Micromodelling of polyethylene materials

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PRESENTATION OUTLINE

1. Research objectives
2. Modelling of crystalline polyethylene
3. Modelling of semicrystalline polyethylene
4. Conclusions

PROBLEM STATEMENT

Motivation

- To understand the interplay between the microstructure and the overall macroscopic behaviour of semicrystalline polyethylene.

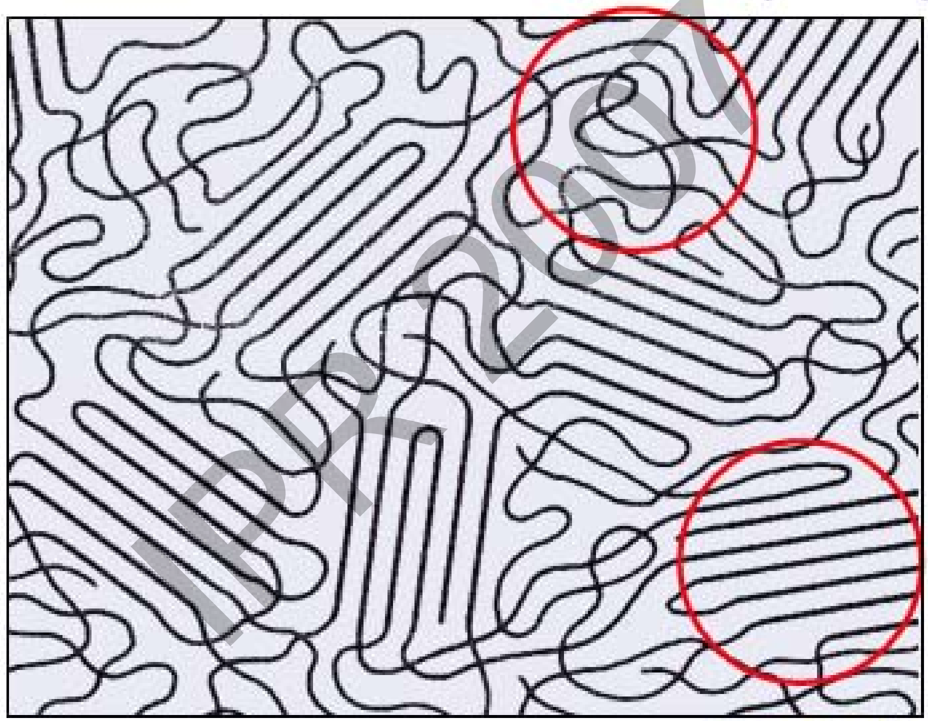
Goal

- To understand the deformation process of polyethylene
- To develop constitutive models to predict the mechanical behaviour of polyethylene considering the damage processes occurring at large deformations.

POLYETHYLENE PHASES

Polyethylene structure

Amorphous phase



Crystalline phase

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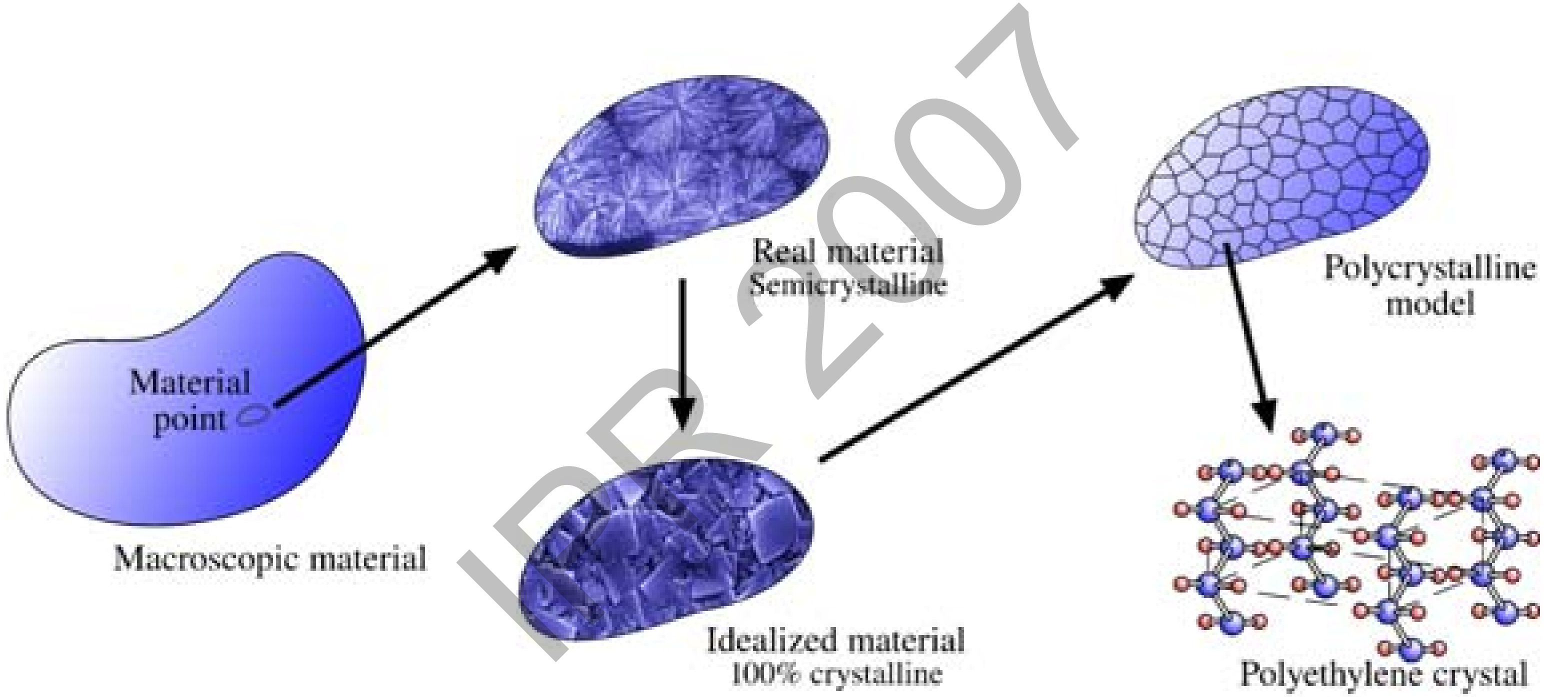
MODELLING APPROACH

