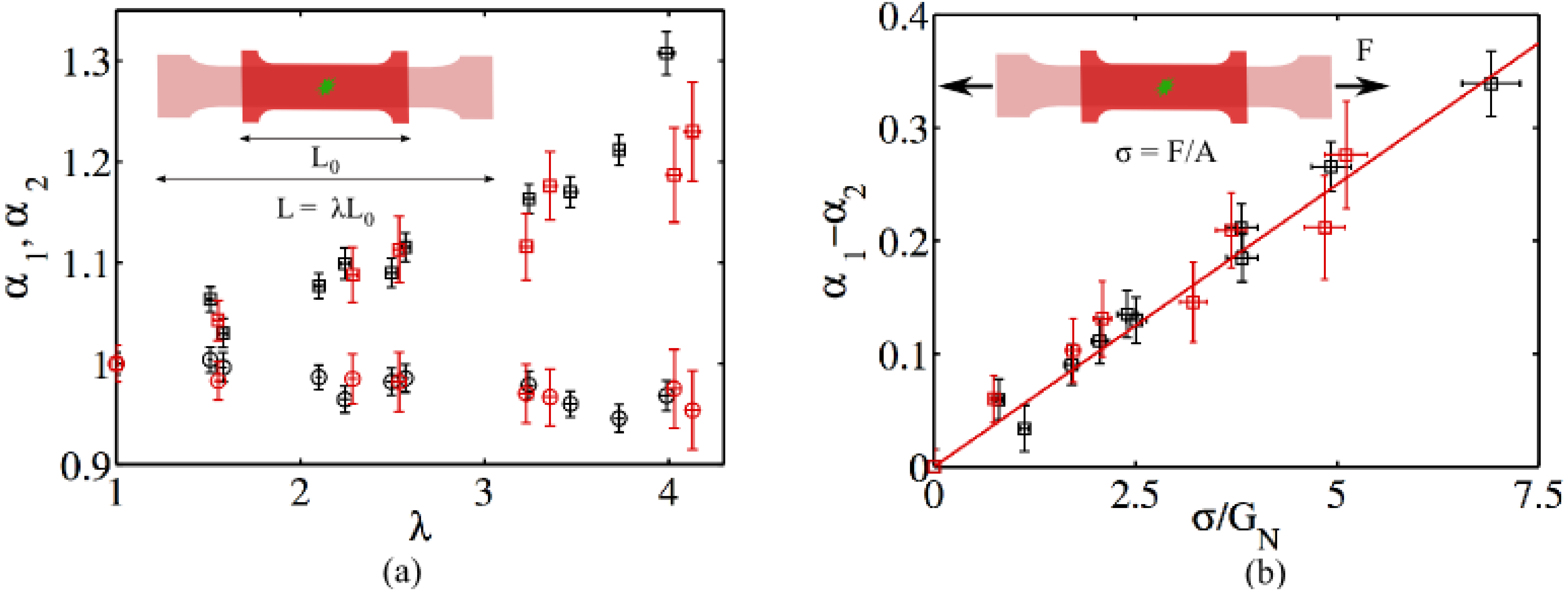


Stretched sample, $\lambda = 4.129$,

$\alpha_1 = 1.23 \pm 0.049$ and $\alpha_2 = 0.954 \pm 0.039$

Nieto Simavilla et al. Journal of Heat Transfer. 2014

Comparison FRS and IRT



Nieto Simavilla et al. Journal of Heat Transfer. 2014

Key Findings: Universality…

Stress-Thermal Coefficients for several polymeric materials

Material	Deformation –	G_N [kPa]	C_t x 10^4 [kPa^{-1}]	$C_\mathrm{t} G_\mathrm{N}$ –	C x 10^9 [Pa^{-1}]
PIB 85k[7]	Shear	320 [1]	1.9	0.061 ± 0.024	1.45
PIB 130k[7]	Shear	320 [1]	1.2	0.038 ± 0.022	1.45
xl-PDMS[6]	Uniax.	200 [1]	1.3	0.026 ± 0.008	0.13-0.26
xl-PBD 200k[5]	Uniax.	760 [1]	0.73	0.051 ± 0.011	3.5
xl-PBD 150k[5]	Uniax.	760 [1]	0.93	0.059 ± 0.014	3.5
xl-PI 100k[4]	Uniax.	370 [2]	0.37	0.014 ± 0.005	2.2
PS 260k[3]	Uniax.	200 [1]	1.65	0.033 ± 0.007	-4.8
PMMA 83k[3]	Uniax.	310 [1]	1.7	0.054 ± 0.011	0.16

$$\boxed{C_\mathrm{t} G_\mathrm{N} \sim 0.04}$$

(1) Fetters et al. Macromolecules 27, 17 (1994)
(2) Fetters et al. Macromolecules 37 (2004)
(3) Gupta et al. Journal of Rheology 57 (2013)
(4) Nieto Simavilla et al. J. Pol. Sci. B 50 (2012)
(5) Venerus et al. Macromolecules 42 (2009)
(6) Broerman et al. J.Chem. Phys. 111 (1999)
(7) Venerus et al. Phys. Rev. Lett. 82 (1999)

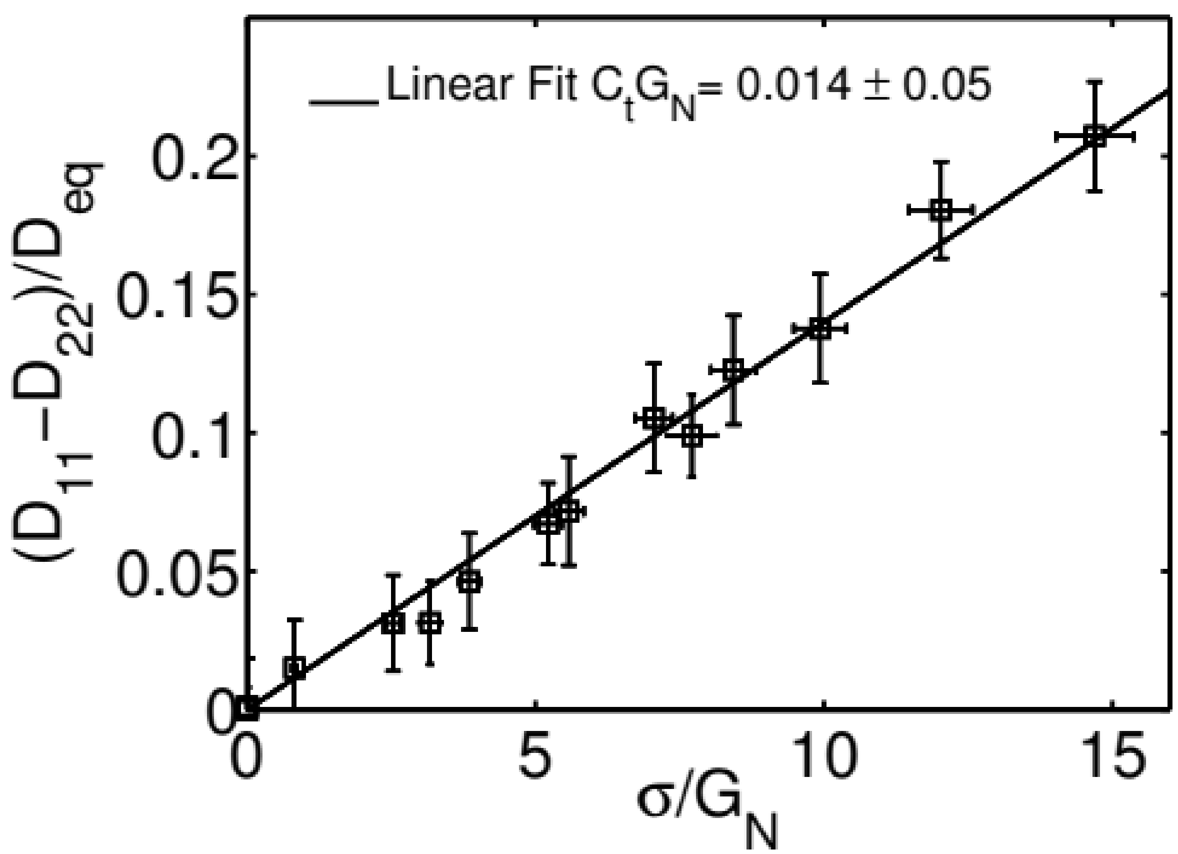
Stress-thermal Rule:

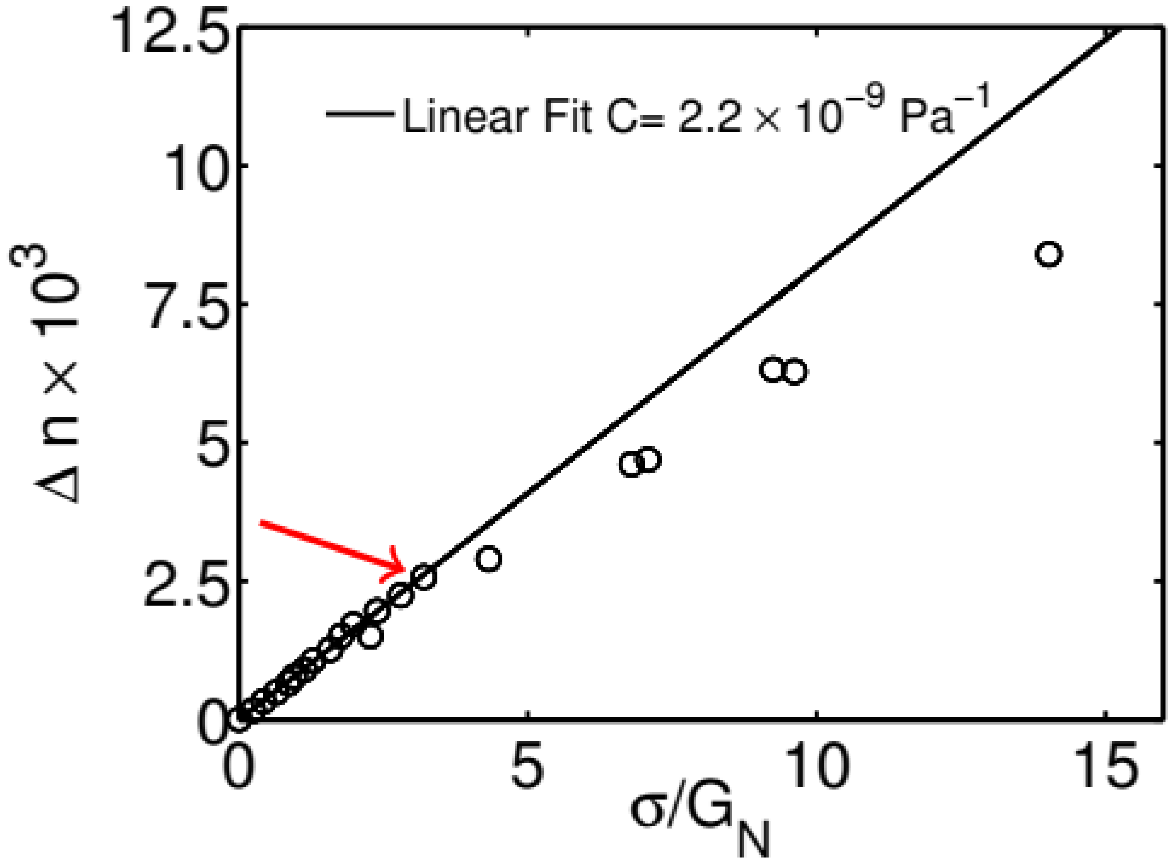
$$\boldsymbol{k} - \frac{1}{3}\mathrm{tr}(\boldsymbol{k})\boldsymbol{\delta} = k_\mathrm{eq} C_\mathrm{t}(\boldsymbol{\tau} - \frac{1}{3}\mathrm{tr}(\boldsymbol{\tau})\boldsymbol{\delta})$$

Stress-optic Rule:

$$\boldsymbol{n} - \frac{1}{3}\mathrm{tr}(\boldsymbol{n})\boldsymbol{\delta} = C(\boldsymbol{\tau} - \frac{1}{3}\mathrm{tr}(\boldsymbol{\tau})\boldsymbol{\delta})$$

Key Findings: …Beyond Finite Extensibility





The STR stays valid where the SOR fails!

Nieto Simavilla et al. J. Pol. Sci. B 2012

Anisotropic Thermal Conduction

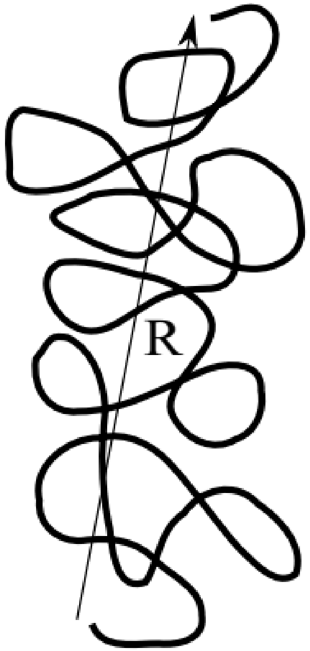
Fourier's Law: Thermal transport in deformed polymers is diffusive and anisotropic.

$$\boxed{\boldsymbol{q} = -\boldsymbol{k} \cdot \nabla T}$$

$\boldsymbol{k}$ is a tensor!

Observation: k_{eq} increases with molecular weight.

Ueberreiter & Otto-Laupenmühlen, Kolloid Z. 1953



Hypothesis: *Energy transport along the backbone of a polymer chain is more efficient than between chains.*

Simple molecular arguments:

$$\boldsymbol{k} \propto \langle \boldsymbol{RR} \rangle \qquad + \qquad \boldsymbol{\tau} \propto \langle \boldsymbol{RR} \rangle$$

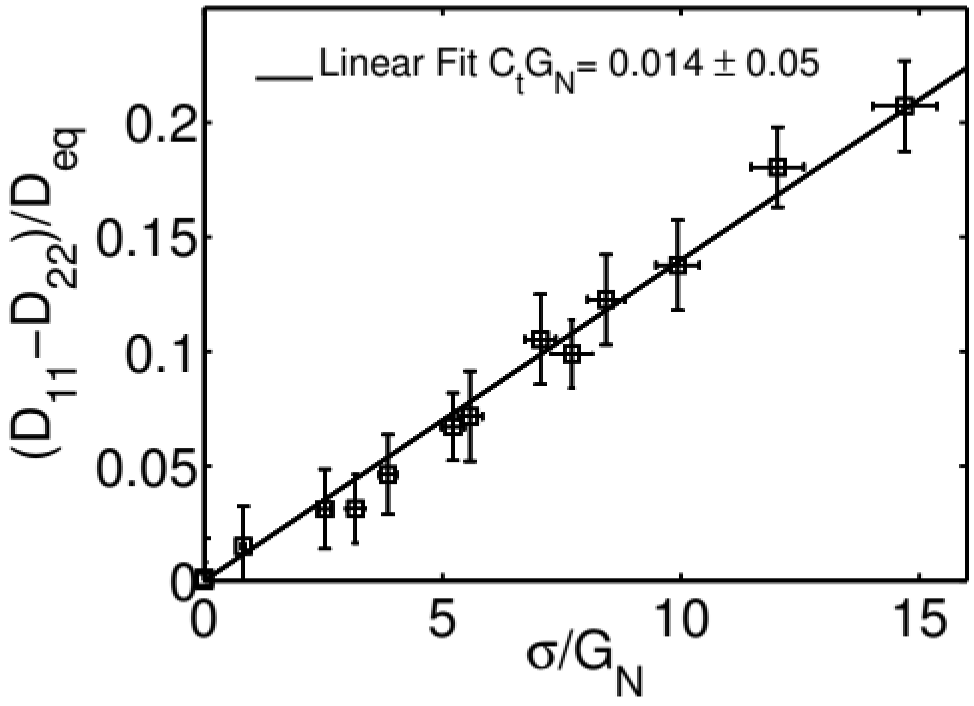
$$\boxed{\boldsymbol{k} - \tfrac{1}{3}\mathrm{tr}(\boldsymbol{k})\boldsymbol{\delta} = k_{\mathrm{eq}} C_{\mathrm{t}} \left[\boldsymbol{\tau} - \tfrac{1}{3}\mathrm{tr}(\boldsymbol{\tau})\boldsymbol{\delta}\right]}$$

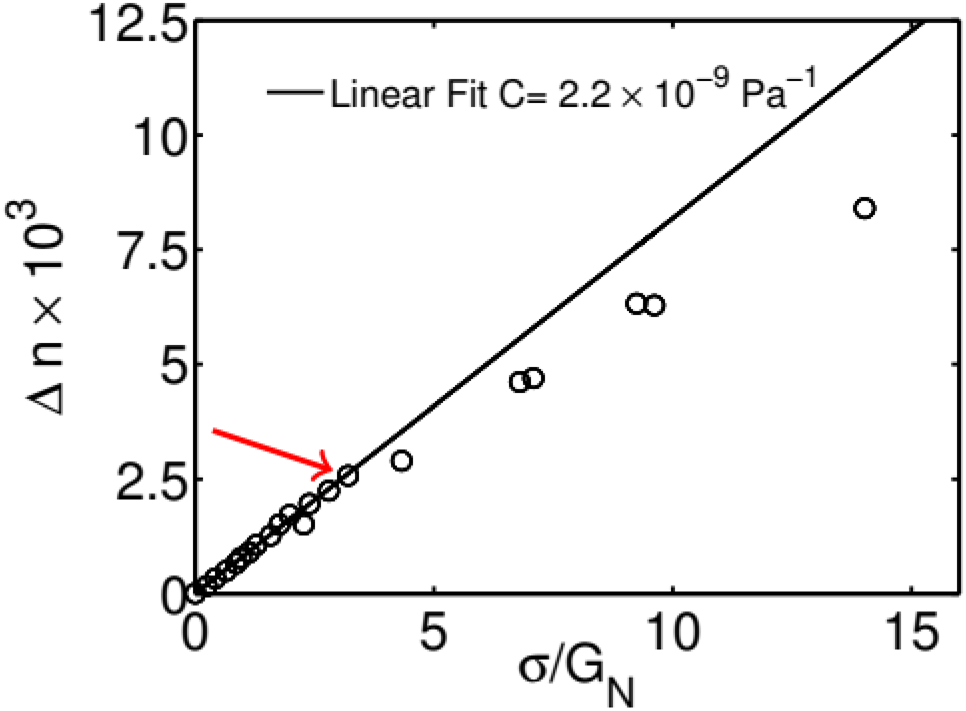
The Stress-Thermal Rule

B.H.A.A. van den Brule, Rheol Acta 1989.
Öttinger and Petrillo, J. Rheol. 40 (5) 1996.
Curtiss and Bird, J. Chem. Phys. 107 (13) 1997.

$$C_t \propto \frac{n k_B^2 T}{\zeta}$$

Key Findings: …Beyond Finite Extensibility





The STR stays valid where the SOR fails!

