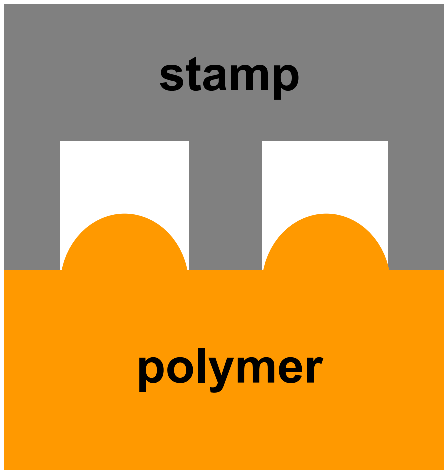
Computationally efficient modelling of pattern dependencies in the micro-embossing of thermoplastic polymers

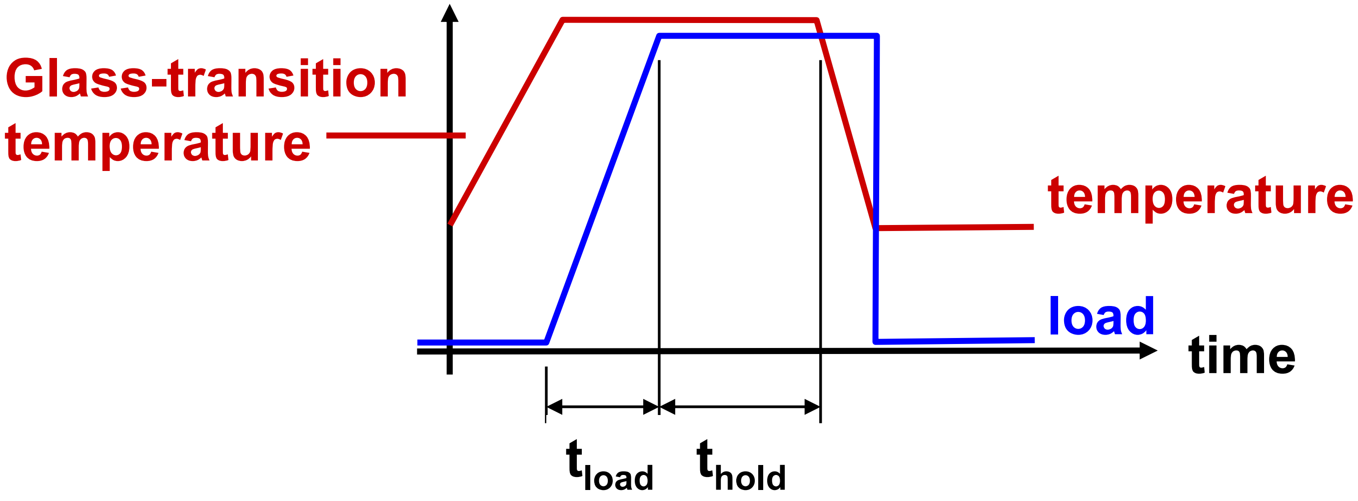
Hayden Taylor and Duane Boning
Microsystems Technology Laboratories
Massachusetts Institute of Technology

Ciprian Iliescu and Bangtao Chen
Institute of Bioengineering and Nanotechnology, Singapore

24 September 2007

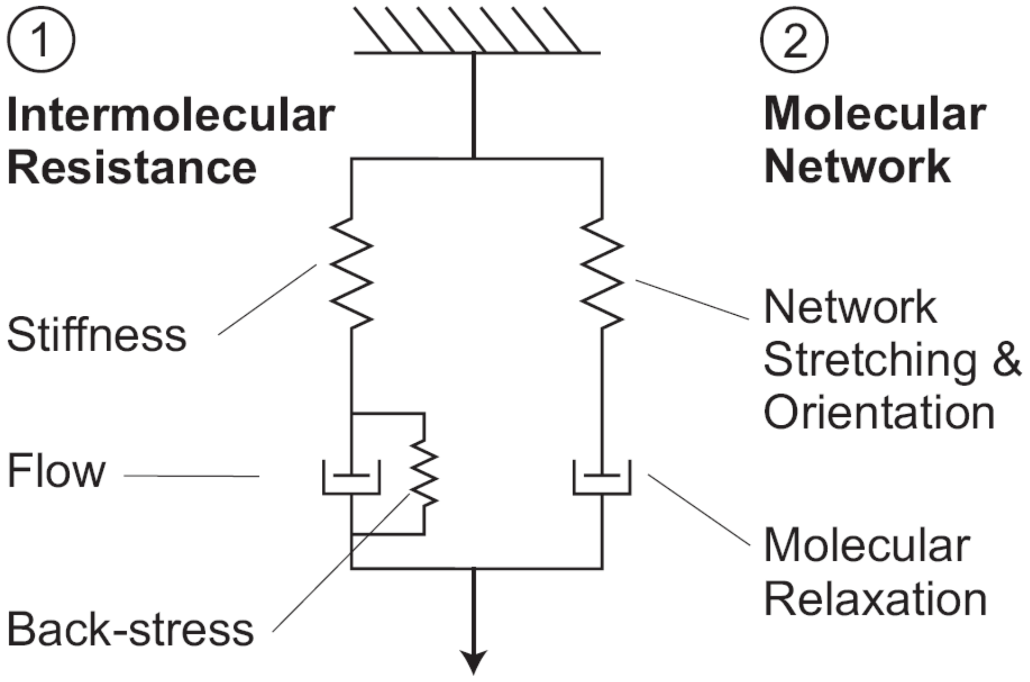
Hot micro- and nano-embossing





- **To choose an optimal process, we need to assign values to**
  - Heat
  - Time
- **Our load and temperature are constrained by**
  - Equipment
  - Stamp and substrate properties