Idealized 100% crystalline polyethylene

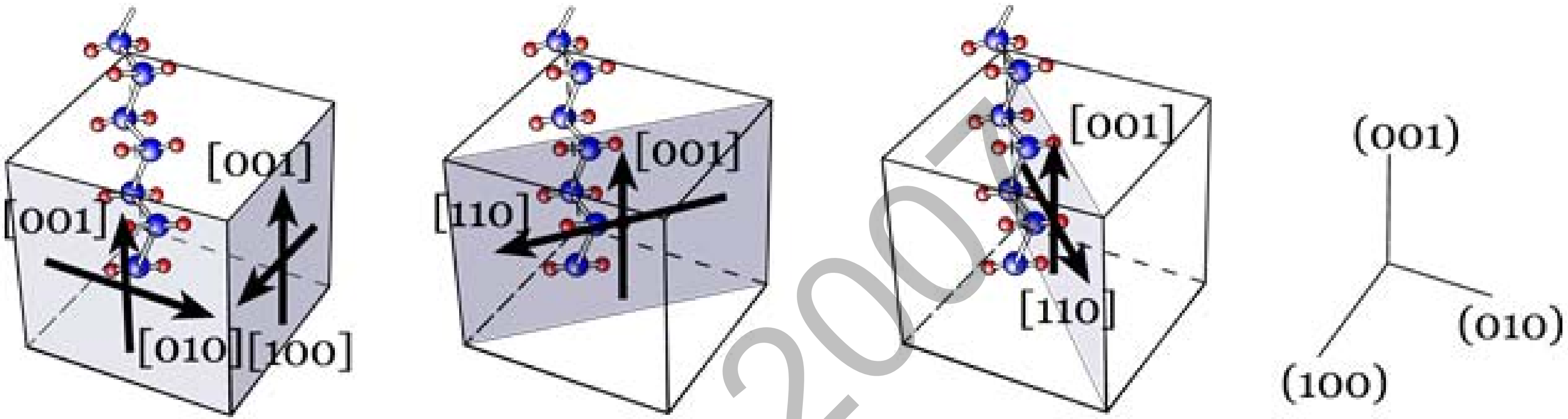


Macroscale

Microscale

DEFORMATION MECHANISMS

Crystallographic slip systems



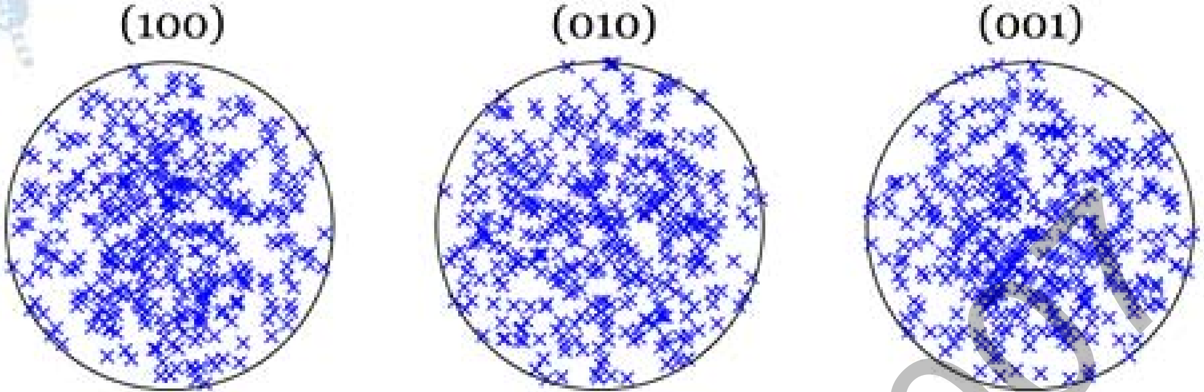
Critical shear strength

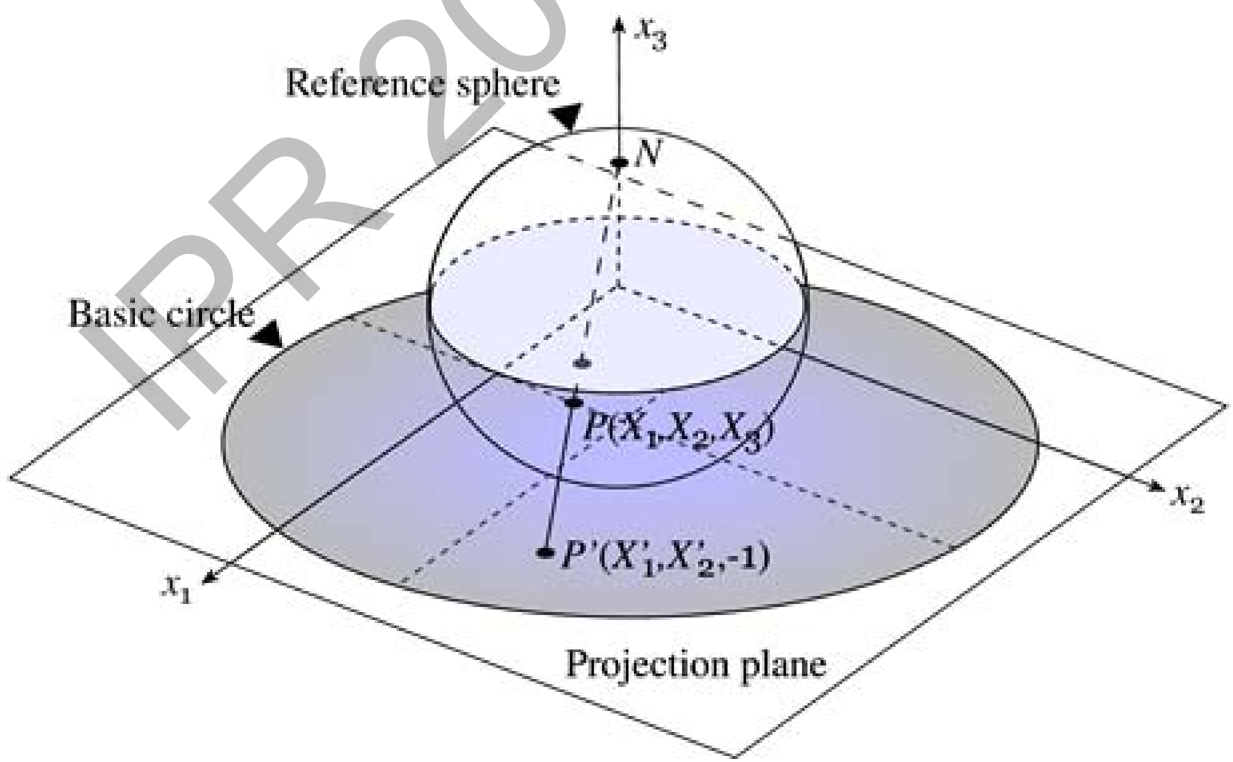
Slip system	g^{a} (MPa)
(100) [001]	7.2
(010) [001]	15.6
{110} [001]	13.0
(100) [010]	12.3

Bartczak *et al*, 1992

CRYSTAL AGGREGATE

Crystallographic texture





CRYSTALLINE POLYETHYLENE

Summary - Viscoplastic model

Schmid tensor

$$\mathbf{T}^\alpha = \mathbf{n}^\alpha \otimes \mathbf{s}^\alpha$$

EQUILIBRIUM

Resolved shear stress

$$\boldsymbol{S} = \boldsymbol{\sigma} - tr(\boldsymbol{\sigma})\boldsymbol{I}$$

$$\tau^\alpha = \mathbf{S} : \mathbf{T}^\alpha$$

Stress-strain relationship

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left(\frac{\tau^\alpha}{g^\alpha} \right)^n$$

$\dot{\gamma}^\alpha$ Shear strain rate

τ^α Resolved shear stress

COMPATIBILITY

Deformation rate and spin

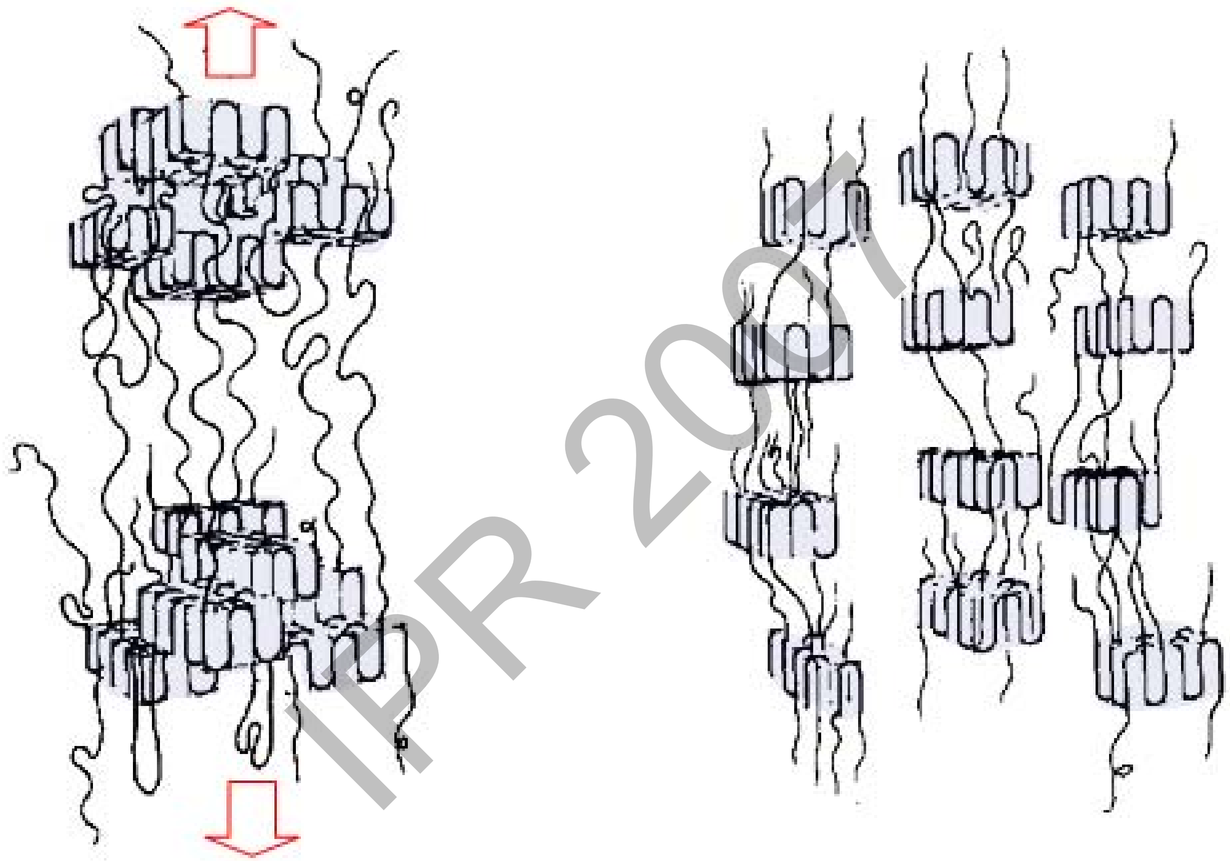
$$\mathbf{D}^p = \sum_\alpha \dot{\gamma}^\alpha \mathrm{sym}(\mathbf{T}^\alpha) \qquad \mathbf{W}^p = \sum_\alpha \dot{\gamma}^\alpha \mathrm{skw}(\mathbf{T}^\alpha)$$