Nieto Simavilla et al. J. Pol. Sci. B 2012

The Stress-Thermal Rule can be applied:

1. To any melt just by knowing stress and G_N
2. At high strain and strain rates beyond the onset of finite extensibility effects

Constitutive Model: eXtended Pom-Pom

- What physics are in the model?

$$\overset{\nabla}{\boldsymbol{\tau}} + \boldsymbol{\lambda}(\boldsymbol{\tau})^{-1}\cdot\boldsymbol{\tau} - 2G_0\mathbf{D}_u = \mathbf{0}$$

$$\alpha \neq 0 \rightarrow \Psi_2 \neq 0$$

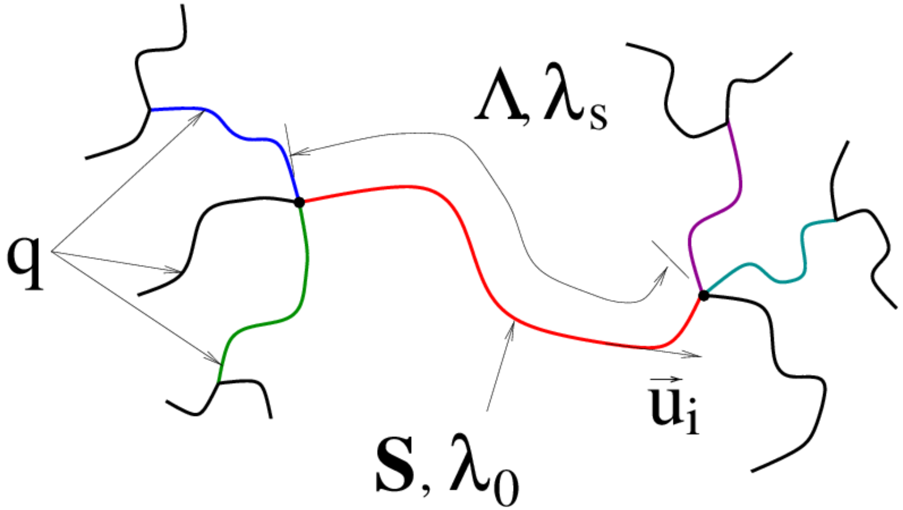
$$\boldsymbol{\lambda}(\boldsymbol{\tau})^{-1} = \frac{1}{\lambda_{0b}}\left[\frac{\alpha}{G_0}\boldsymbol{\tau} + f(\boldsymbol{\tau})^{-1}\boldsymbol{I} + G_0\left(f(\boldsymbol{\tau})^{-1} - 1\right)\boldsymbol{\tau}^{-1}\right]$$

$$\Lambda = \sqrt{1 + \frac{I_{\boldsymbol{\tau}}}{3G_0}}$$

$$\frac{1}{\lambda_{0b}}f(\boldsymbol{\tau})^{-1} = \frac{2}{\lambda_s}\left(1 - \frac{1}{\Lambda}\right) + \frac{1}{\lambda_{0b}}\left(\frac{1}{\Lambda^2} - \frac{\alpha I_{\boldsymbol{\tau}\cdot\boldsymbol{\tau}}}{3G_0^2\Lambda^2}\right)$$

$$\lambda_s = \lambda_{0s}\, e^{-\frac{2}{q}(\Lambda - 1)}$$

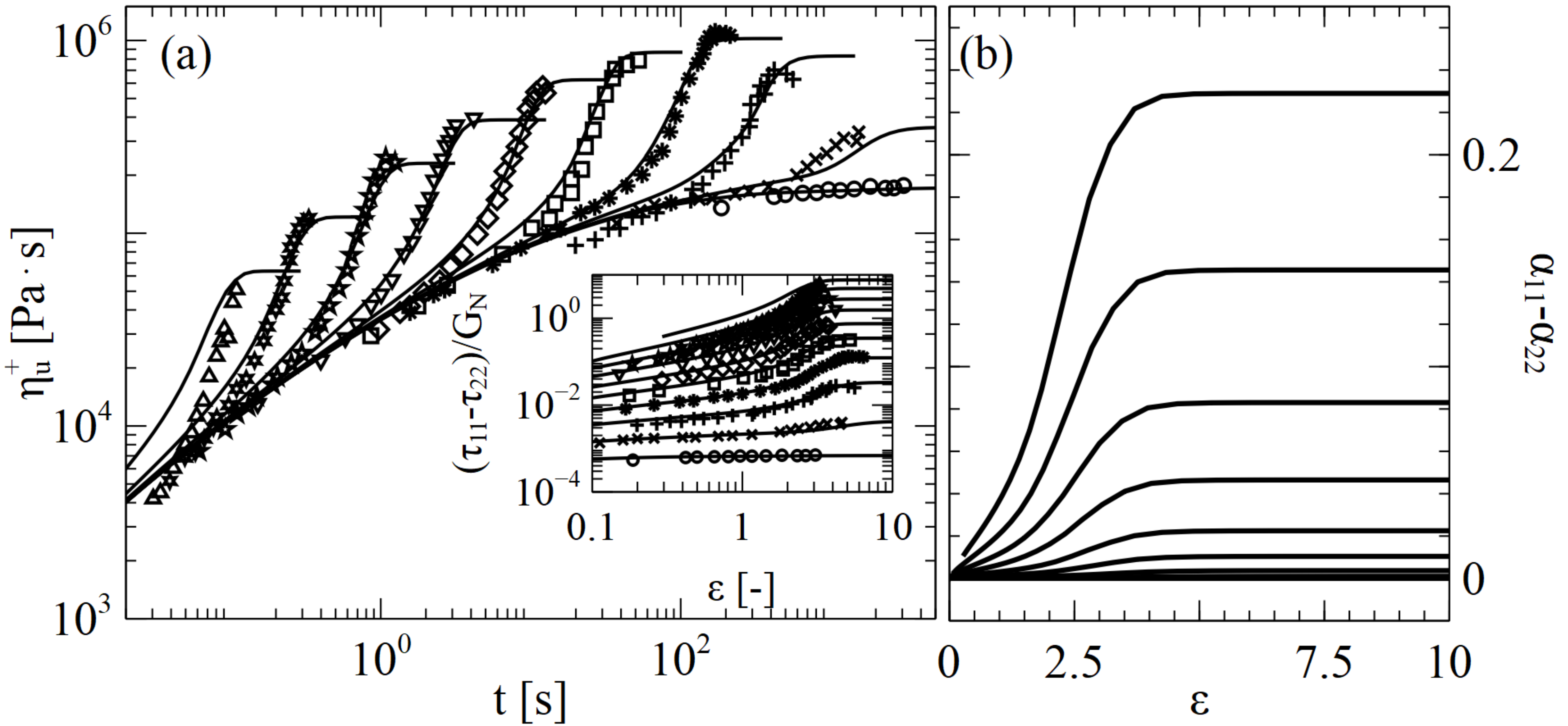
- Why XPP?
  - Amenable to FEM
  - Able to describe non-linear rheology
  - X: Avoids finite extensibility discontinuities
  - X: Includes second normal stress difference



Data: IUPAC_A LDPE melt at 170ºC
Verbeeten et al. JOR 2001

PP: McLeish and Larson. JOR 1998
xPP: Verbeeten et al. JOR 2001

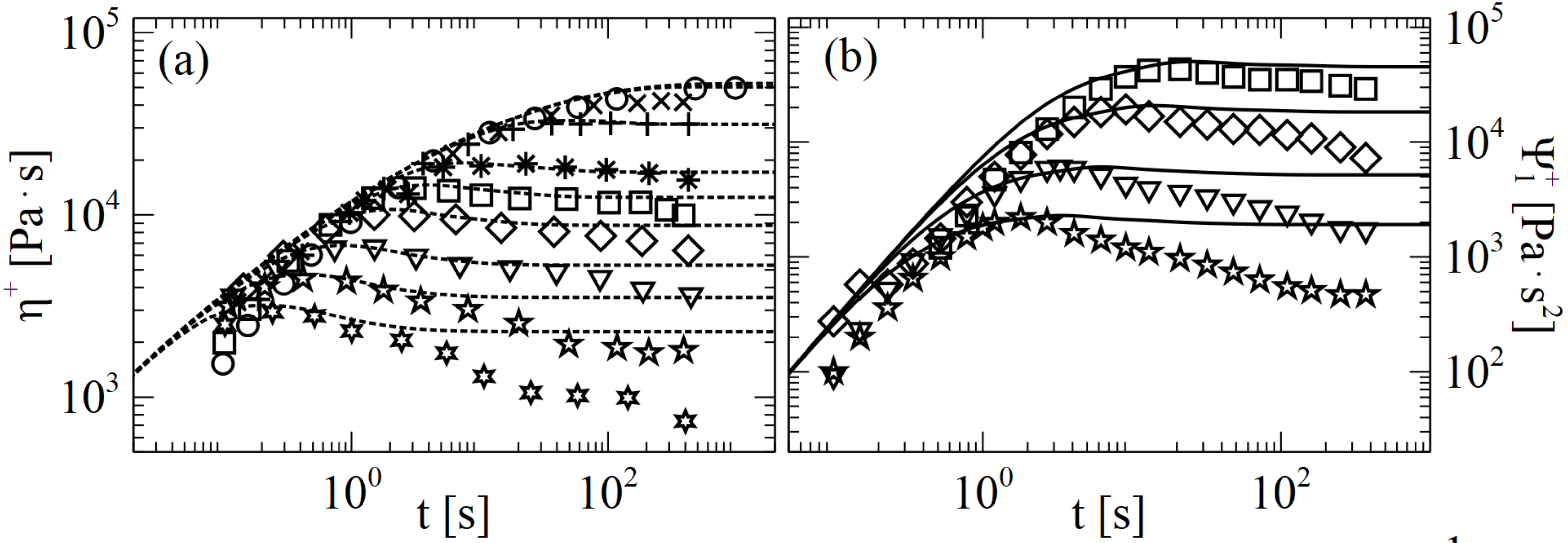
Transient Start-up: Uniaxial IUPAC_A LDPE



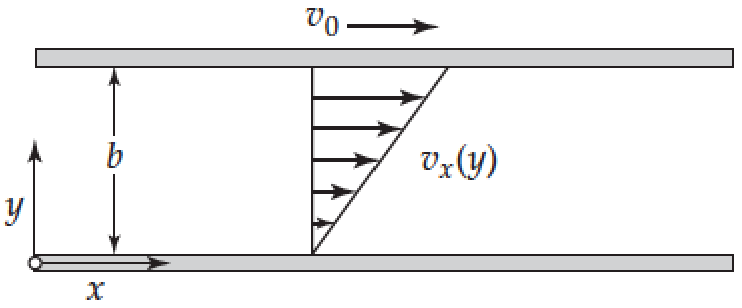
The anisotropy in TC is comparable to that observed in PS and PMMA melts ~20%.

