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Continuum mechanical modeling of processing induced initial anisotropy in the finite strain deformation of amorphous thermoplastic polymers

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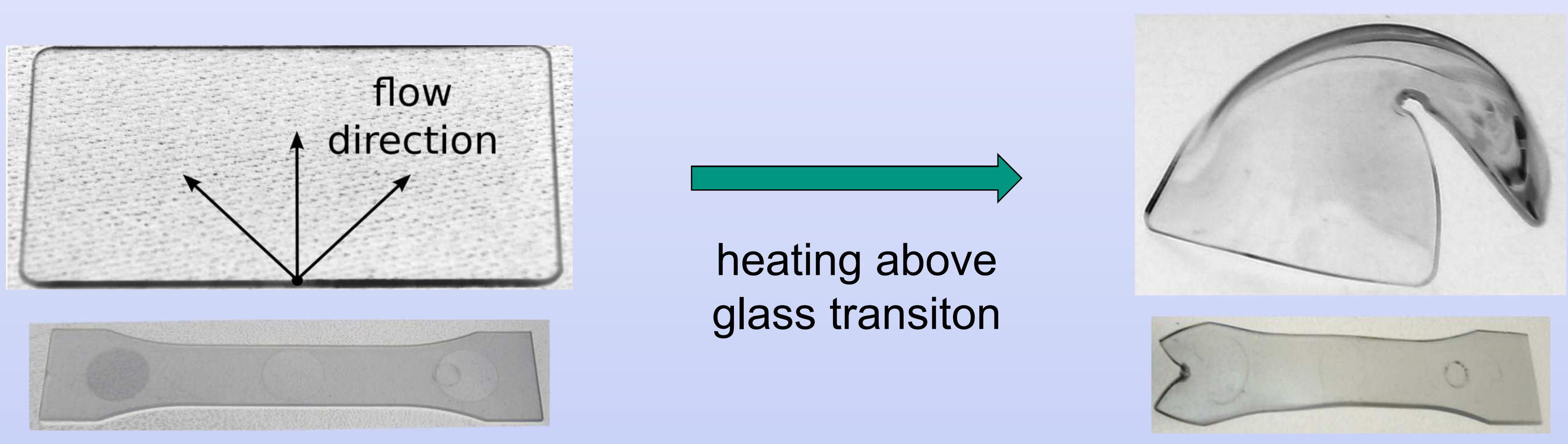
Motivation

- injection molding of plastic components gives rise to "frozen-in" molecular stretch and orientation
- examples (injection molded plate and tensile test specimen, PMMA)



- molecular orientation visible under polarized light

bright ≙ high molecular orientation

no orientation left after annealing at 120° C

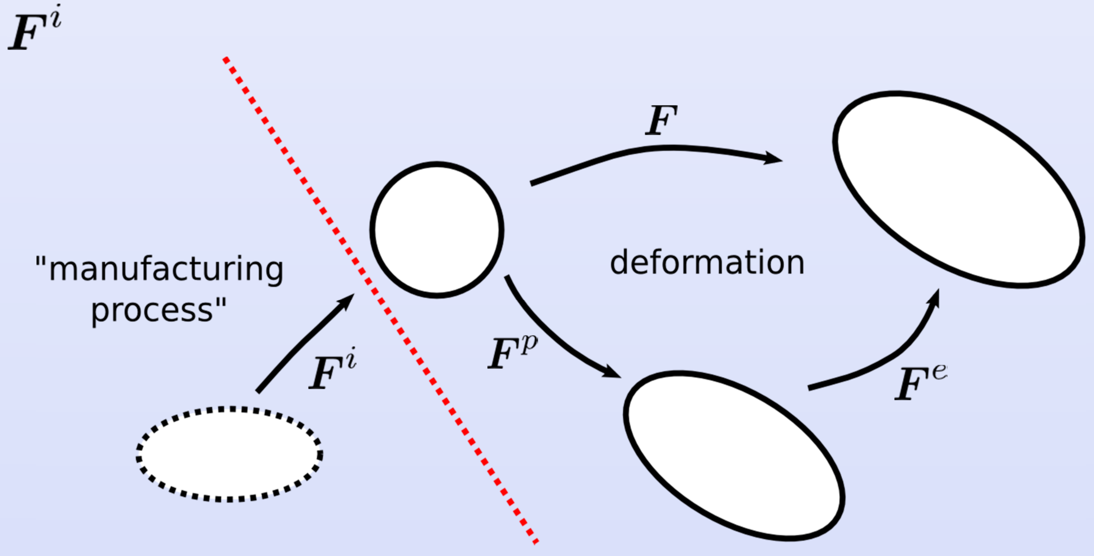
- **aim of this work:**
  predictive modeling accounting for processing influence