$\mathbf{D}^p$ Deformation rate

$\mathbf{W}^p$ Spin

DAMAGE MODEL

Stress-strain state in single crystals

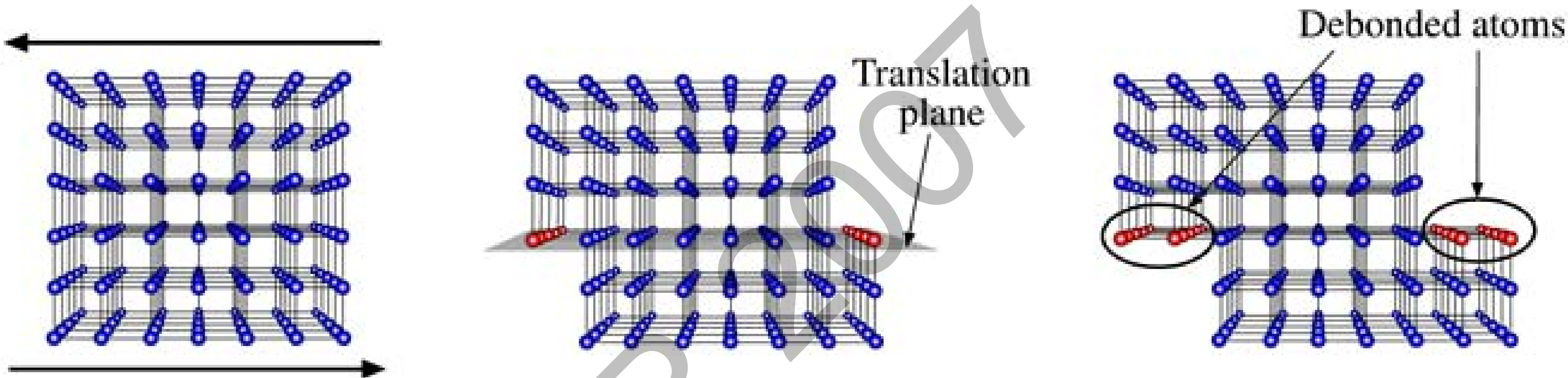


$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left(\frac{\tau^{\alpha}}{g^{\alpha}} \right)^{n}$$

Stress-strain relationship with no damage

DAMAGE MODEL

Stress-strain state in single crystals



Undamaged crystal

Damage crystal

$$\Omega^{\alpha} = \frac{\text{Current number of atomic debonds}}{\text{Initial number of atomic bonds}} = \frac{\text{Total area of defects}}{\text{Initial area}}$$

DAMAGE MODEL

Stress-strain state in single crystals

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left(\frac{\tau^{\alpha}}{g^{\alpha}} \right)^n$$

Classic viscoplastic model

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left(\frac{\tau^{\alpha}}{(1-\Omega^{\alpha}) g^{\alpha}} \right)^n$$

Stress-strain relationship

$$\frac{d\Omega^{\alpha}}{d\tau^{\alpha}} = \dot{\Omega}_0 \left| \frac{\tau^{\alpha}}{(1-\Omega^{\alpha}) g^{\alpha}} \right|^m$$

Damage evolution law

$$\frac{dg^{\alpha}}{d\gamma^{\alpha}} = h_0 \sec h^2 \left(\frac{h_0}{c} \hat{\gamma} \right)$$

Hardening law

Damage model

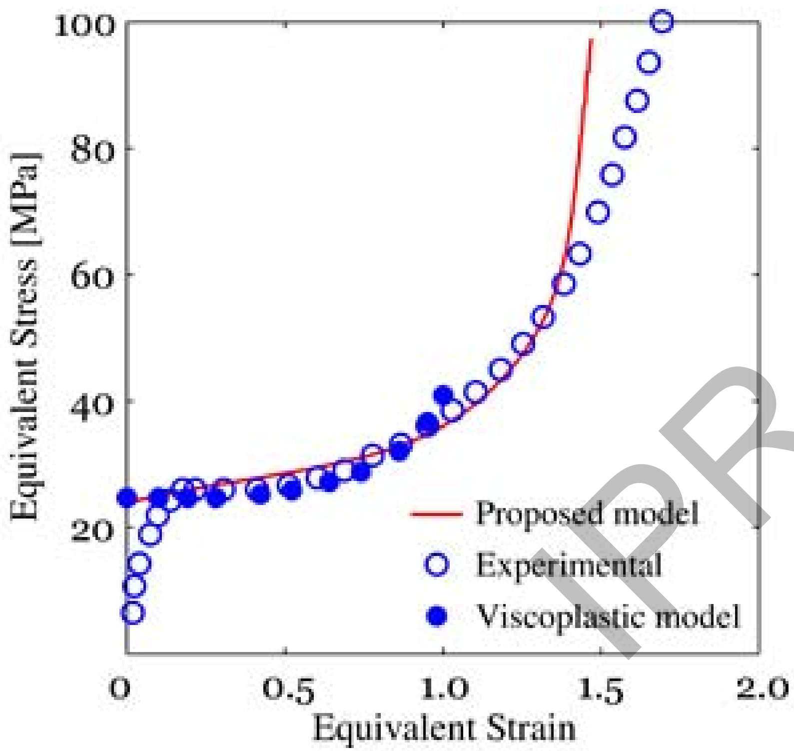
PRELIMINARY RESULTS

Proposed damage model

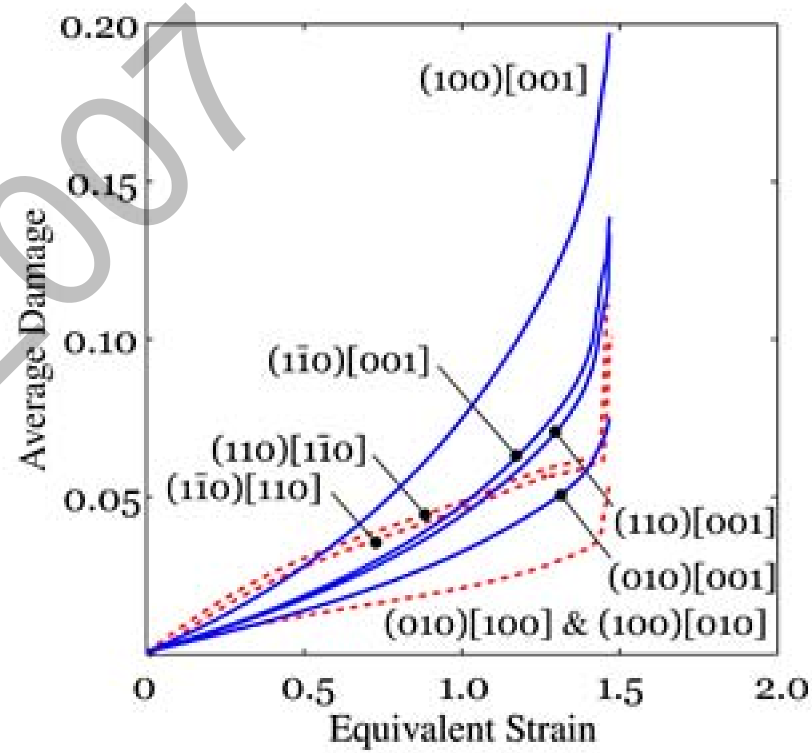
- Idealized 100% crystalline polyethylene.
- 100 randomly oriented crystals.
- Initially isotropic texture.
- Uniaxial tension and simple shear