Gupta et al. Journal of Rheology 57, 2013.

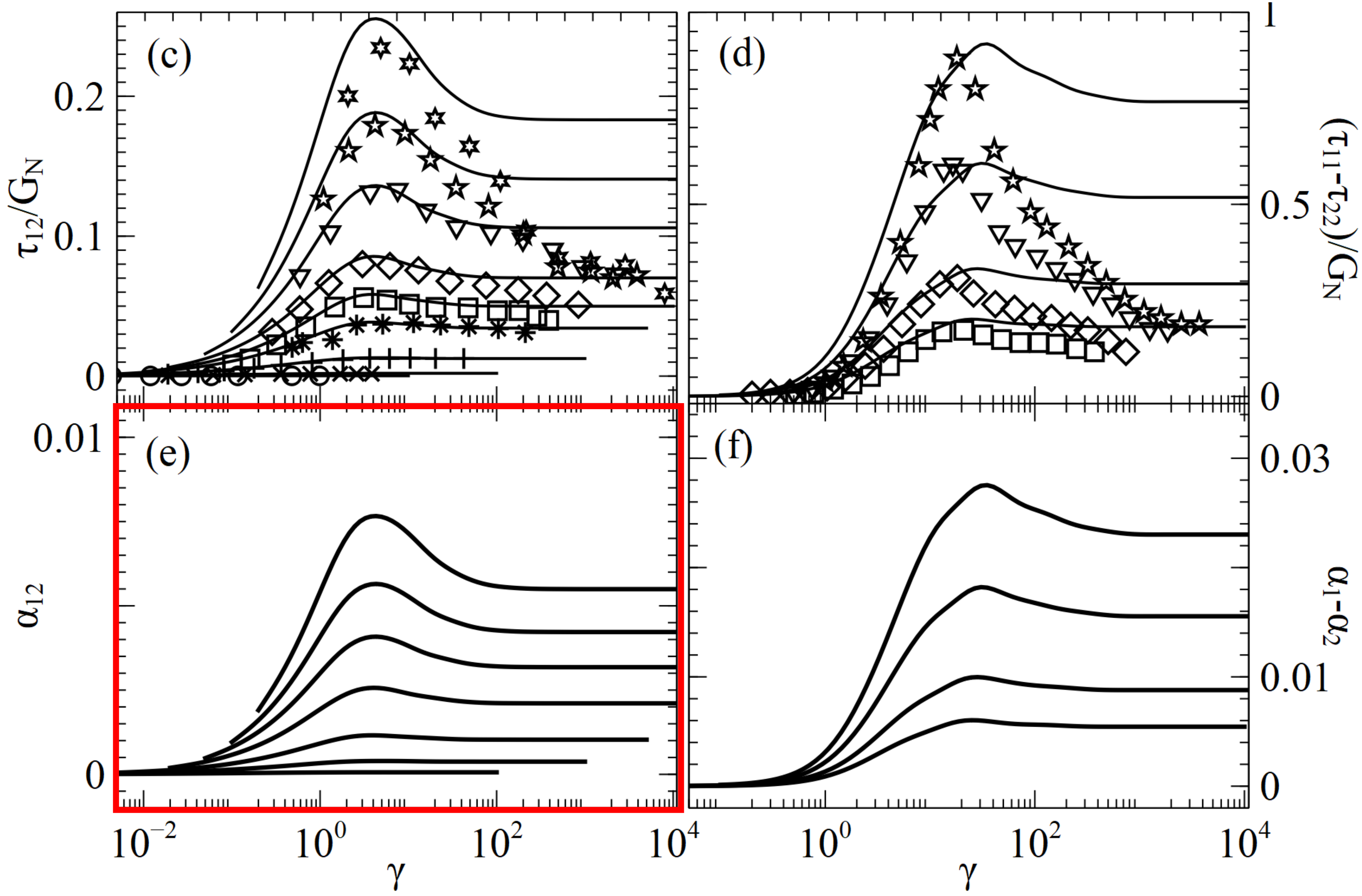
Transient Start-up: Shear Rheology IUPAC_A LDPE



1



Transient Start-up: Shear IUPAC_A LDPE



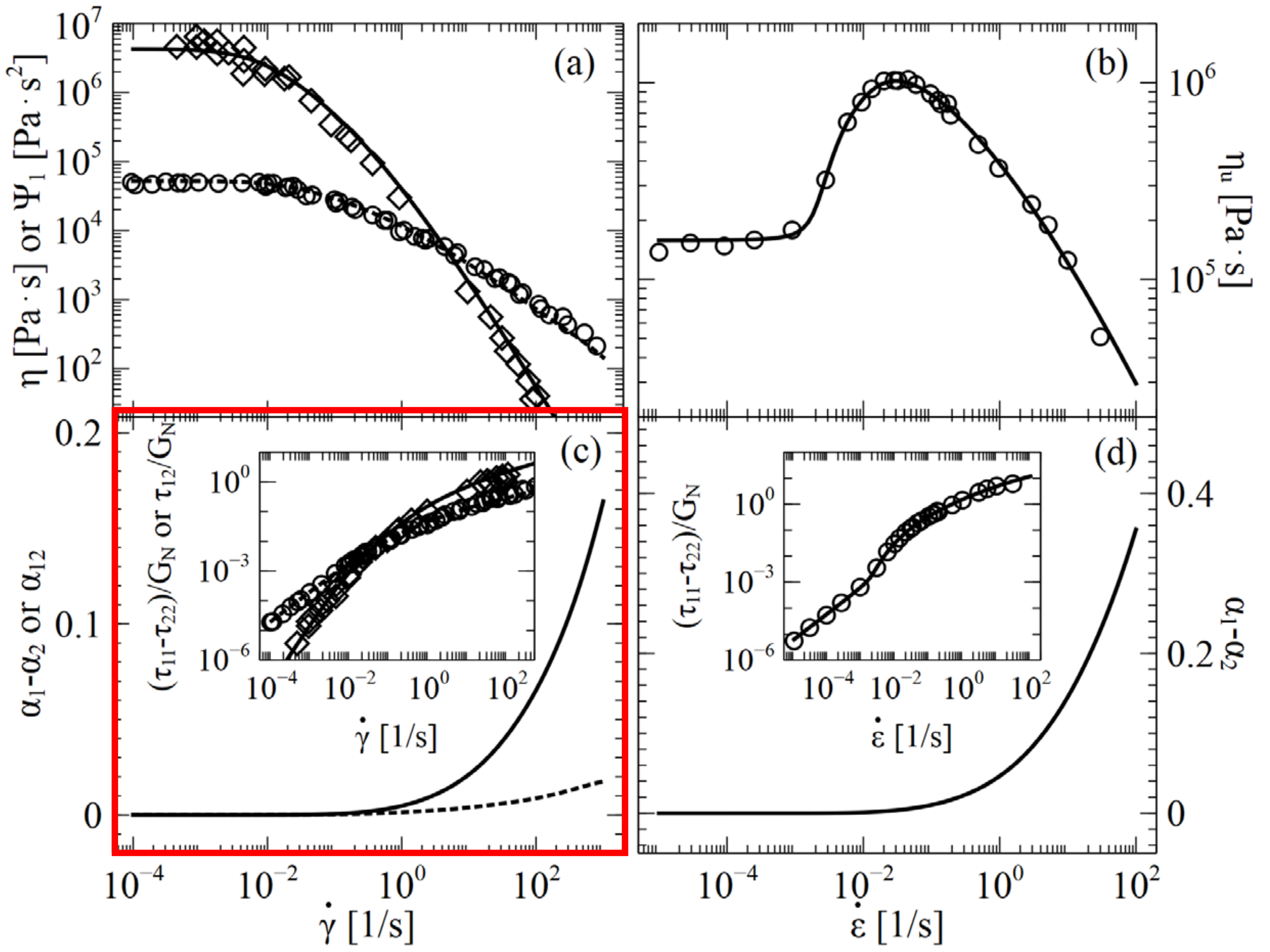
There is a non-zero off-diagonal component in shear flows

$$\boldsymbol{k} = \begin{pmatrix} k_{11} & k_{12} & k_{13} \\ & k_{22} & k_{23} \\ & & k_{33} \end{pmatrix}$$

$$\boldsymbol{q} = \boldsymbol{k} \cdot \boldsymbol{\nabla} T$$

A temperature gradient in the 1-direction can generate heat flow in the 2-direction: ***Thermal Hall Effect***

Steady-State: Shear and Uniaxial Ext. IUPAC_A LDPE



There is a non-zero off-diagonal component in shear flows

$$\boldsymbol{k} = \begin{pmatrix} k_{11} & k_{12} & k_{13} \\ & k_{22} & k_{23} \\ & & k_{33} \end{pmatrix}$$

$$\boldsymbol{q} = \boldsymbol{k} \cdot \boldsymbol{\nabla} T$$

A temperature gradient in the 1-direction can generate heat flow in the 2-direction: ***Thermal Hall Effect***