Constitutive modeling

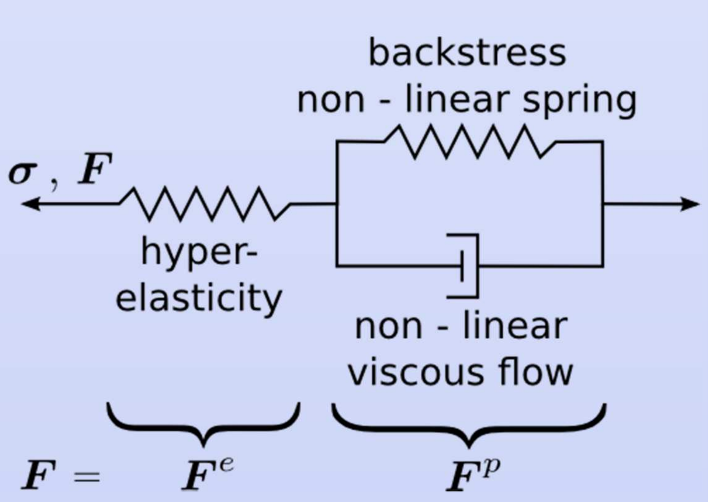
- including pre-deformation of molecular network with initial inelastic deformation gradient $\boldsymbol{F}^i$

total network deformation gradient (Boyce et al., 1989)

$$\boldsymbol{F}^n = \boldsymbol{F}^p \boldsymbol{F}^i$$



- **constitutive model** (Boyce et al., 1988,...)



  - elastic part (Neo-Hooke)

$$\boldsymbol{\sigma} = \frac{\mu}{J^e}(\boldsymbol{B}^e - \mathbf{I}) + \lambda(J^e - 1)\mathbf{I}$$

$$\boldsymbol{B}^e = \boldsymbol{F}^e \boldsymbol{F}^{eT} \quad , \quad J^e = \det \boldsymbol{F}^e$$

  - flow rule for inelastic rate of deformation tensor in intermediate configuration

$$\hat{\boldsymbol{D}}^p = \dot{\gamma}^p \frac{\bar{\boldsymbol{\Sigma}}'}{|\bar{\boldsymbol{\Sigma}}'|} \,, \quad \bar{\boldsymbol{\Sigma}}' = \boldsymbol{\Sigma}' - \hat{\boldsymbol{b}}' \,, \quad \boldsymbol{\Sigma} = \det(\boldsymbol{F})\, \boldsymbol{F}^{eT} \boldsymbol{\sigma} \boldsymbol{F}^{e-T}$$

  - backstress (8-chain-model, Arruda & Boyce ,1993)

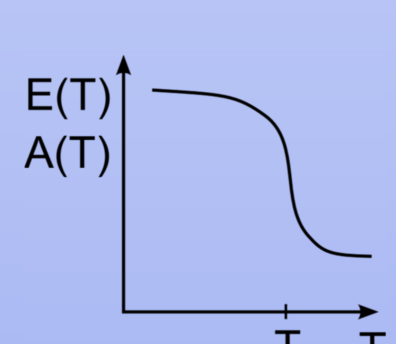
$$\hat{\boldsymbol{b}} = \frac{1}{3} C^R \frac{\sqrt{N}}{\lambda_c} \mathcal{L}^{-1}\left(\frac{\lambda_c}{\sqrt{N}}\right) \hat{\boldsymbol{B}}^n \,, \quad \hat{\boldsymbol{B}}^n = \boldsymbol{F}^n \boldsymbol{F}^{nT} \,, \quad \lambda_c^2 = \frac{1}{3} \mathrm{tr} \hat{\boldsymbol{B}}^n$$

effect of current inelastic deformation and initial network deformation

  - inelastic strain rate (Argon, 1973)