UNIAXIAL TENSION

Idealized 100% crystalline



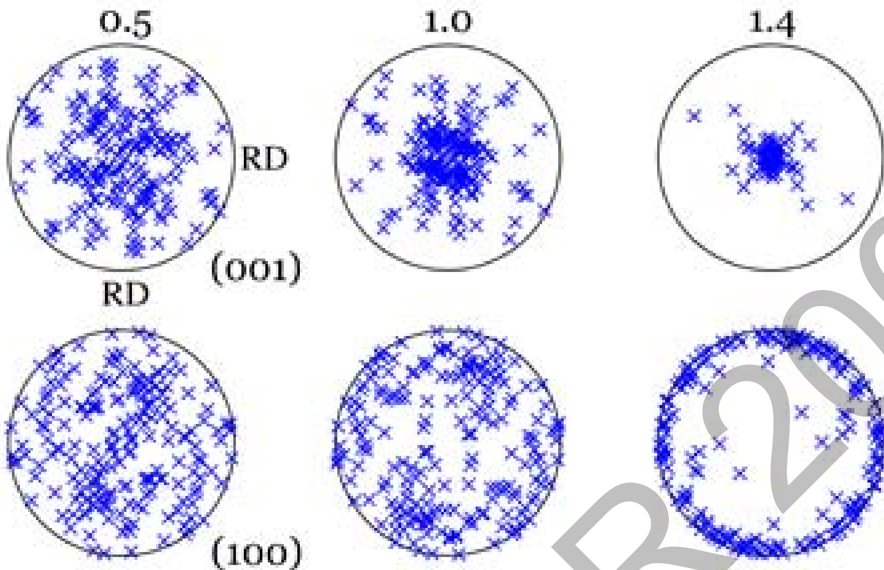
Stress-strain behaviour

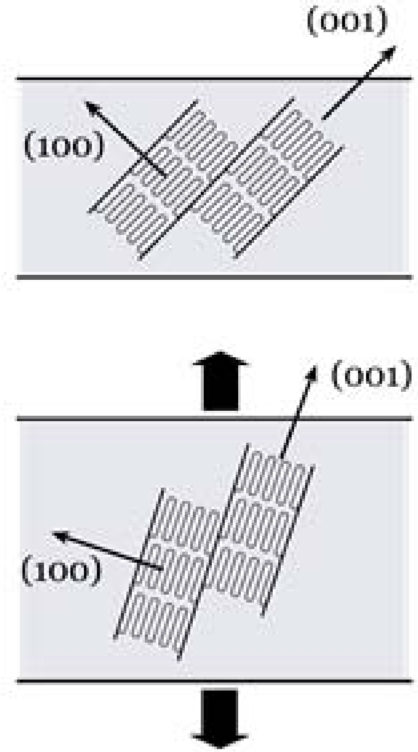


Slip systems damage

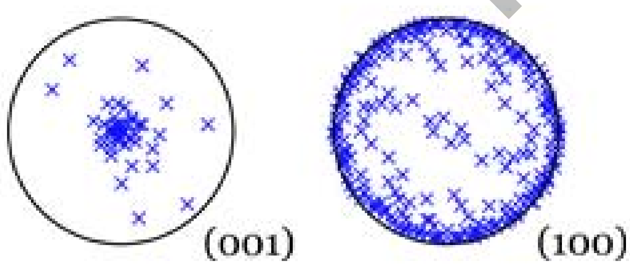
UNIAXIAL TENSION

Crystallographic textures

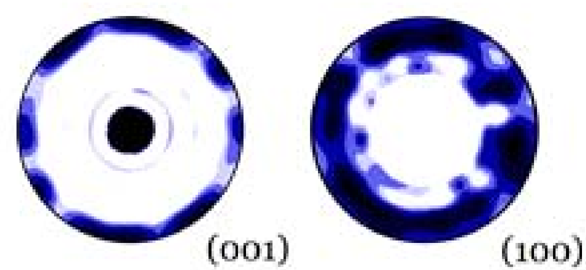




Projection perpendicular to the loading direction



Parks & Ahzi (1.0)



Experimental (1.8)

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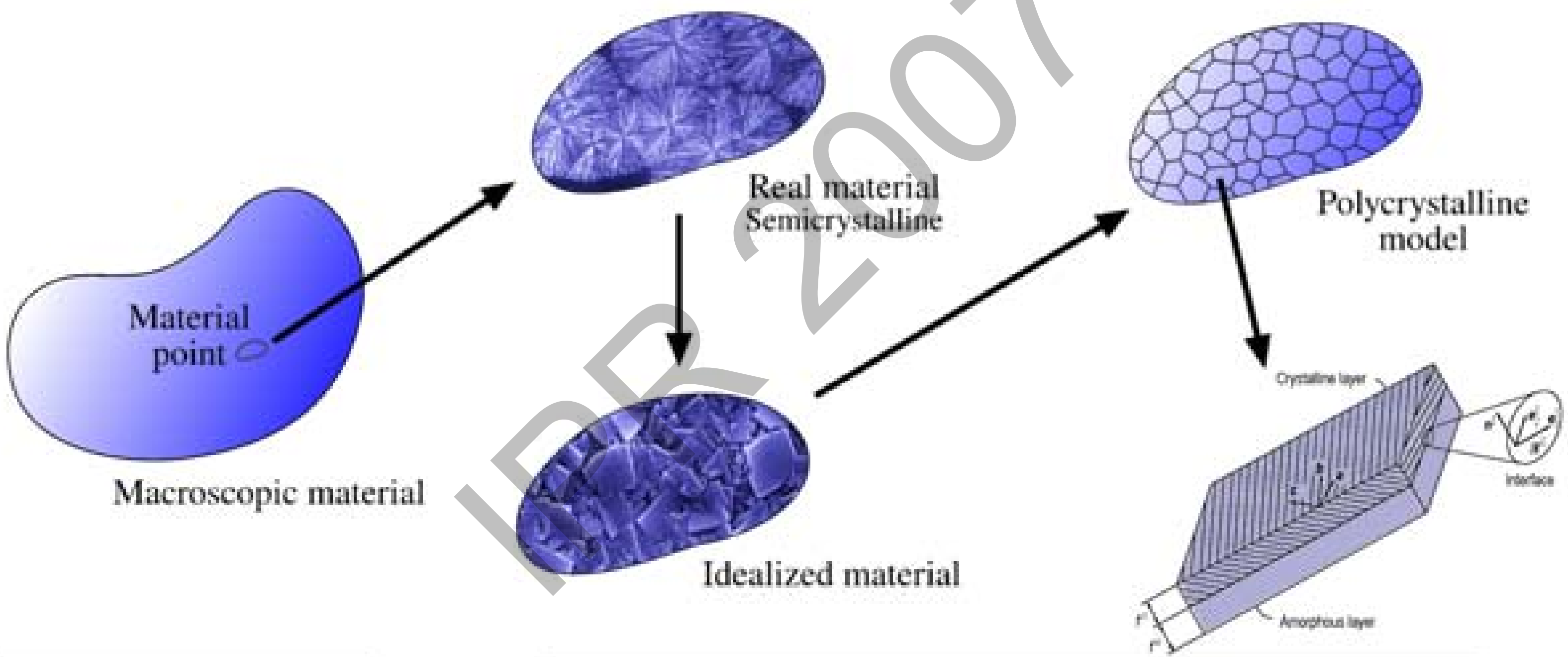
MODELLING APPROACH