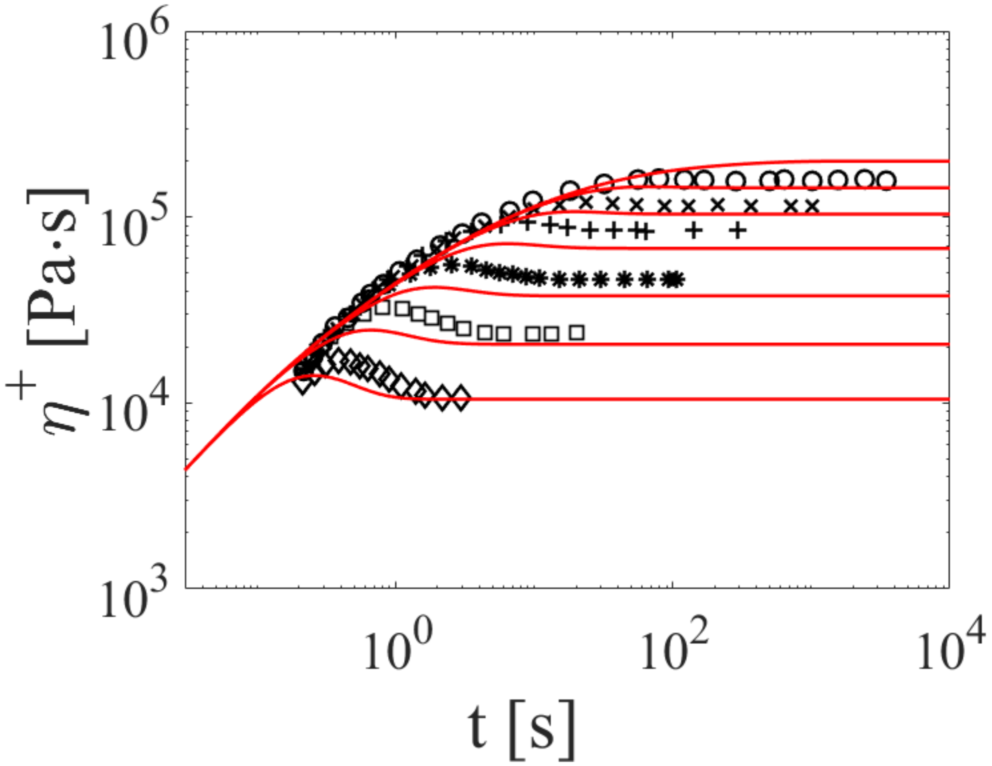
Constitutive Model: Rolie Poly

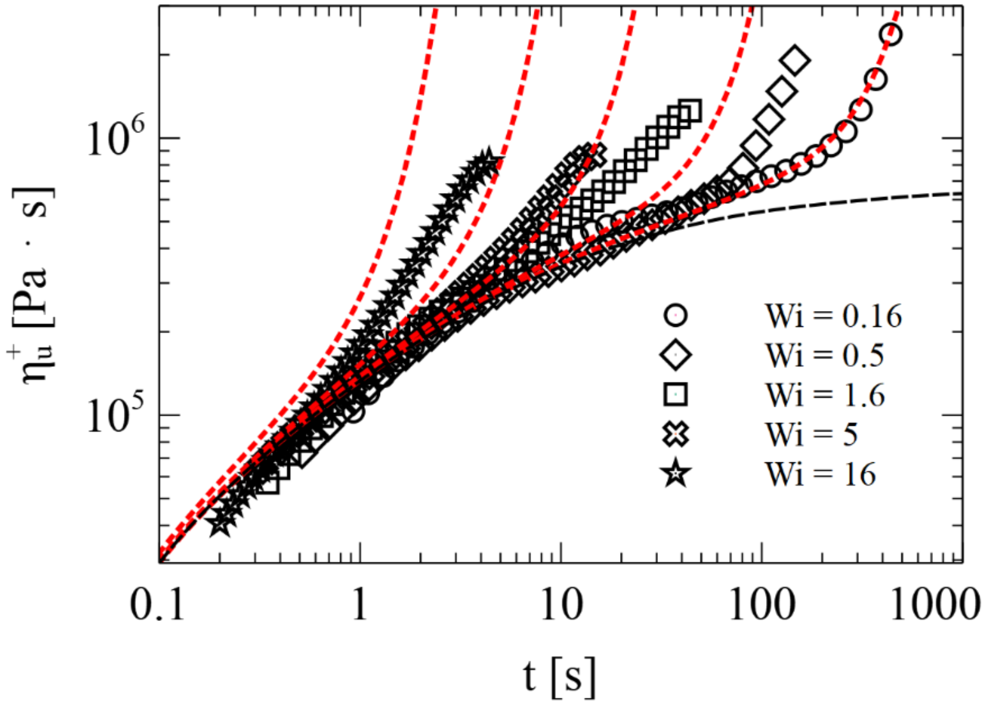
Graham et al. JOR 2003
Likhtman et al. JNNFM 2003

- Rolie Poly Model: ROuse LInear Entangled POLYmers

$$\frac{d\boldsymbol{\sigma}}{dt} = \boldsymbol{\kappa}\cdot\boldsymbol{\sigma} + \boldsymbol{\sigma}\cdot\boldsymbol{\kappa}^{T} - \frac{1}{\tau_d}(\boldsymbol{\sigma} - \boldsymbol{I}) - \frac{2\left(1-\sqrt{(3/\mathrm{tr}\boldsymbol{\sigma})}\right)}{\tau_R}\left(\boldsymbol{\sigma} + \beta\left(\frac{\mathrm{tr}\boldsymbol{\sigma}}{3}\right)^{\delta}(\boldsymbol{\sigma} - \boldsymbol{I})\right)$$