PMMA in compression



① **Intermolecular Resistance**

Stiffness

Flow

Back-stress

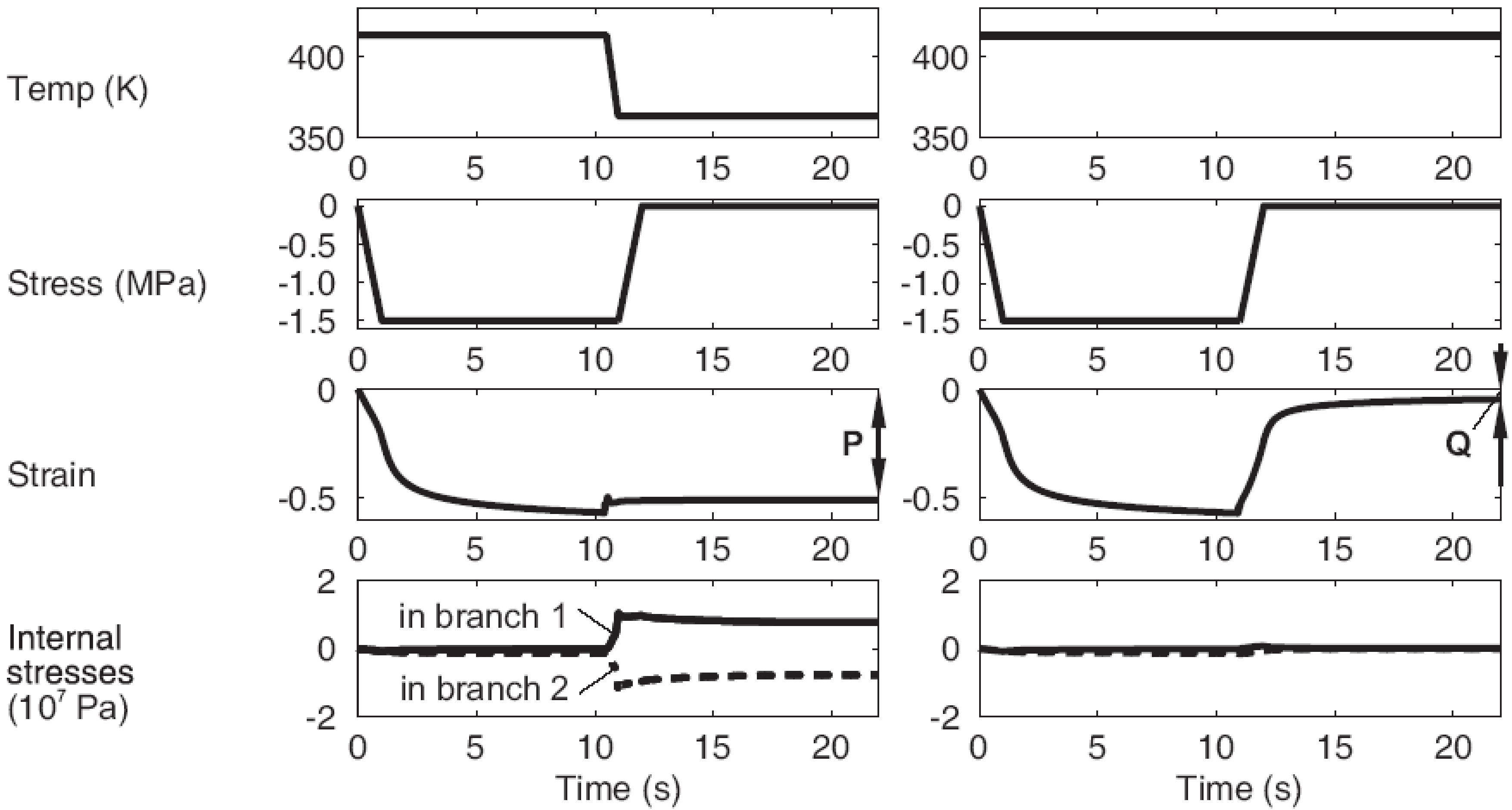
② **Molecular Network**

Network Stretching & Orientation

Molecular Relaxation

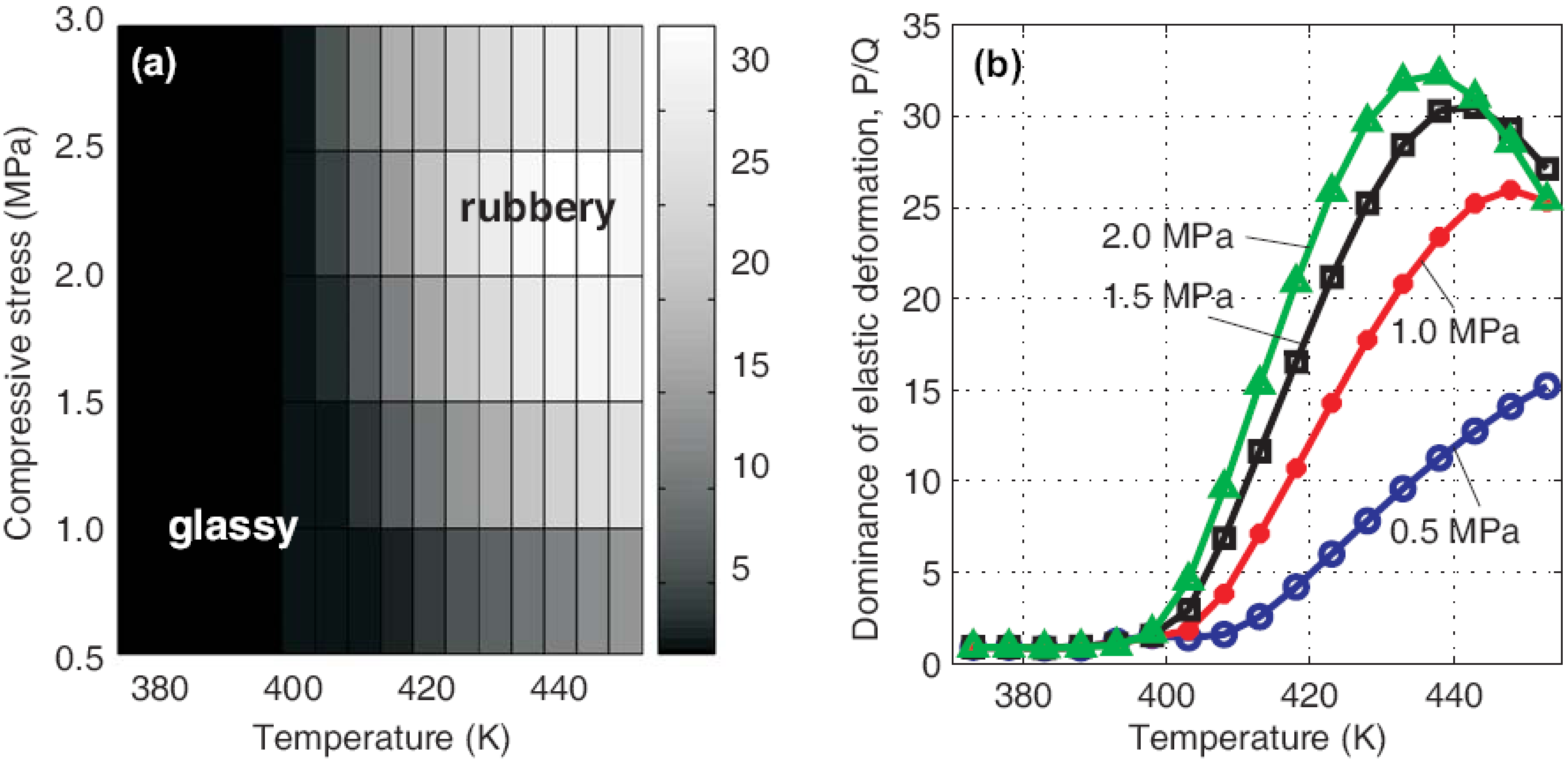
N.M. Ames, Ph.D. thesis, MIT, 2007

PMMA in compression, 140 °C



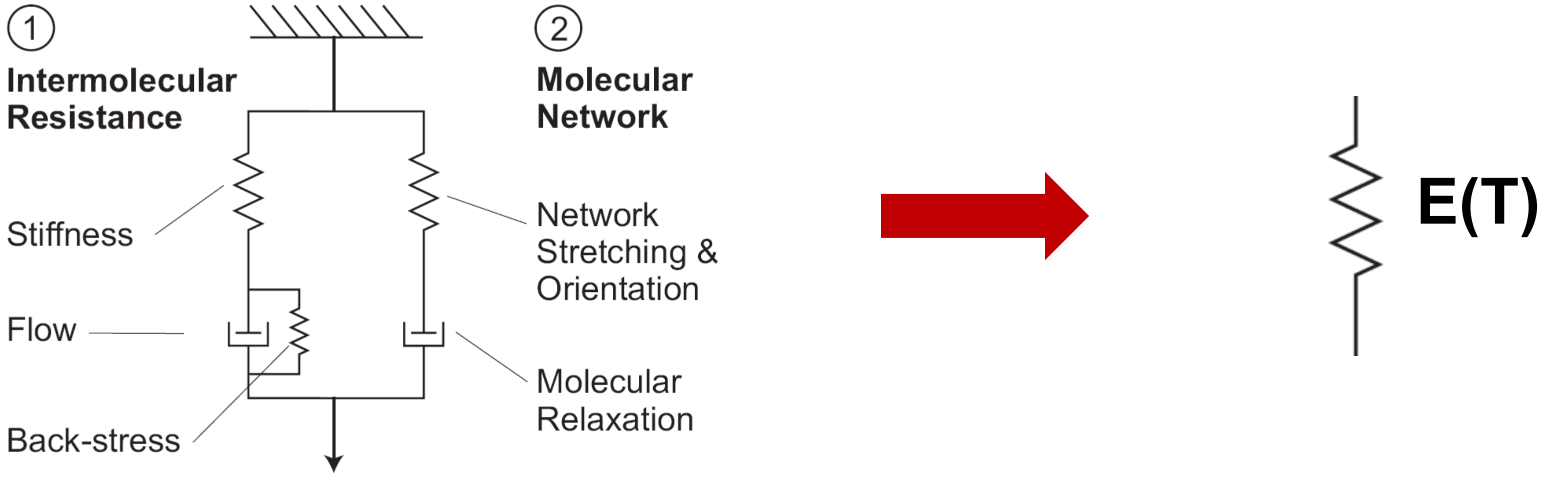
using model of N.M. Ames, Ph.D. thesis, MIT, 2007

PMMA in compression (T_g = 105 °C)



using model of N.M. Ames, Ph.D. thesis, MIT, 2007

Starting point: linear elastic material model

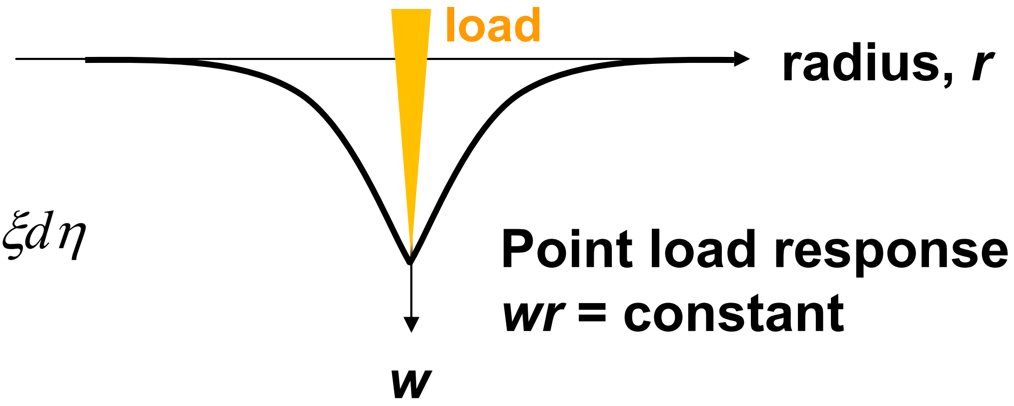


- **Embossing done at high temperature, with low elastic modulus**