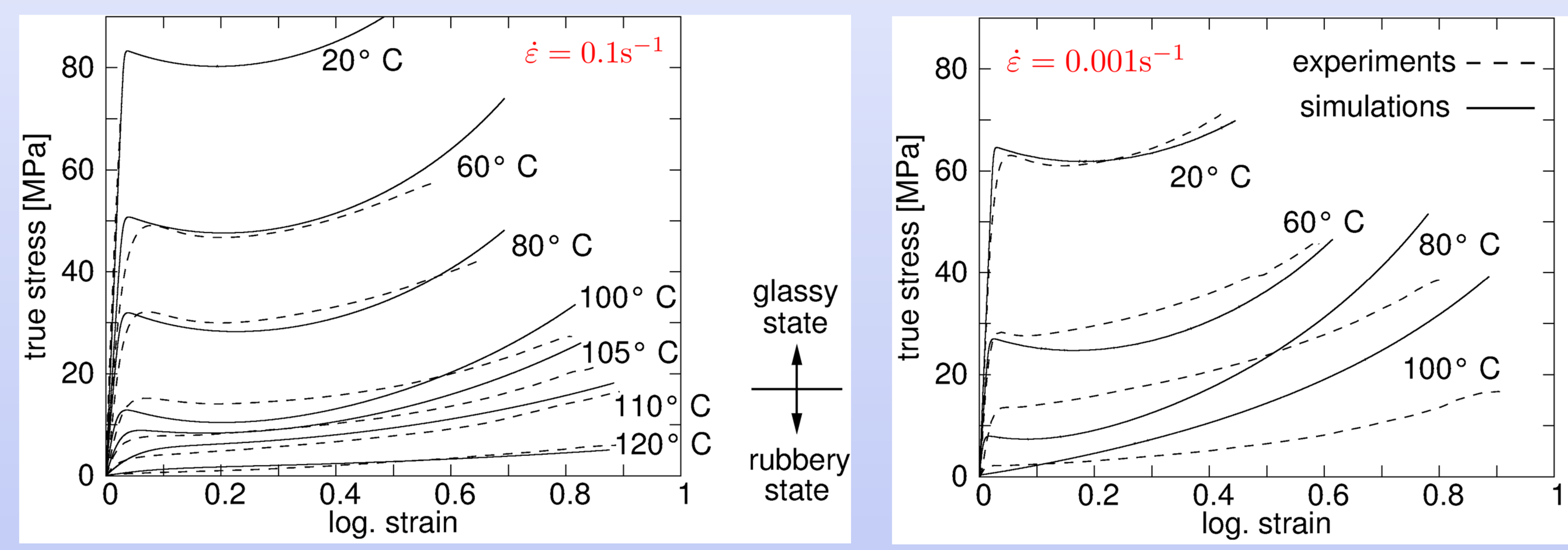
$$\dot{\gamma}^p = \dot{\gamma}_0^p \exp\left[-\frac{As}{T}\left(1 - \left(\frac{|\bar{\boldsymbol{\Sigma}}'|}{s}\right)^{\frac{5}{6}}\right)\right]$$

- **model extension beyond glass transition**
  - **intermolecular resistance**: temperature dependent stiffness and activation energy (Dupaix & Boyce, 2007)
  - **network resistance:** density of entanglements n(T) decreases with increasing temperature (Raha & Bowden, 1972)