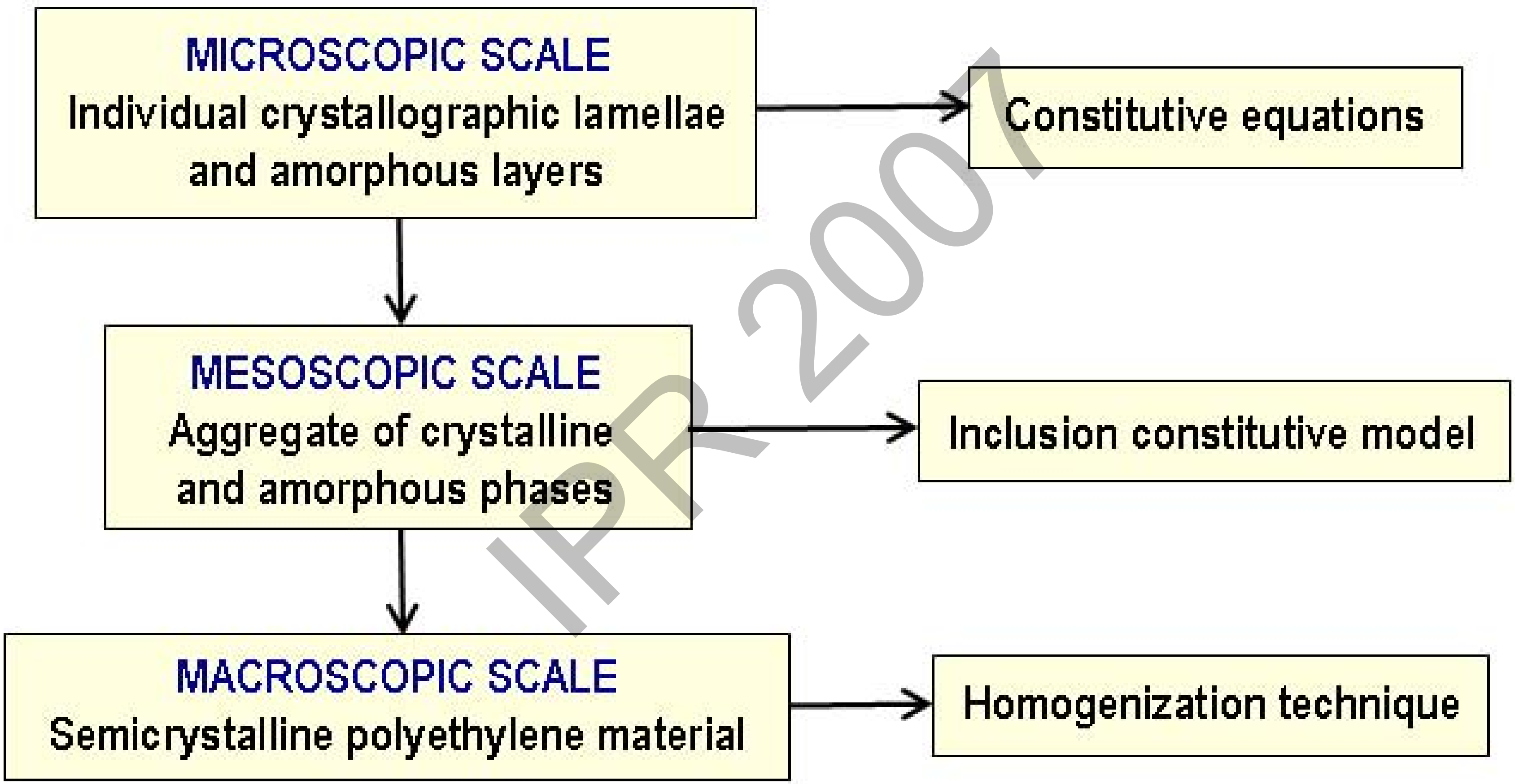
Semicrystalline polyethylene



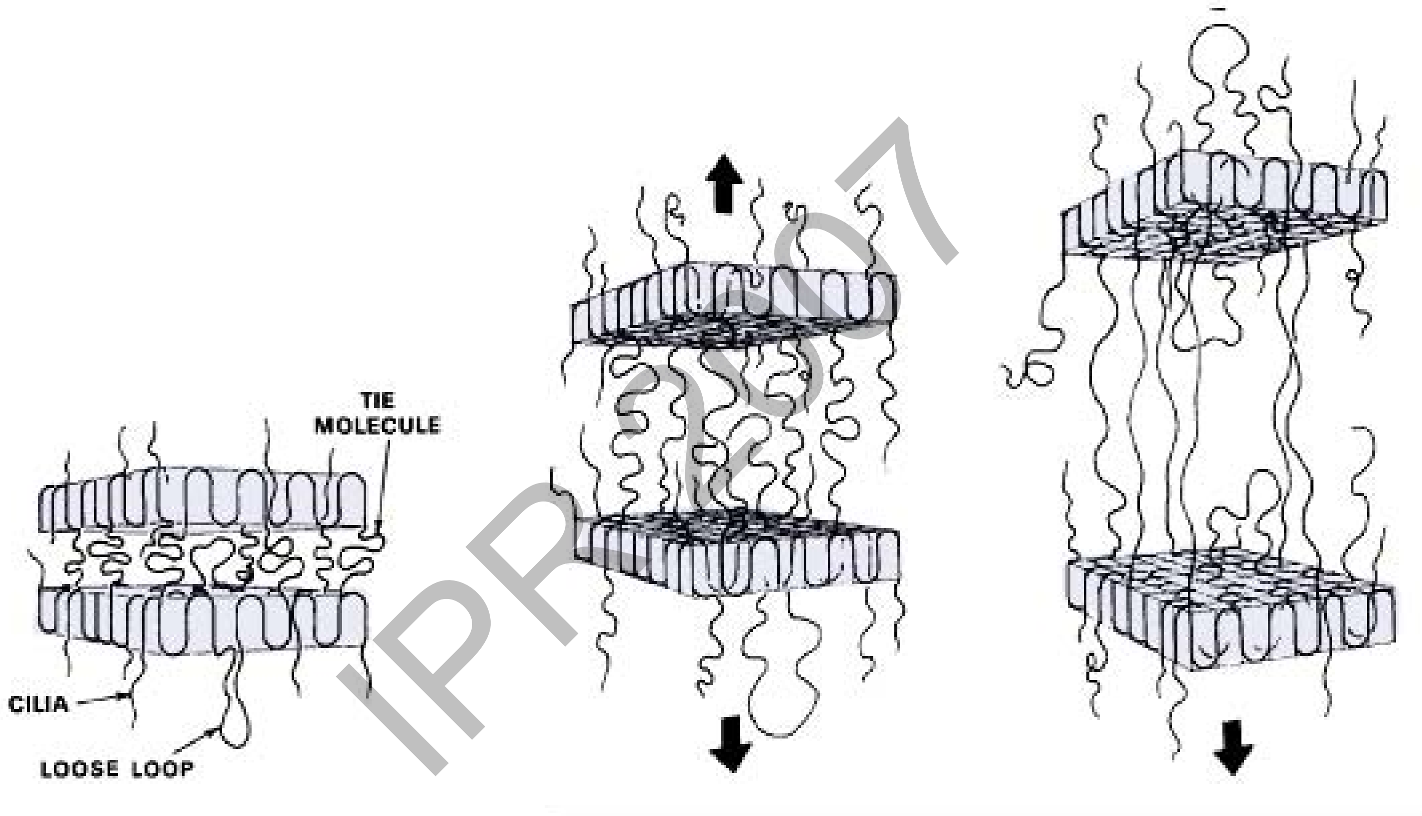
Macroscale

Microscale

MULTISCALE MODELLING



AMORPHOUS POLYETHYLENE

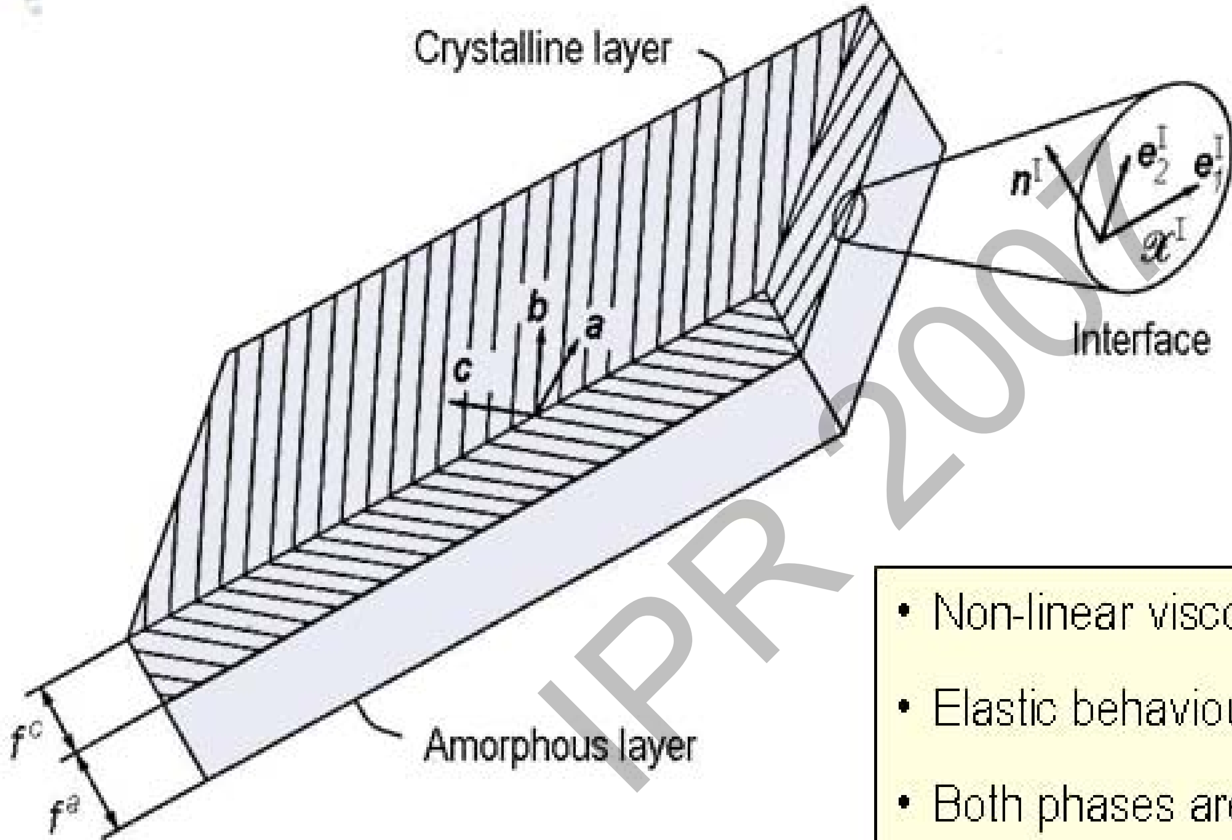


Unstrained state

Strained state

COMPOSITE INCLUSION

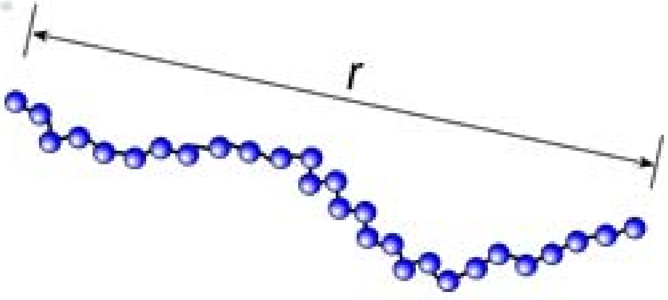
Inclusion constitutive model

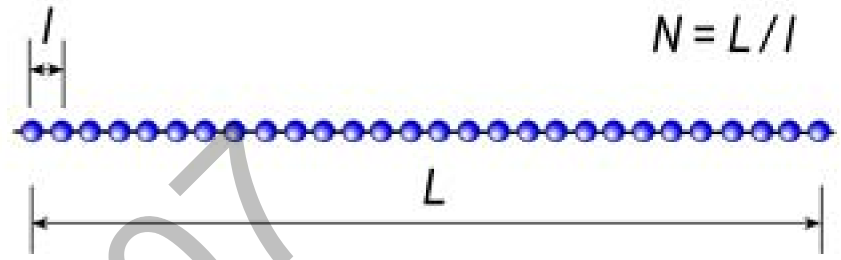


- Non-linear viscoplastic behaviour.
- Elastic behaviour is not included.
- Both phases are incompressible.
- Insensitive to pressure deformation
- Deformation and stress are uniform.