- Predictions

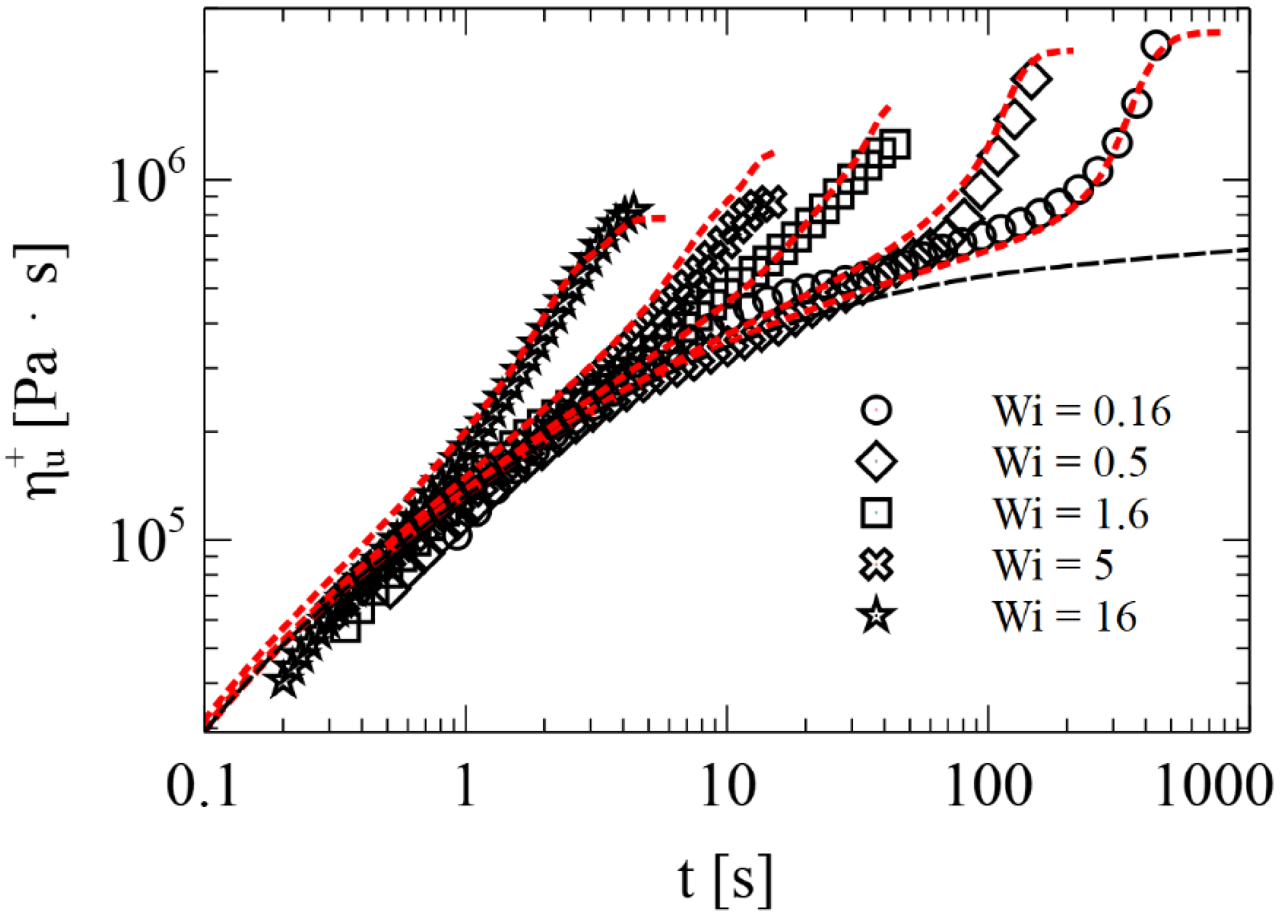




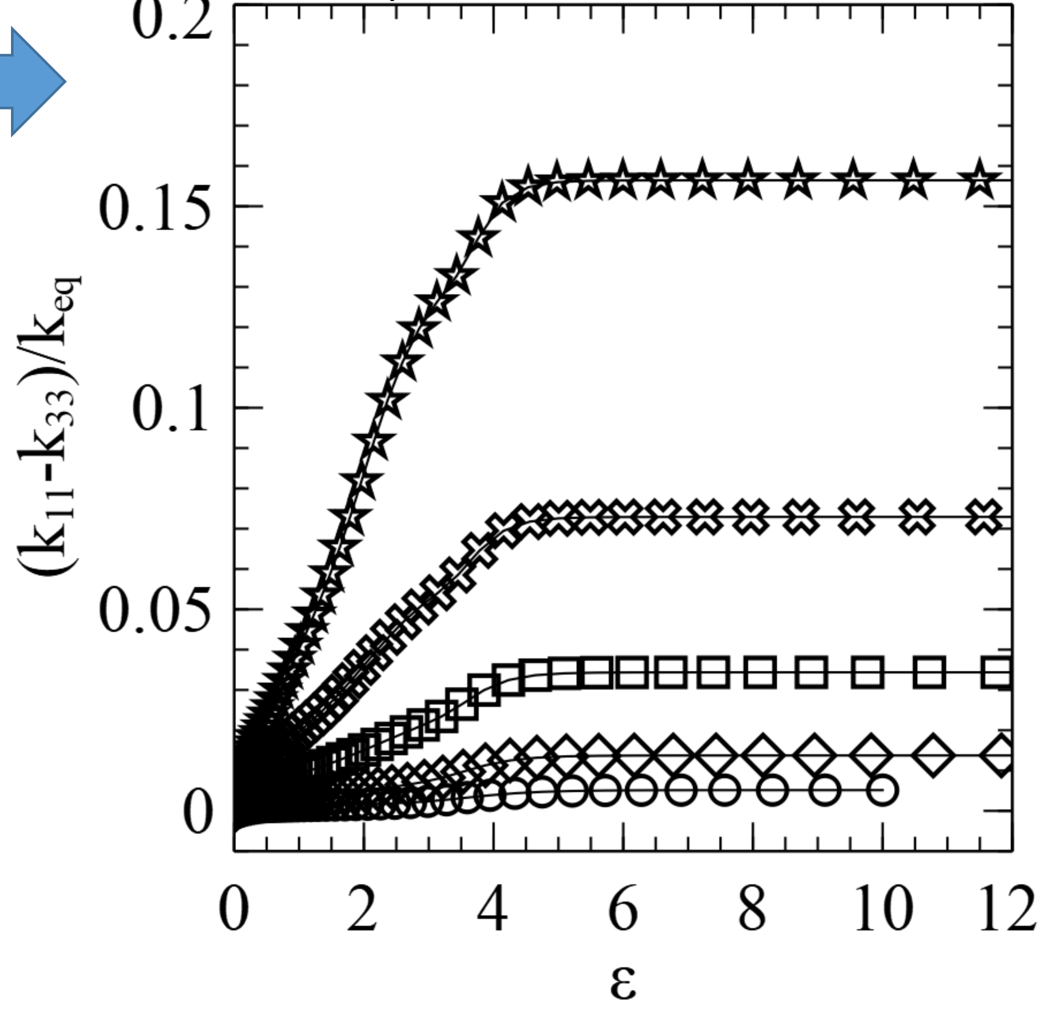
- Future Work: Implement Finite extensibility. Kabameni et al. Rheol Acta 2009

Transient Start-up: Uniaxial PS

Dashed lines → XPP Model



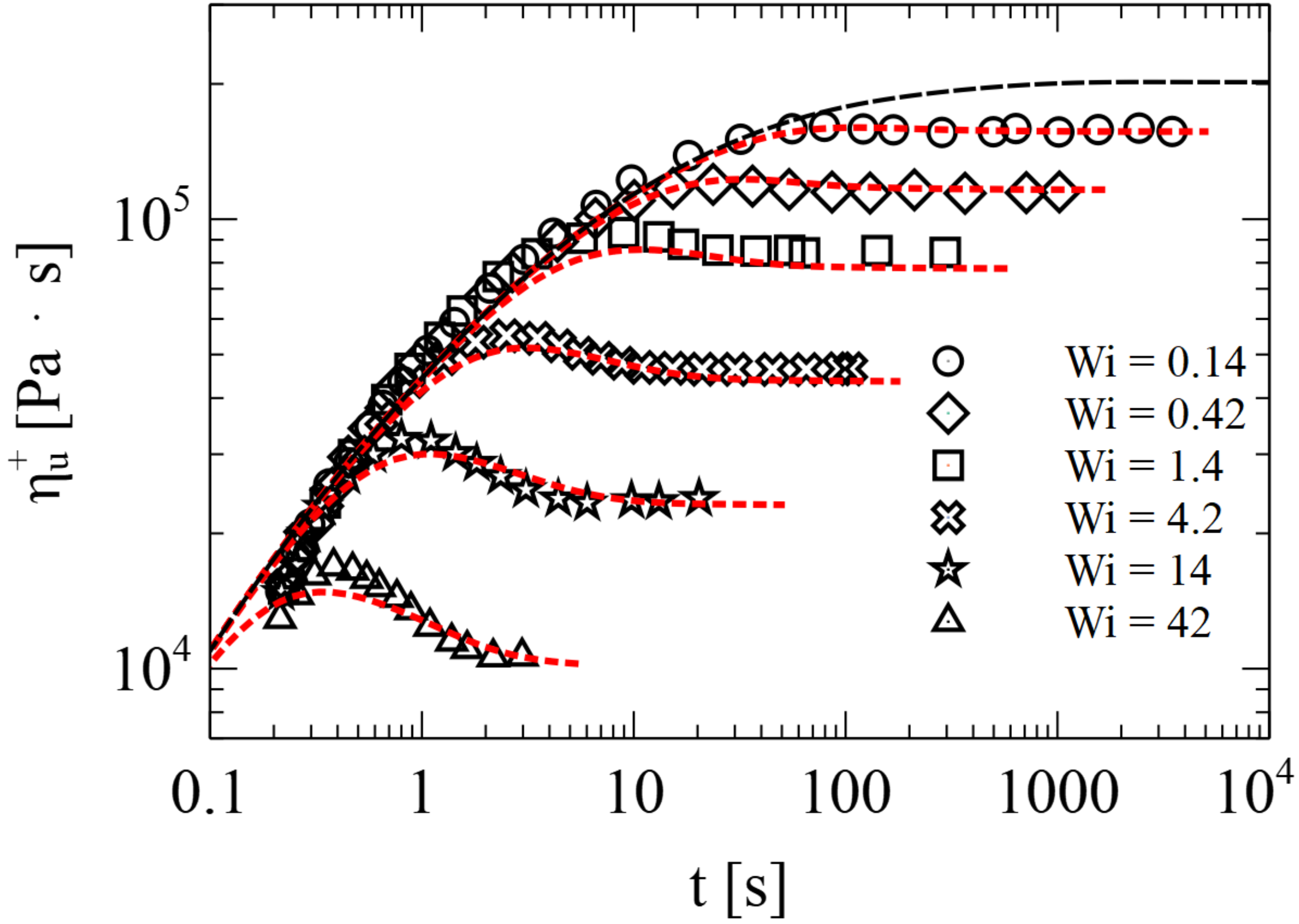
XPP + STR Model prediction.
No experimental data.