Model response vs. experimental data

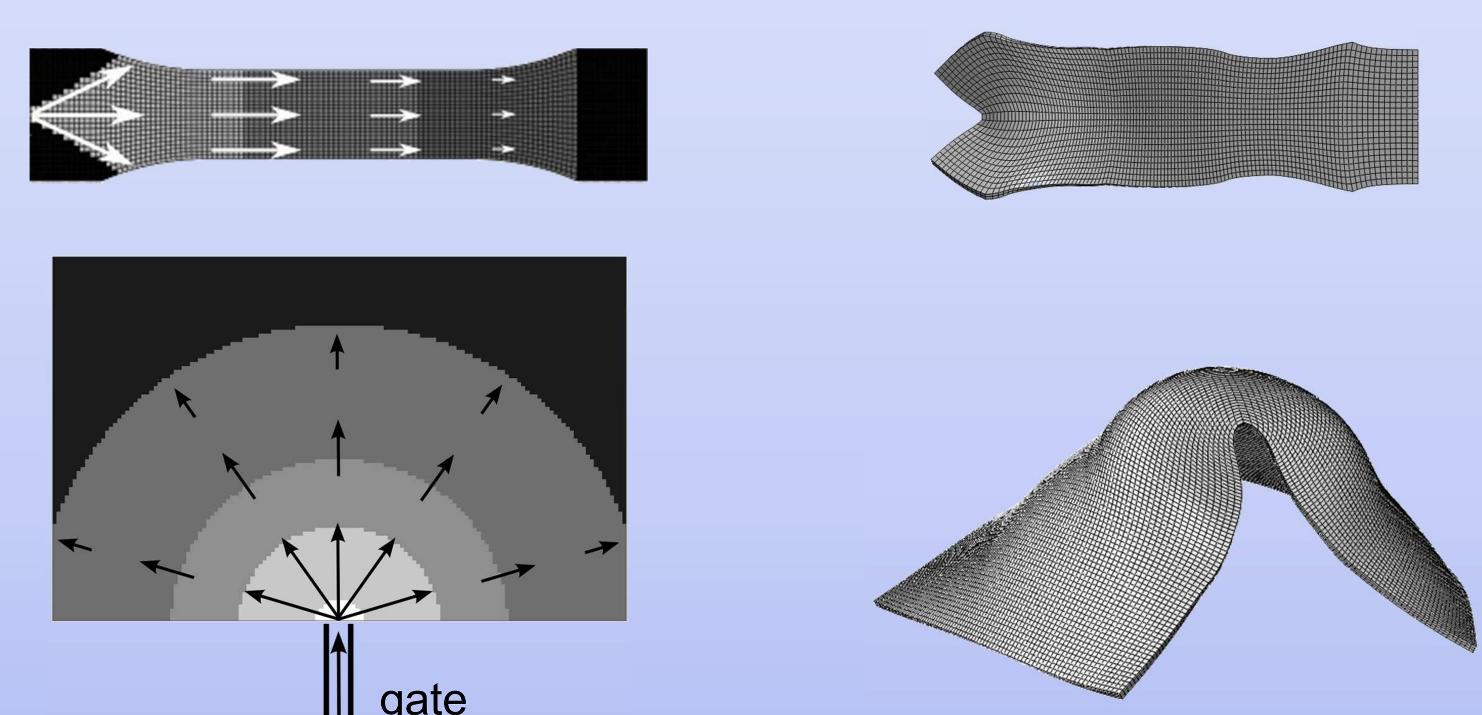
- uniaxial tensile tests at different strain rates and temperatures on PMMA (below and above glass transition)



- glass transition temperature strain rate dependent
- **requirement for model extension:**
  reduced hardening at high temperatures and low rates (molecular reptation)

Computational examples

- simulation of annealing experiments with injection molded components
- **key issue:** estimation of "frozen-in" network stretch and orientation from flow field and mapping to FE model
- 5 regions with different initial stretch



- **reasonable agreement** of stress-free deformation after heating above glass transition temperature

Conclusions & Outlook

- thermo-mechanical model for large strain deformation of amorphous thermoplastics considering initial network stretch from manufacturing process
- calibrated from experiments over a wide range of temperatures
- reasonable esimate of stress-free deformation during heating

future work:

- estimation and mapping of molecular stretch and orientation from mold filling simulations
- improvement of temperature dependent network model
- application: forming simulations including manufacturing influence (process chain)