AMORPHOUS POLYETHYLENE

Molecular chain entropy





Boltzmann's Principle

$$S = k \ln W$$

$k = 1.38 \times 10^{-23}\ JK^{-1}$

Probability density of a molecular chain

$$\ln W = \text{constant} - N\left(\frac{r}{Nl}\beta + \ln\frac{\beta}{\sinh\beta}\right)$$

$\beta = \mathcal{L}^{-1}(r/Nl)$

$\mathcal{L}(\beta) = \coth\beta - 1/\beta$

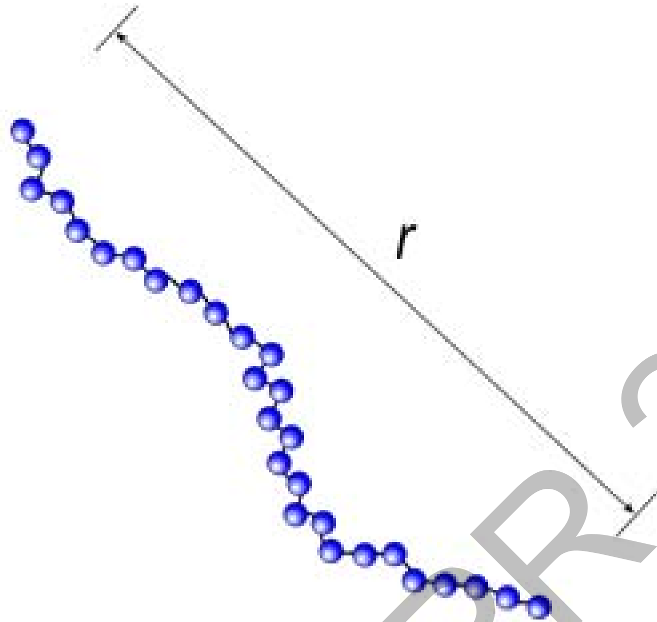
Molecular chain entropy

$$S = \text{constant} - kN\left(\frac{r}{Nl}\beta + \ln\frac{\beta}{\sinh\beta}\right)$$

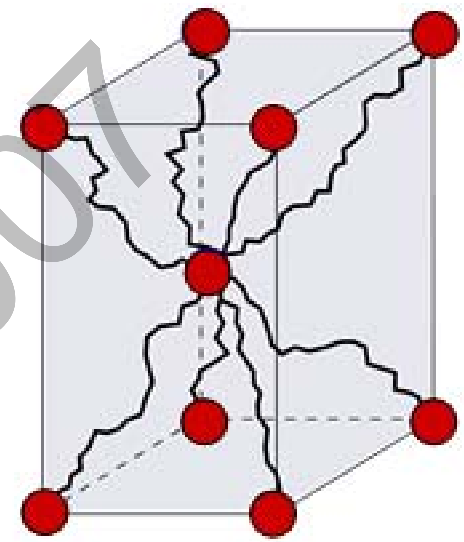
Kuhn & Grun, 1952

AMORPHOUS POLYETHYLENE

Kinematic hardening – Back-stress tensor



Idealized molecule



The eight-chain model

Back-stress tensor

$$\boldsymbol{H} = \frac{2}{J}\boldsymbol{B} \cdot \frac{\partial \Psi}{\partial \boldsymbol{B}}$$

Helmholtz free energy $d\Psi = -T dS$

$$\boldsymbol{H} = \frac{nkT}{3}\sqrt{\frac{3N}{I_1}}\mathcal{L}^{-1}\left(\sqrt{\frac{I_1}{3N}}\right)\boldsymbol{B}$$

AMORPHOUS POLYETHYLENE

Summary – Viscoplastic model

Deviatoric Cauchy stress

$$S = \sigma - tr(\sigma) I$$

Deviatoric back-stress

$$H' = \frac{nkT}{3}\sqrt{\frac{3N}{I_1}}\,\mathcal{L}^{-1}\left(\sqrt{\frac{I_1}{3N}}\right)\left(B - \tfrac{1}{3} I\right)$$

Resolved shear stress

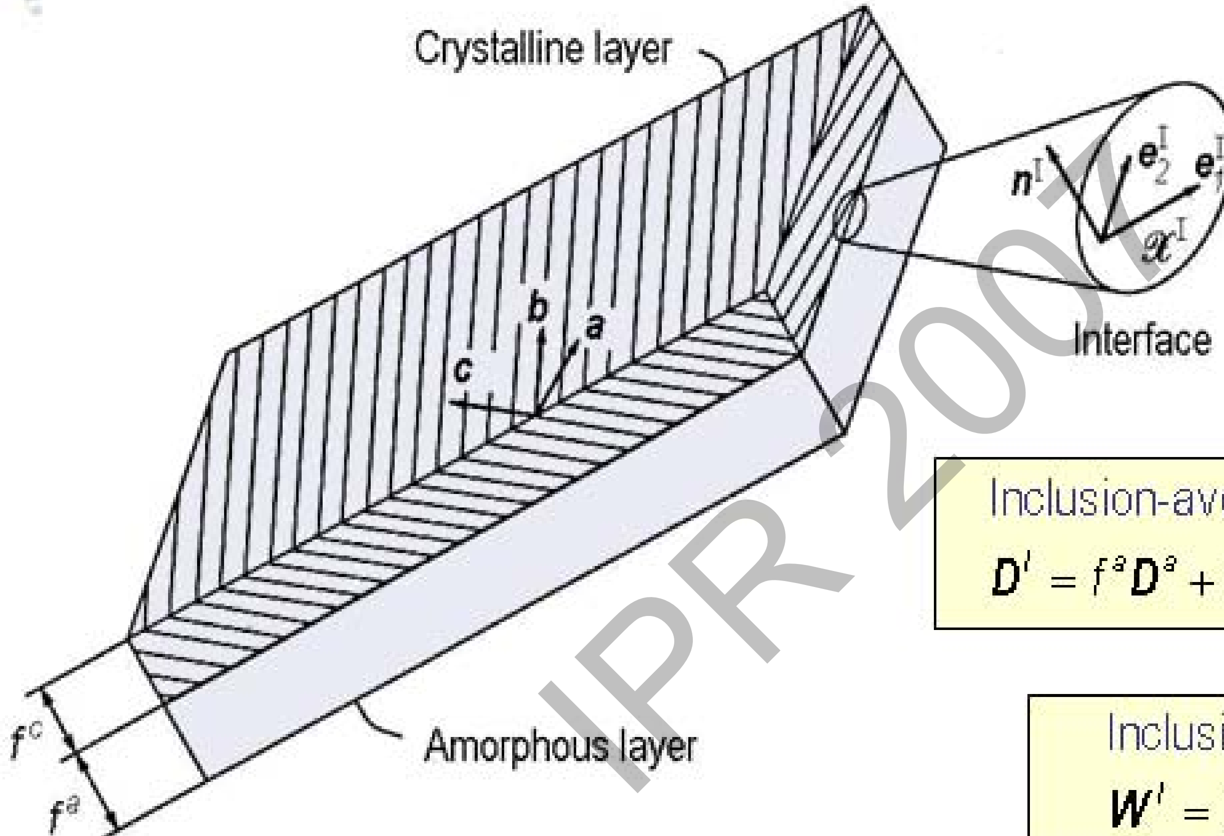
$$\tau = \left[\tfrac{1}{2}(S - H') : (S - H')\right]^{1/2}$$

Deformation rate

$$D^p = \dot{\gamma}_0 \left(\frac{\tau}{\tau_0}\right)^{m-1} \left(\frac{S - H'}{\tau_0}\right)$$

INCLUSION VOLUME-AVERAGING

Homogenization technique



Inclusion-averaged deformation rate

$$\boldsymbol{D}^I = f^a \boldsymbol{D}^a + f^c \boldsymbol{D}^c = (1 - f^c)\boldsymbol{D}^a + f^c \boldsymbol{D}^c$$