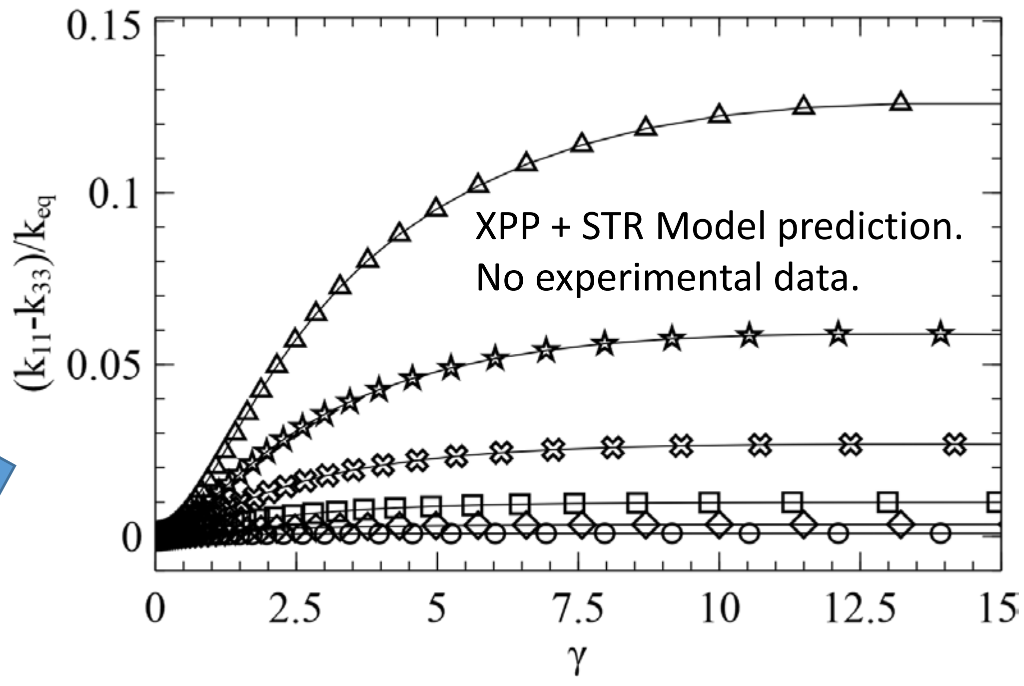
Data: Venerus et al. JOR 1999

Transient Start-up: Shear Rheology PS

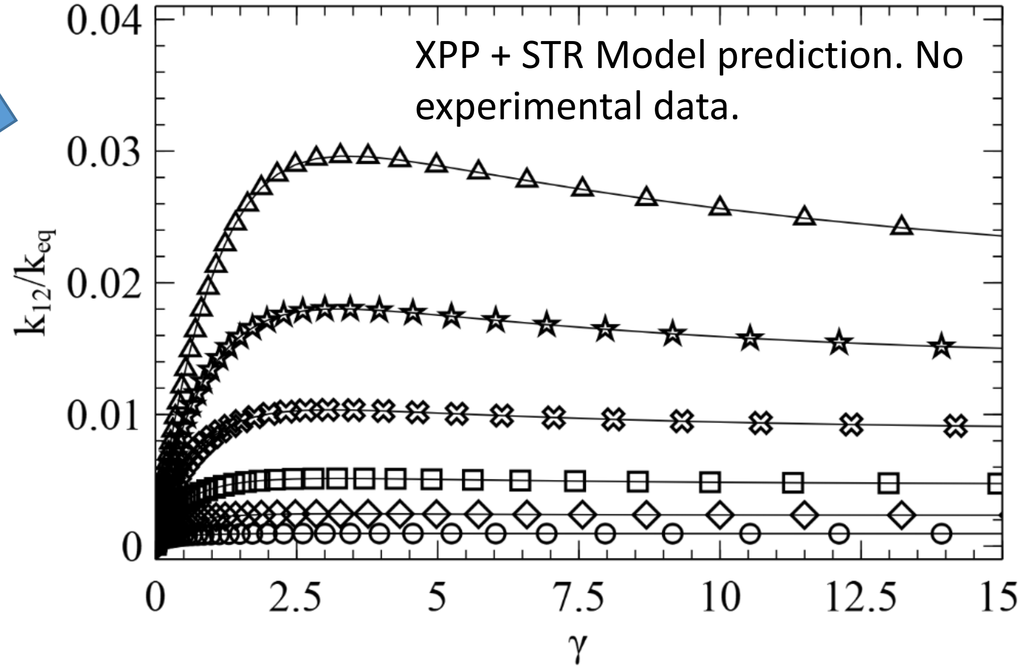
Dashed lines → XPP Model



Data: Thomas Schweizer Rheol. Acta 2002

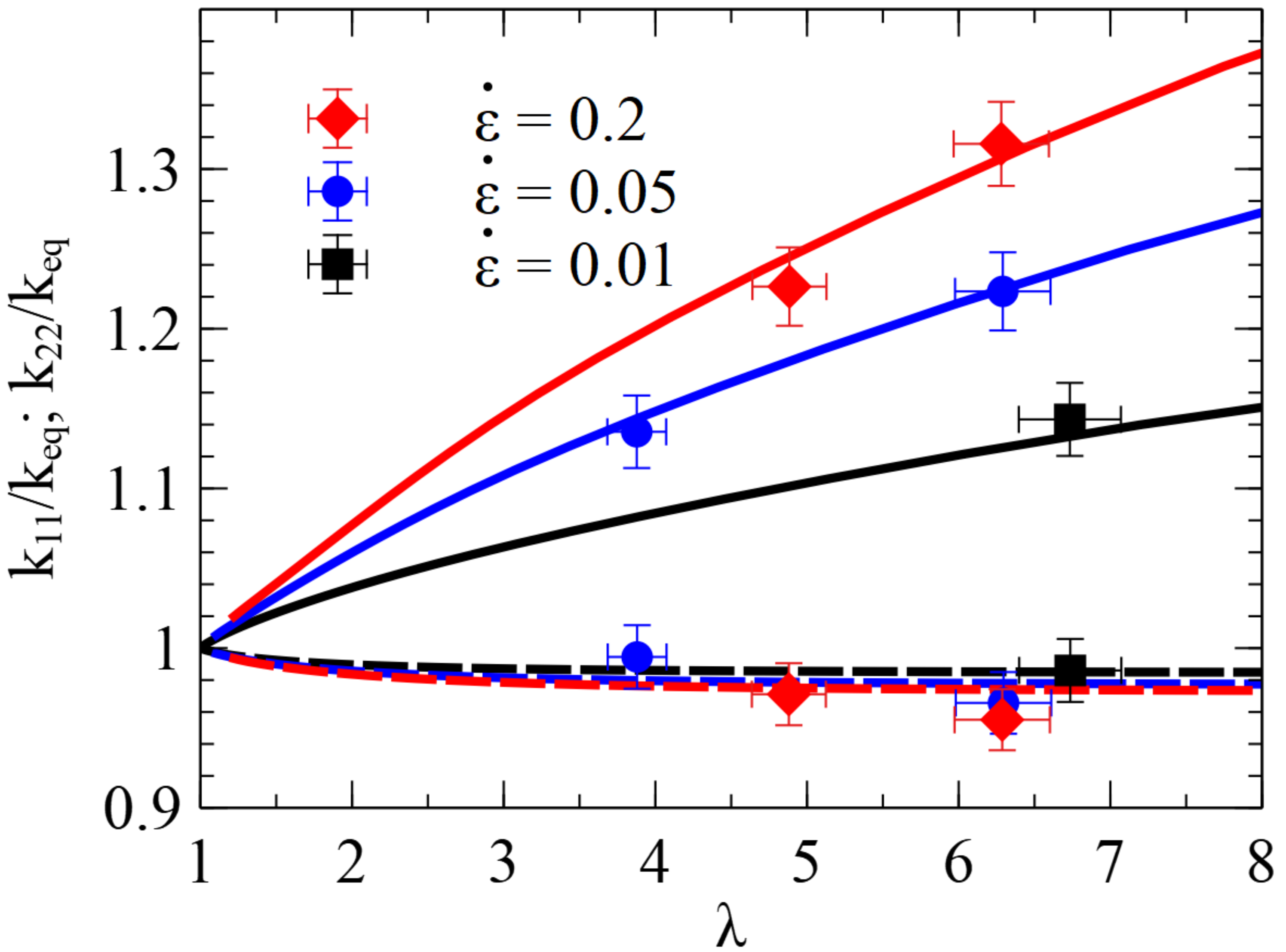


XPP + STR Model prediction. No experimental data.



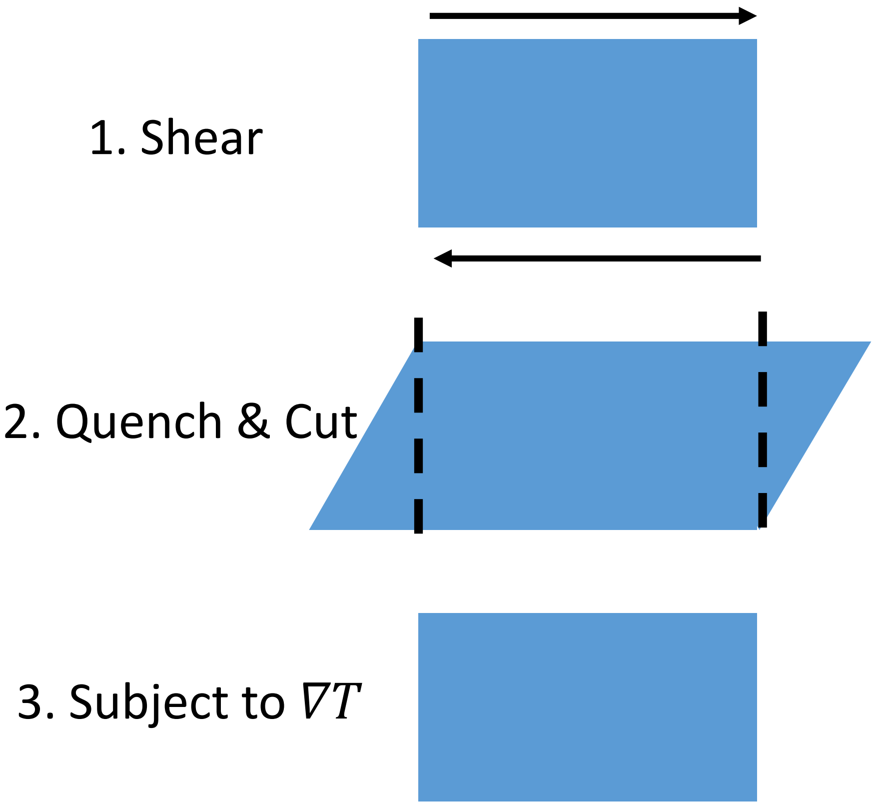
XPP + STR Model prediction. No experimental data.