- **Deformation ‘frozen’ in place by cooling before unloading**
- **Wish to compute deformation of a layer when embossed with an arbitrarily patterned stamp**
- **Take discretized representations of stamp and substrate**

Response of material to unit pressure at one location

General load response:

$$w(x,y)=\frac{1-\nu^2}{\pi E}\iint\frac{p(\xi,\eta)}{\sqrt{(x-\xi)^2+(y-\eta)^2}}\,d\xi\, d\eta$$



load

radius, *r*

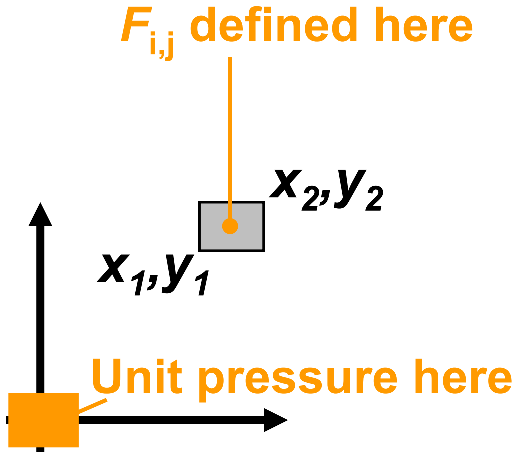
Point load response
***wr* = constant**

w

Response to unit pressure in a single element of the mesh:

$$F_{i,j}=\frac{1-\nu^2}{\pi E}\left[f(x_2,y_2)-f(x_1,y_2)-f(x_2,y_1)+f(x_1,y_1)\right]$$