Inclusion-averaged spin

$$\boldsymbol{W}^I = (1 - f^c)\boldsymbol{W}^a + f^c \boldsymbol{W}^c$$

Inclusion-averaged deviatoric stress

$$\boldsymbol{S}^I = (1 - f^c)\boldsymbol{S}^a + f^c \boldsymbol{S}^c$$

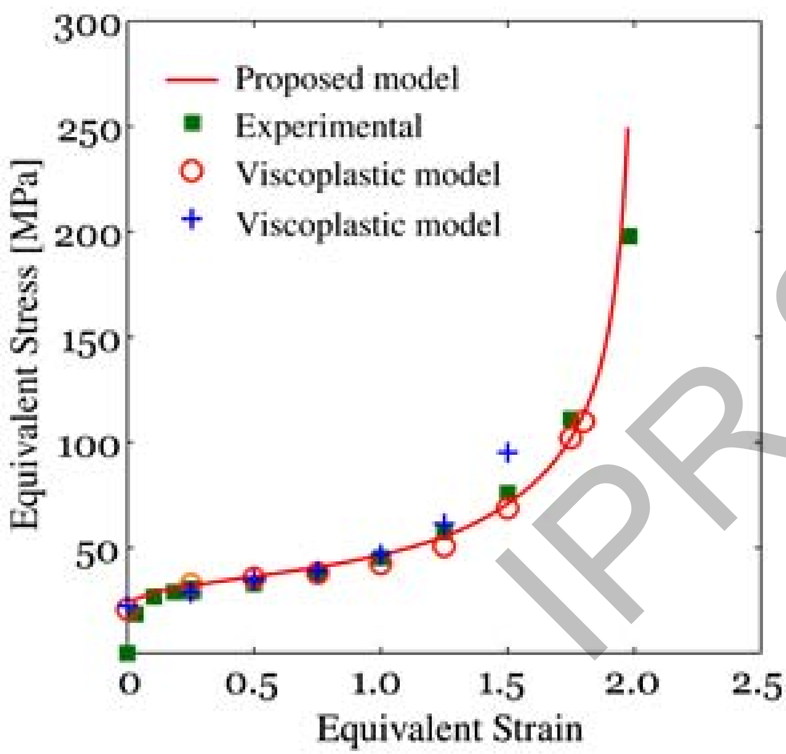
INTERACTION RELATIONS

Homogenization technique

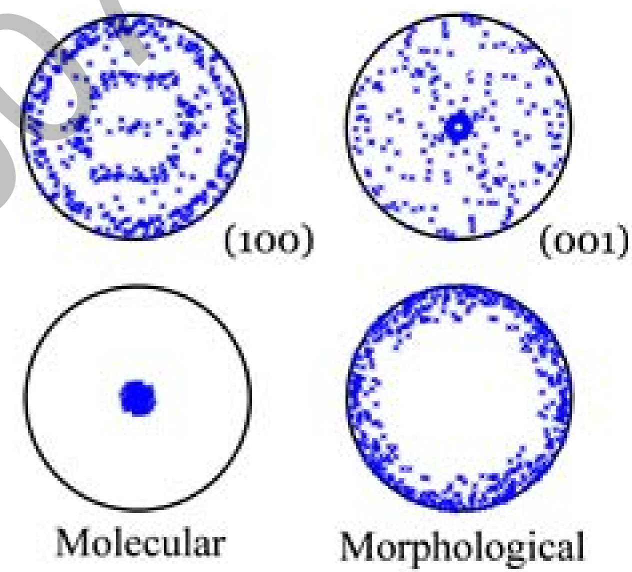
- **Sachs-like Model**
  - Local and global equilibrium are satisfied by considering the stress as uniform in all component parts.
  - Global compatibility is enforced as a global volume average.
  - Local compatibility of the inclusion deformation with the surrounding is not addressed.

UNIAXIAL TENSION

Semi-crystalline



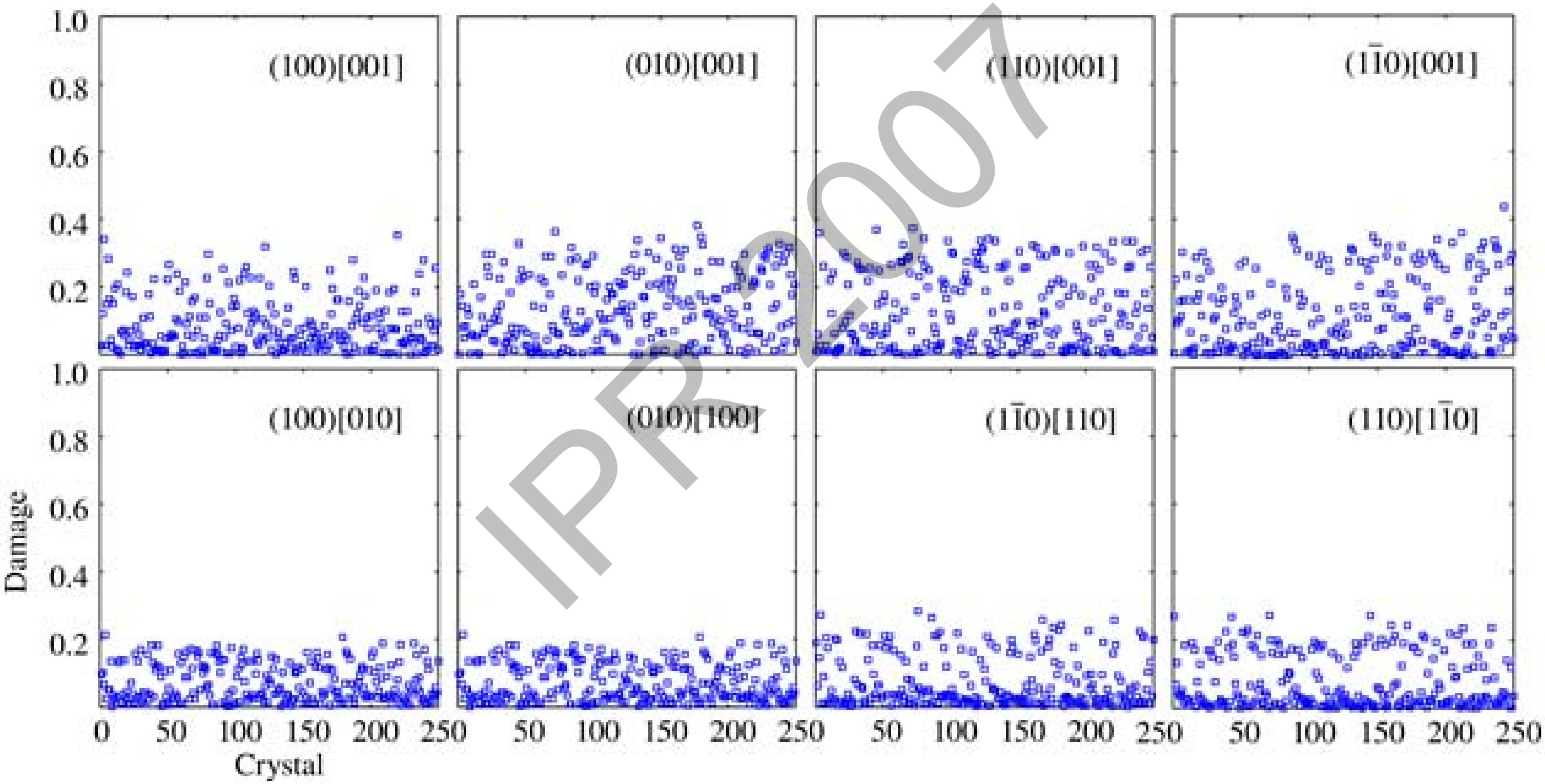
Stress-strain behaviour



Texture

UNIAXIAL TENSION

Semi-crystalline – Slip system damage



UNIAXIAL TENSION

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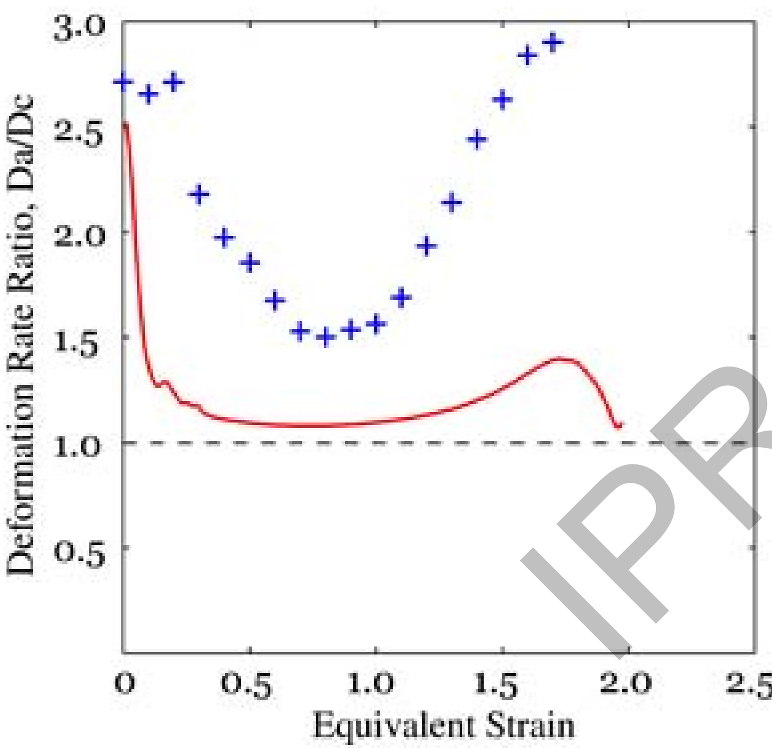
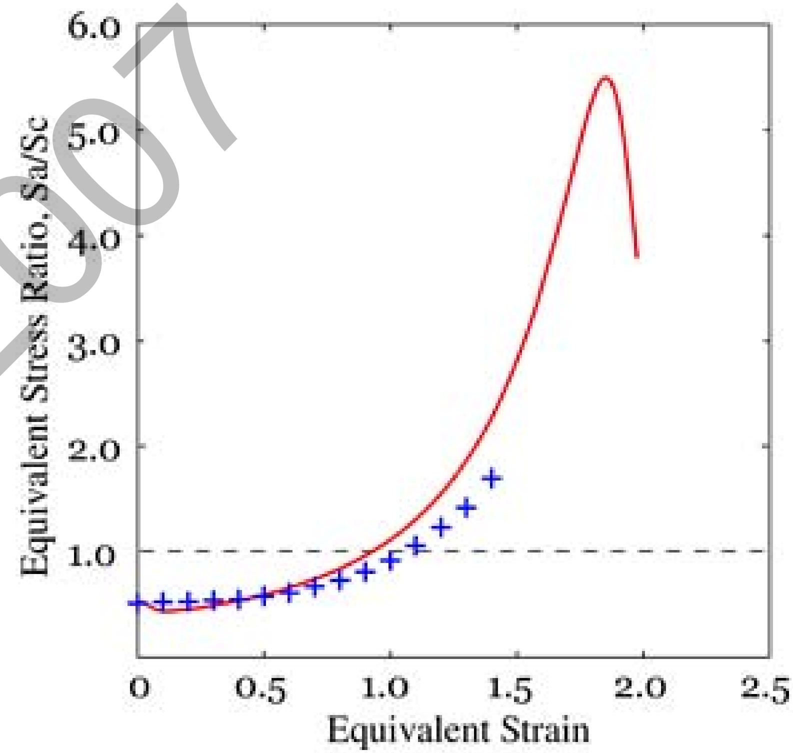