Comparison to experiments: PS



FRS Measurements after quenching. Data from Gupta et al. JOR 2013

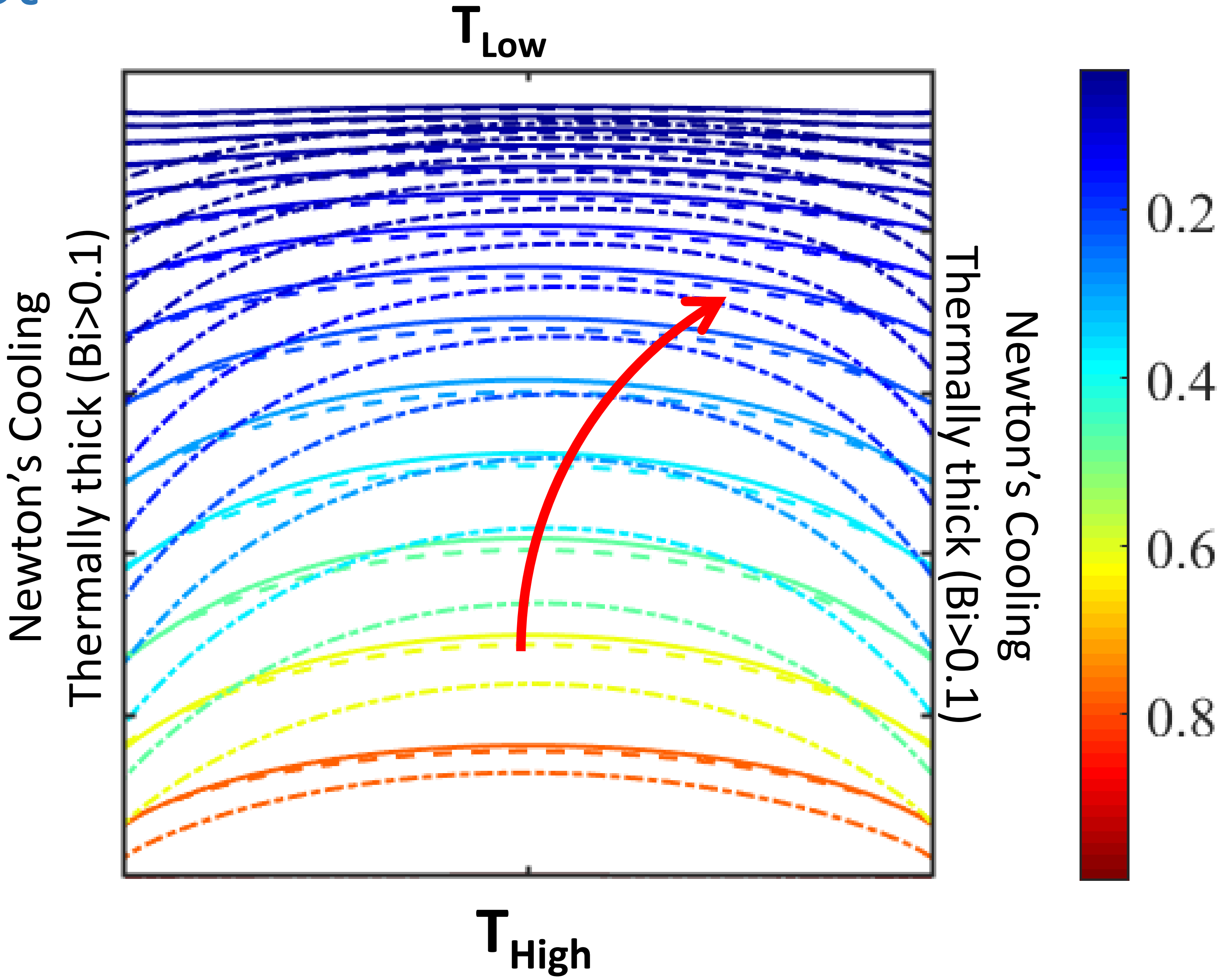
Thermal Hall Effect



1. Shear

2. Quench & Cut

3. Subject to ∇T



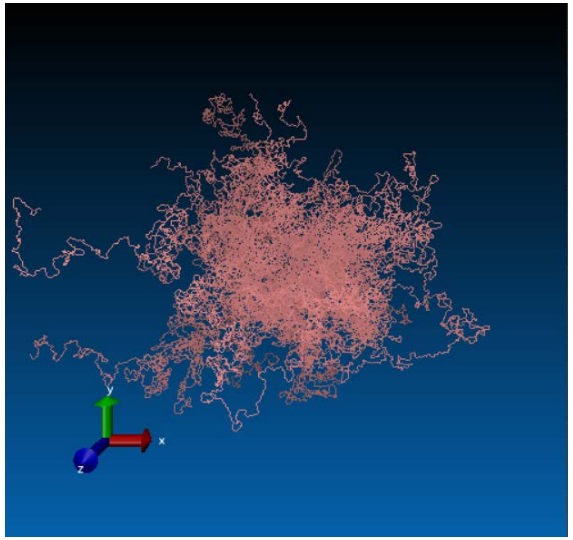
α_{11}=1.00, α_{22}=1.00, α_{12}=0.00

α_{11}=1.20, α_{22}=0.95, α_{12}=0.00

α_{11}=1.20, α_{22}=0.95, α_{12}=0.25

Roadmap for the next six months:

- Previous MD work focus on dimensionality, effect of chemistry, chain length, stiffness…



- C78 (N=48)
- C1000 (N=60)

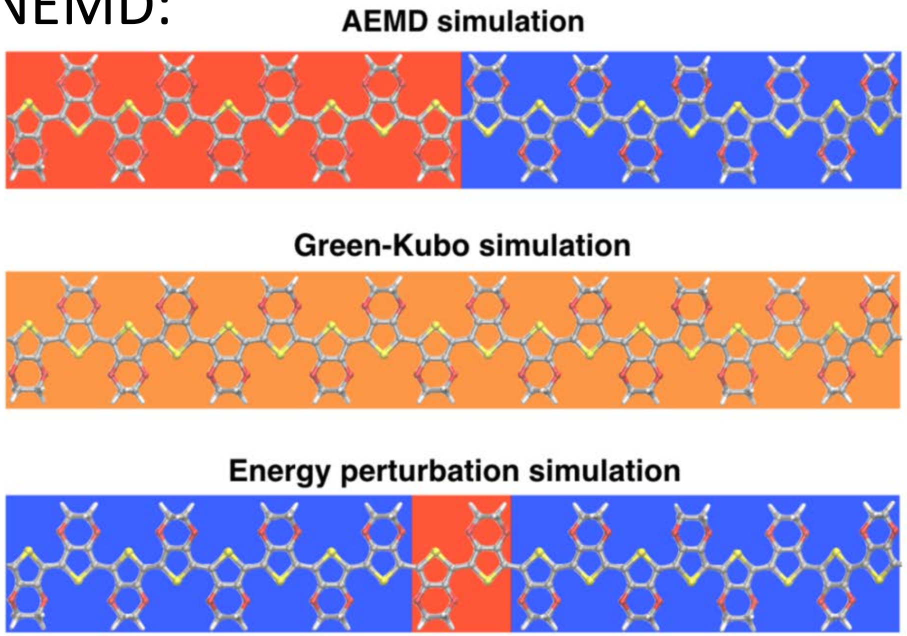
1) MC equilibration under orienting fields ~ deformation rates

2) EMD to obtain structure-property relations:
- k vs. stress
- k vs. structure

$$k_{ij} \propto C_{k,p} v^{i}_{k,p} \lambda^{j}_{k,p}$$

$$\lambda_j \propto L_e?$$

- k Measurement methods:
  - EMD: Green-Kubo
  - AEMD:
  - NEMD:

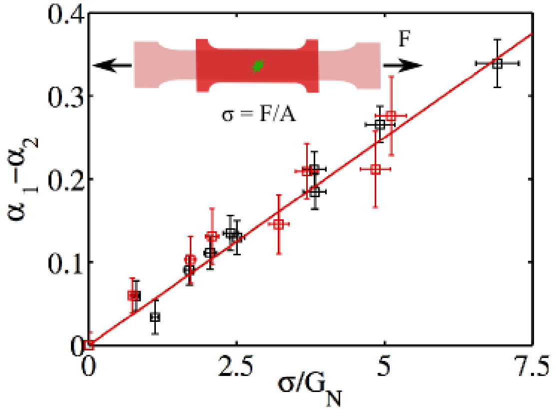


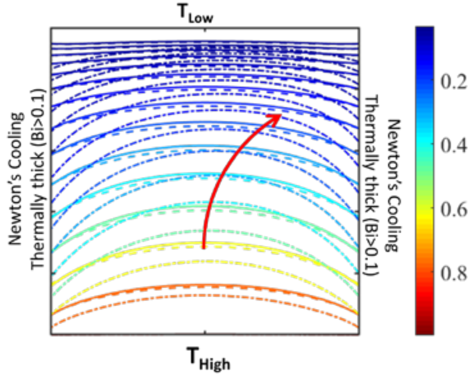
$$k_{ij} = \frac{1}{k_B V T^2} \int_0^{\infty} \langle J_i(t) J_j(0) \rangle dt$$

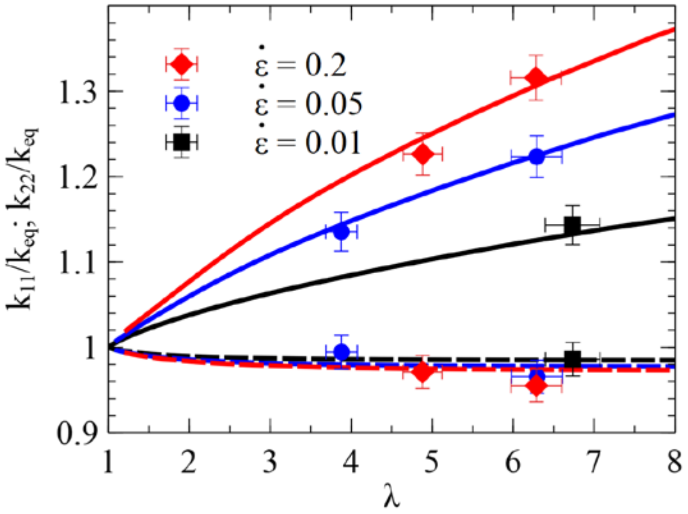
Crnjar et al. Phys. Rev. Mat. 2018

Conclusions

1. Thermal transport becomes anisotropic in polymers subjected to deformation
2. Flow induced anisotropy has significant implications in polymer processing
3. Experimental evidence of:
   - Proportionality to Stress: Stress-Thermal Rule (STR)
   - Universality
   - Beyond Finite Extensibility
4. We can use constitutive models (XPP, RP…) amenable to numerical flow simulations and the STR to include anisotropy in thermal conductivity in non-isothermal flows
5. MD simulations represent a unique tool to gain insight into the open questions regarding thermal transport in polymeric materials.







Thank you!

David C. Venerus and Jay D. Schieber (Illinois Institute of Technology)

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Wilco M.H. Verbeeten (Universidad de Burgos)

Doros N. Theodorou (National Technical University of Athens)

Molecular to Continuum Investigation of Anisotropic Thermal Transport in Polymers
“MCIATTP”
Project # 750985

UNIVERSIDAD
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MARIE CURIE ACTIONS

HORIZON 2020