$$f(x,y)=y\ln\left(x+\sqrt{x^2+y^2}\right)+x\ln\left(y+\sqrt{x^2+y^2}\right)$$



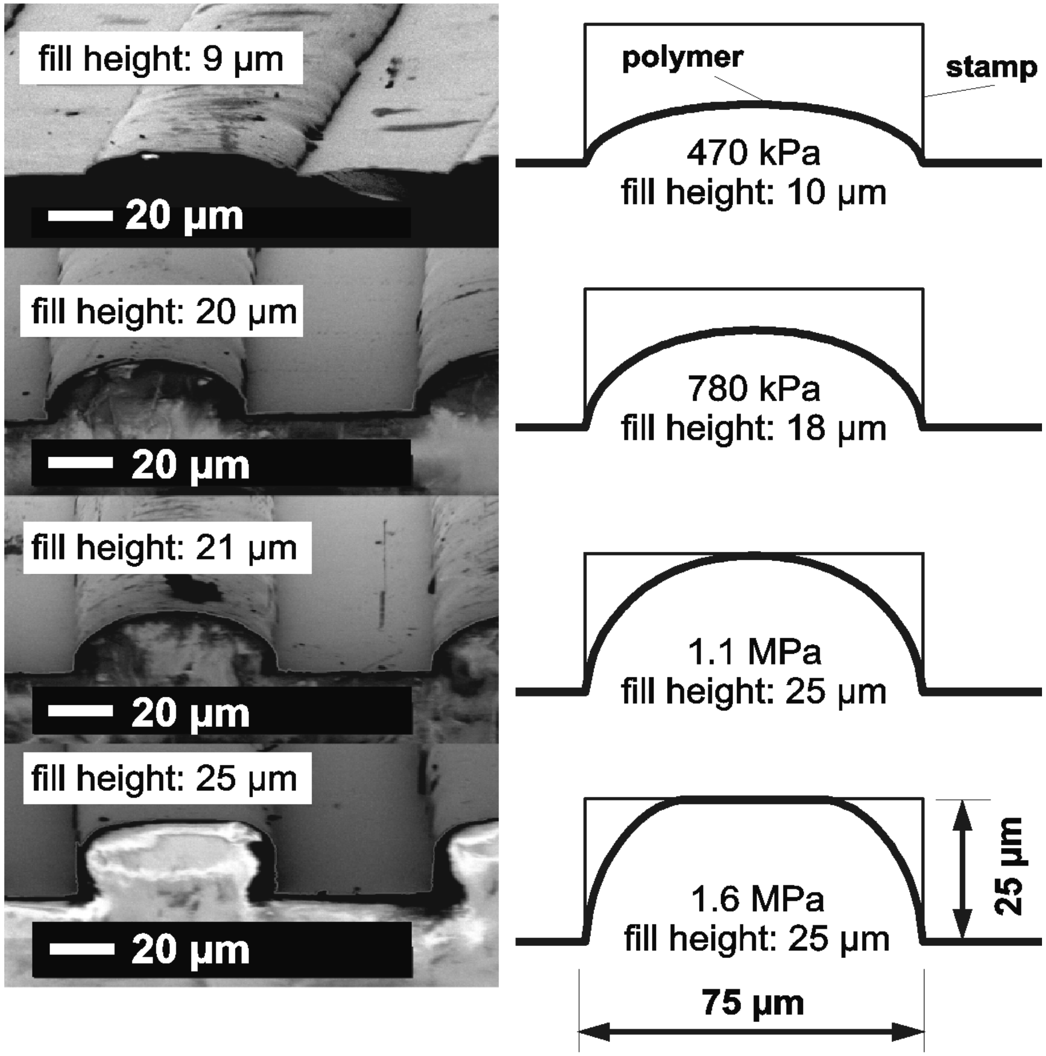
$F_{i,j}$ defined here

x_2,y_2

x_1,y_1

Unit pressure here

1-D verification of approach for PMMA at 130 °C

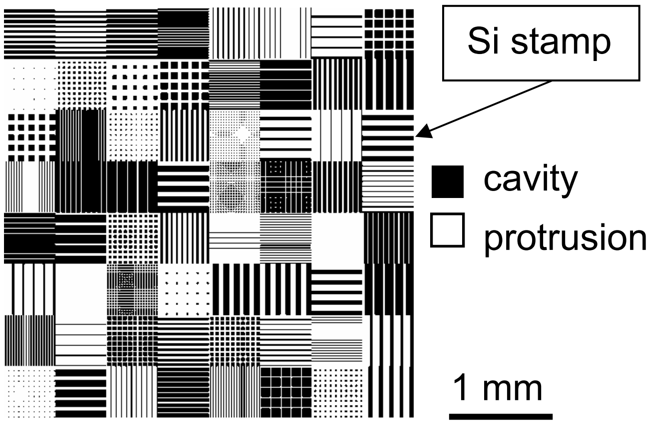


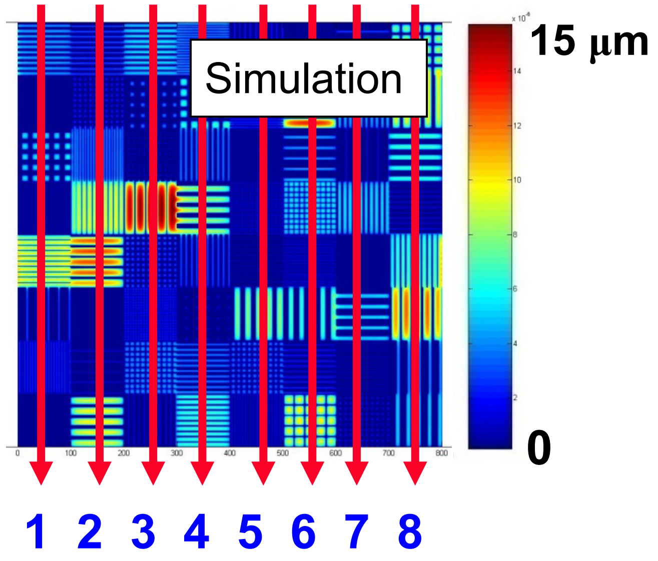
(a) experimental **(b) rubbery model**