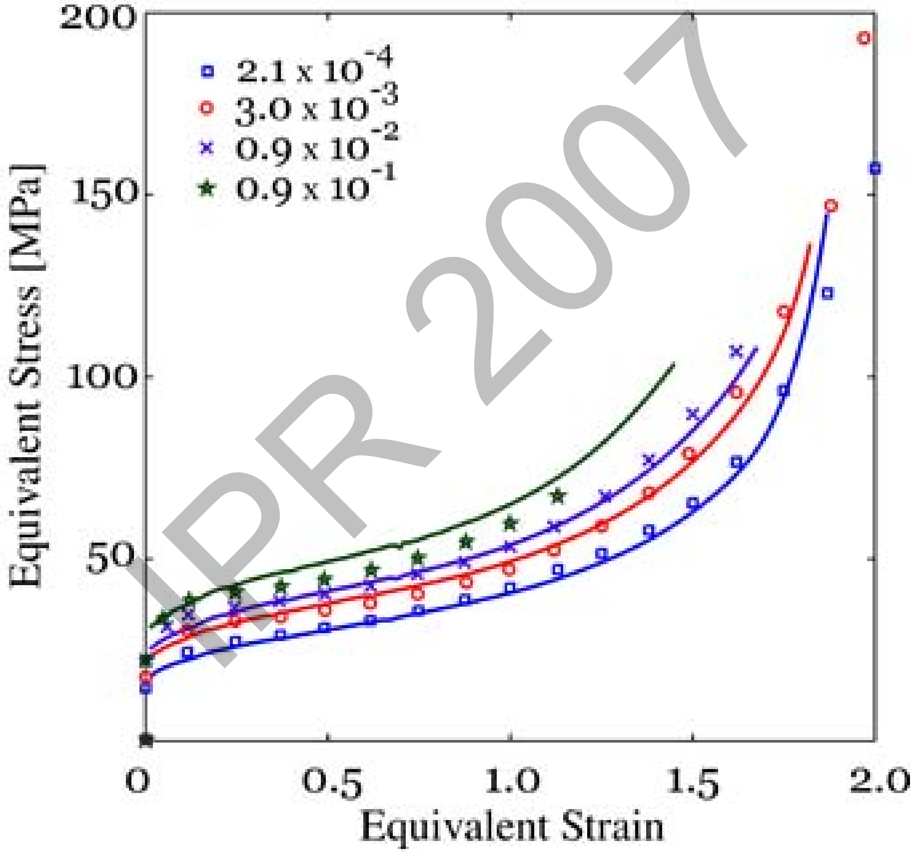
Deformation rate behaviour



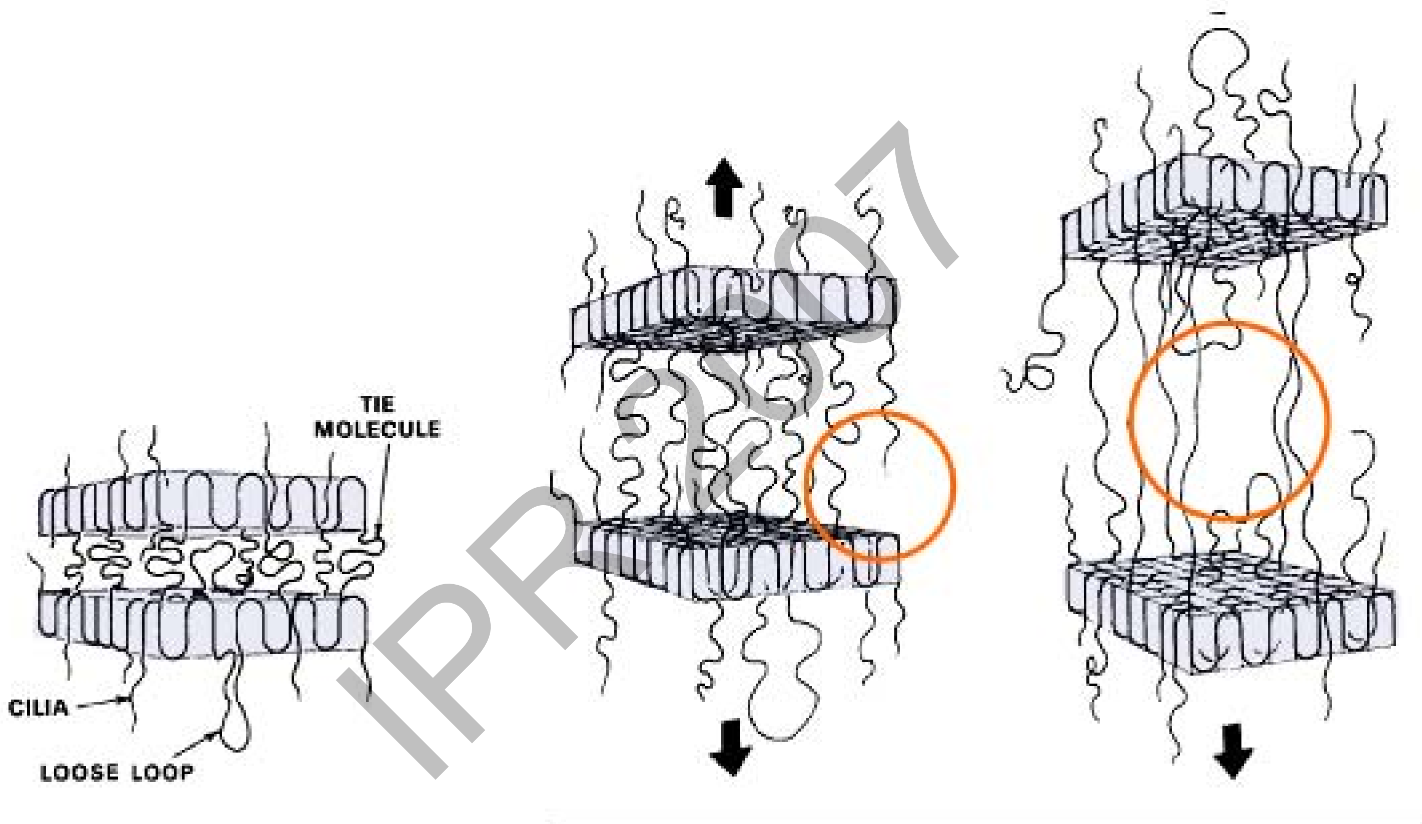
Stress behaviour

UNIAXIAL TENSION

Behaviour at different strain rates



AMORPHOUS POLYETHYLENE



Unstrained state

Strained state

AMORPHOUS POLYETHYLENE

Damage-coupled model

Deviatoric Cauchy stress

$$S = \boldsymbol{\sigma} - tr(\boldsymbol{\sigma}) I$$

Deviatoric back-stress

$$H' = \frac{nkT}{3}\sqrt{\frac{3N}{I_1}}\mathcal{L}^{-1}\left(\sqrt{\frac{I_1}{3N}}\right)\left(B - \tfrac{1}{3}I\right)$$

Equivalent stress

$$\bar{\sigma} = \left[\frac{3}{2}\left(\frac{S}{(1-\Omega^a)} - H'\right) : \left(\frac{S}{(1-\Omega^a)} - H'\right)\right]^{1/2}$$

Deformation rate

$$D^p = \dot{\gamma}\left(\frac{\sigma}{\sigma_0}\right)^{m-1}\left(\frac{\frac{S}{(1-\Omega^a)} - H'}{\sigma_0}\right)$$

Damage evolution law

$$\Omega = \Omega_{cr}\frac{W - W_0}{W} = \Omega_{cr}[1 - \exp(\Delta s/k)]$$

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CONCLUSIONS

- **Two micromechanically based composite models to study plastic deformation and texture evolution in initially isotropic polyethylene have been proposed.**
- The models have been tested in uniaxial tension and simple shear.
- The predicted results agree with the experimental observations of macroscopic stress-strain behaviour and texture evolution in nearly all aspects.
- The models can also be applied to study plastic deformation and texture evolution in other semicrystalline polymers.

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