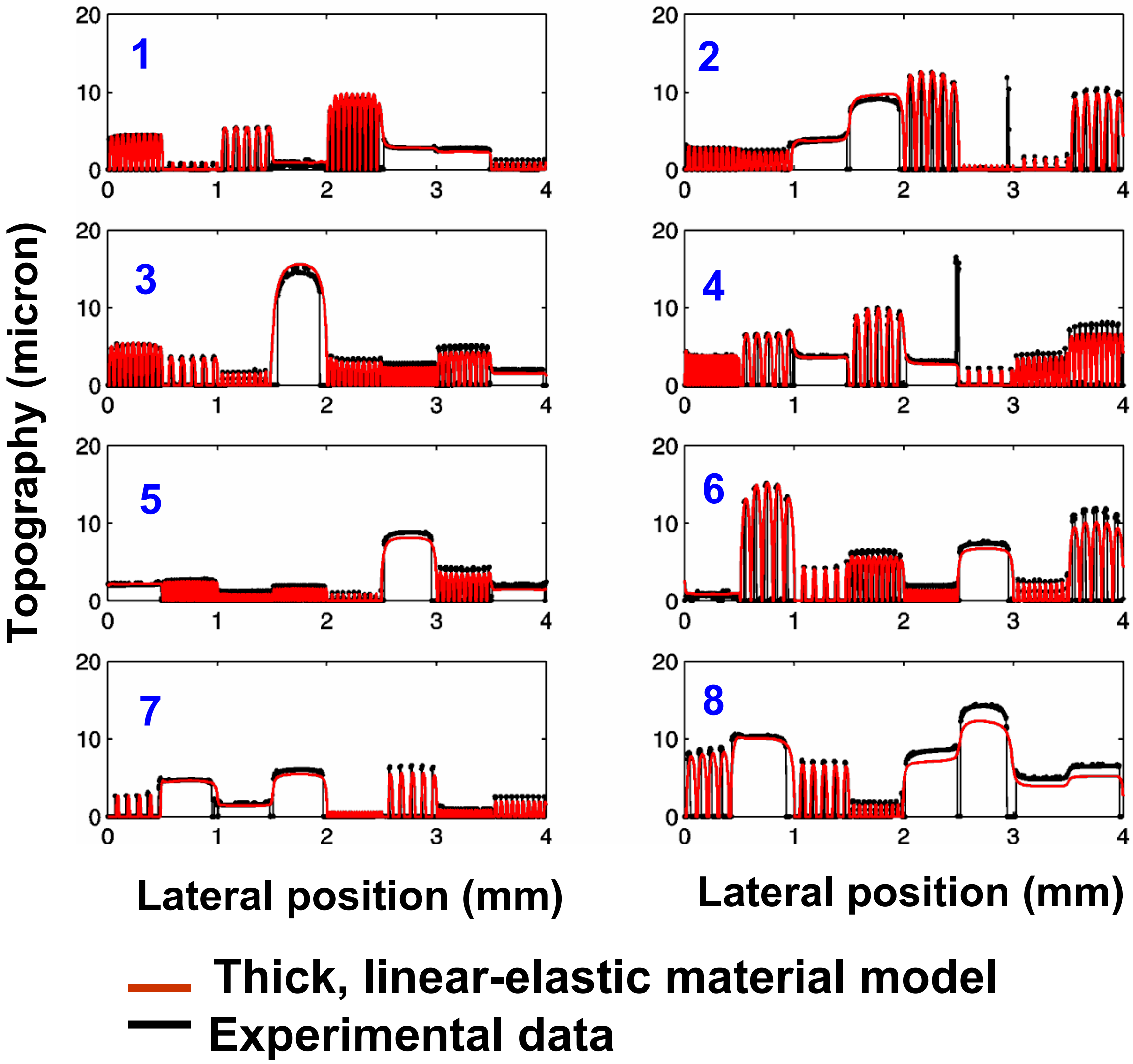
- Iteratively find distribution of pressure consistent with stamp remaining rigid while polymer deforms
- Fit elastic modulus that is consistent with observed deformations

Extracted Young's modulus ~ 5 MPa at 130 °C

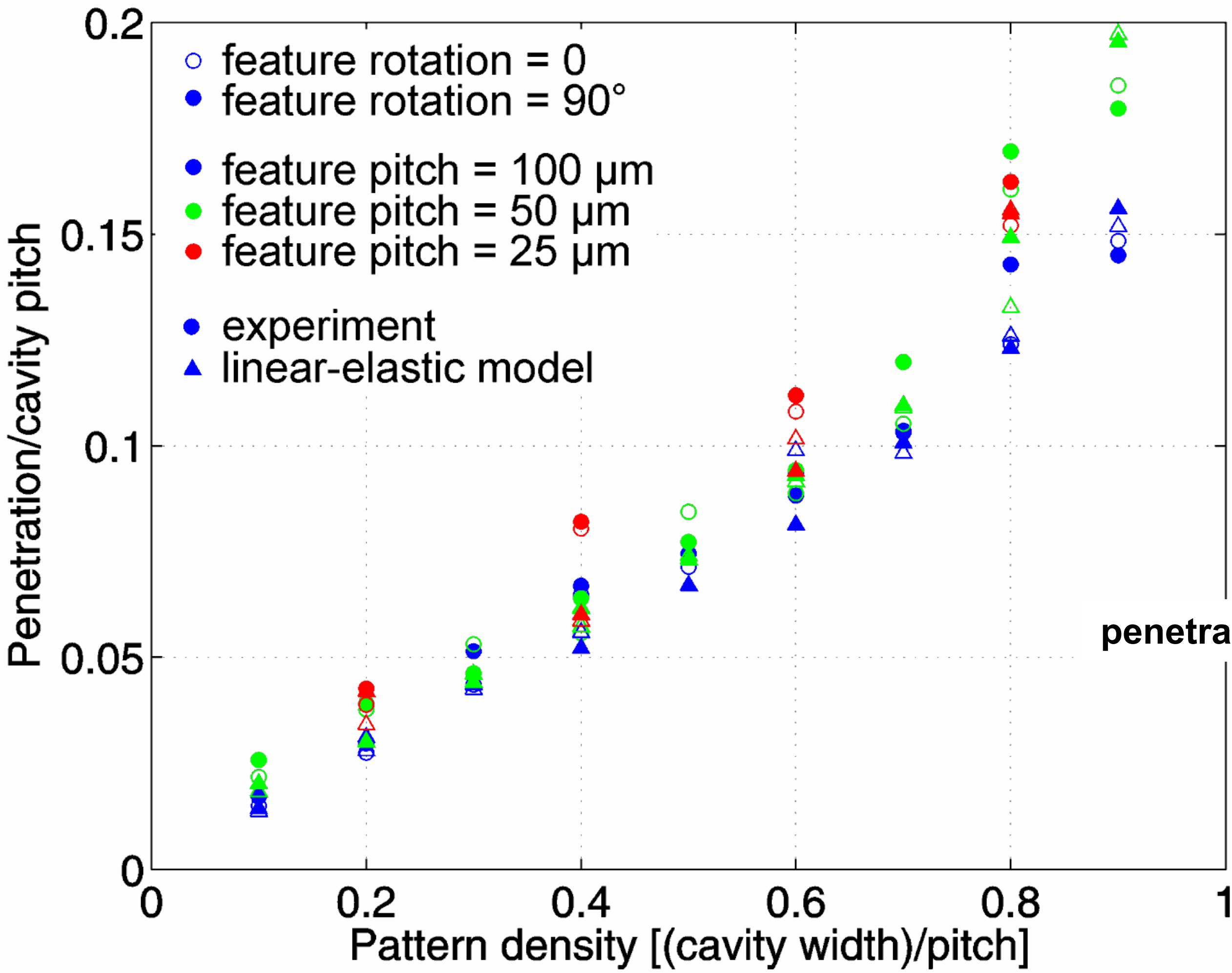
2-D linear elastic model succeeds with PMMA at 125 °C

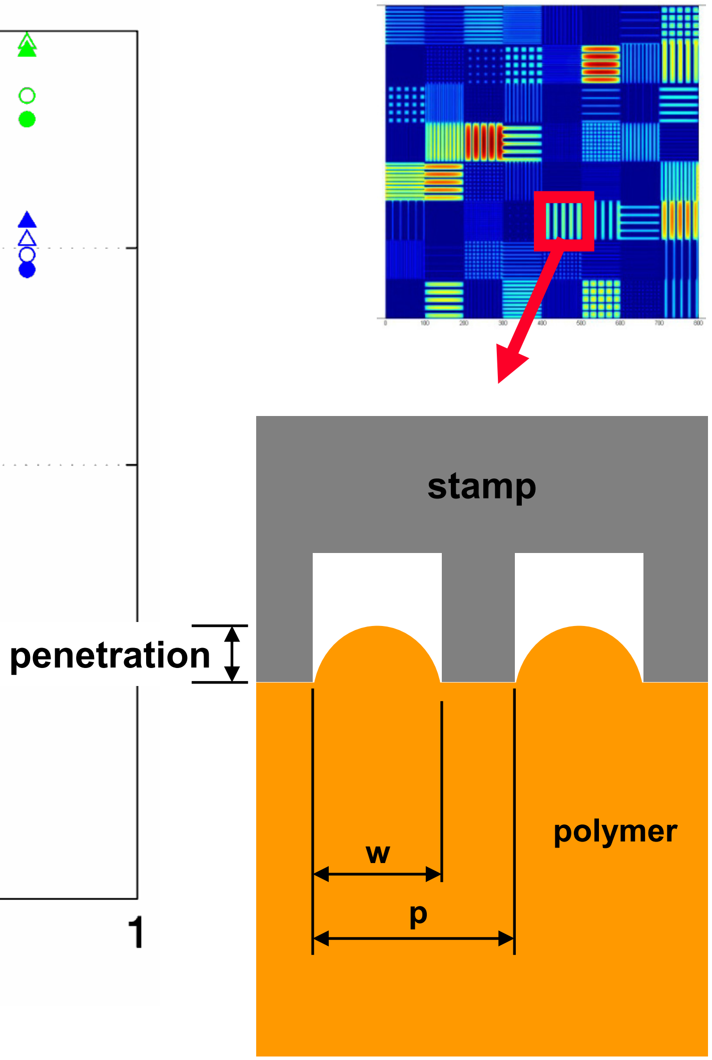




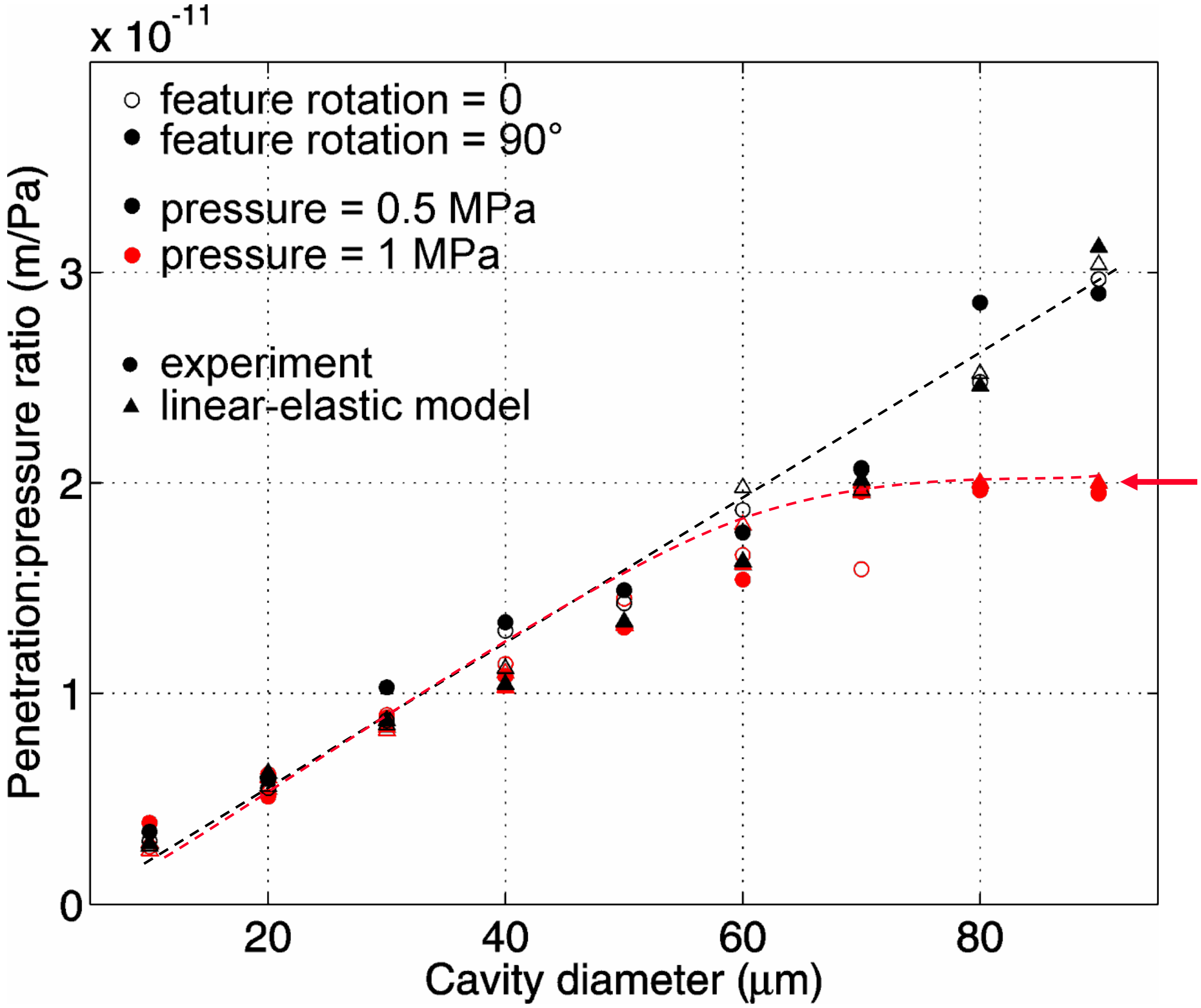


Linear-elastic model succeeds at 125 °C, p_{ave} = 0.5 MPa



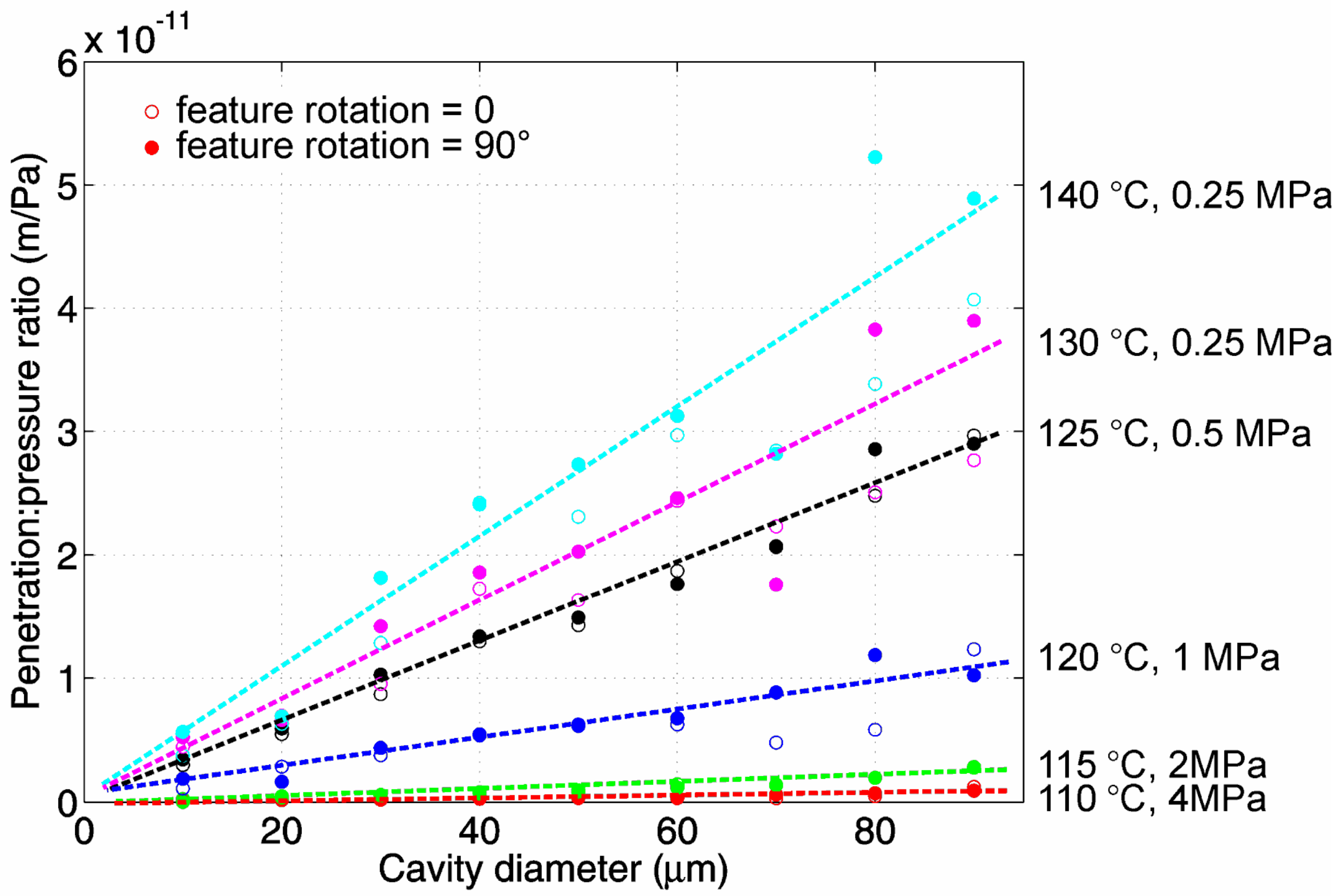


Linear-elastic model succeeds at 125 °C, p_{ave} = 1 MPa

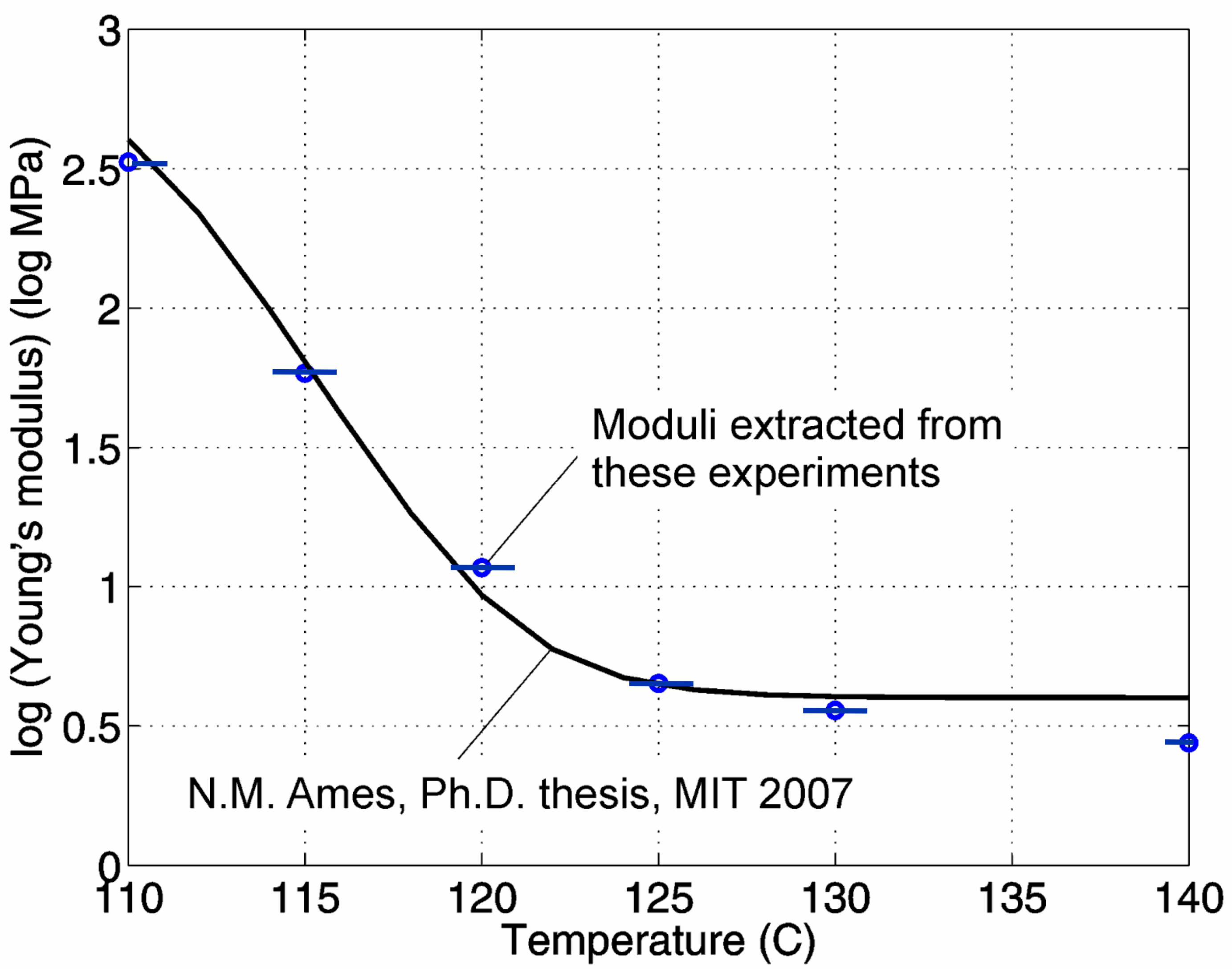


Features filled, 1MPa

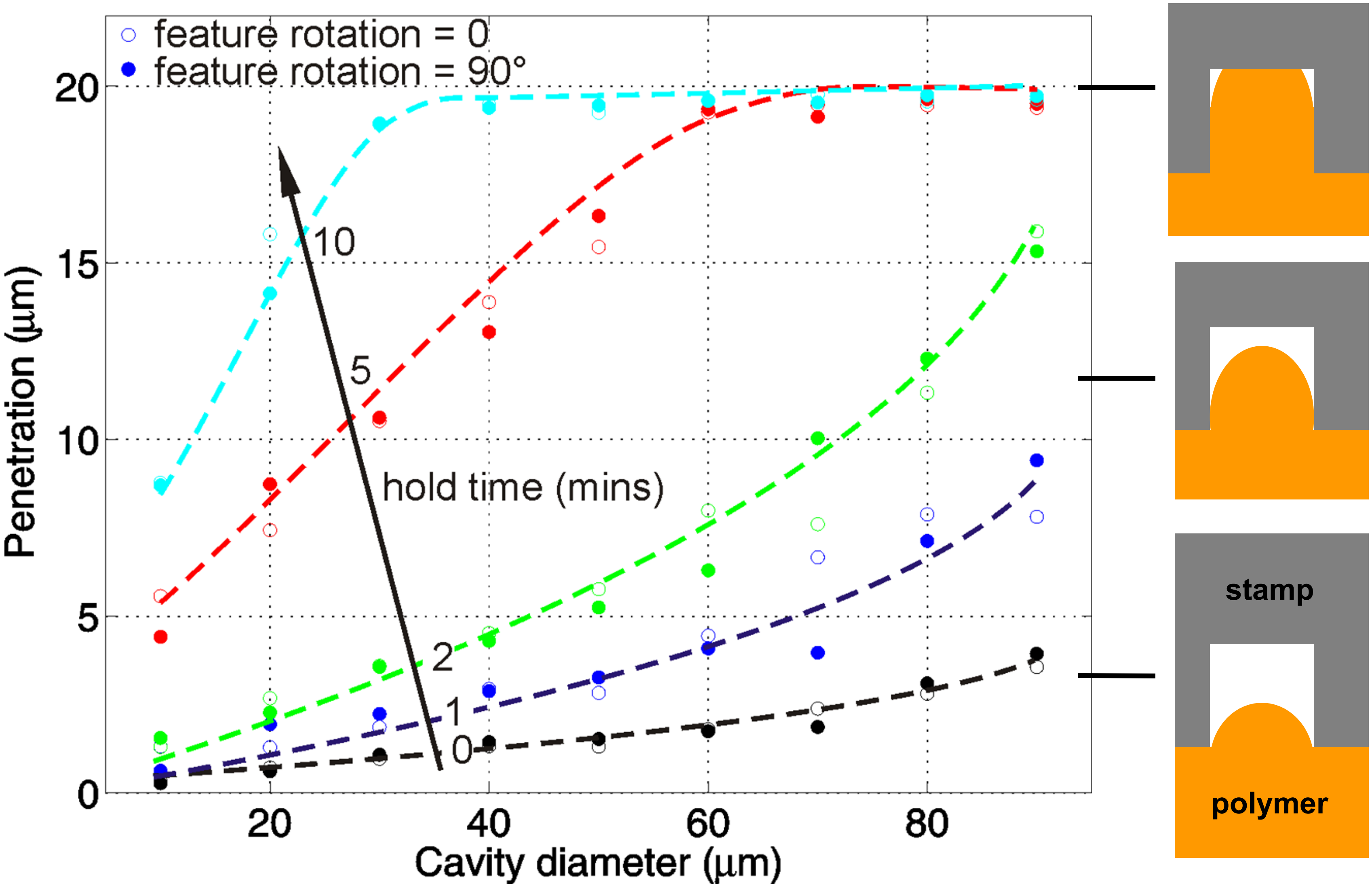
Linear elastic model succeeds below yielding at other temperatures



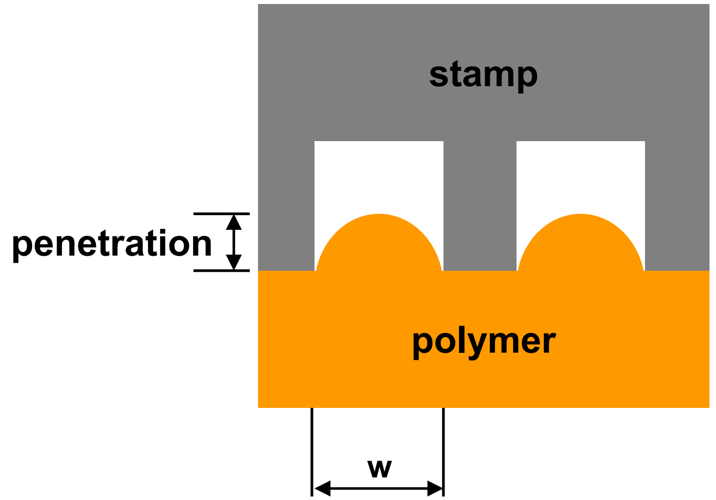
Extracted PMMA Young’s moduli from 110 to 140 °C



Material flows under an average pressure of 8 MPa at 110 °C



Yielding at 110 °C

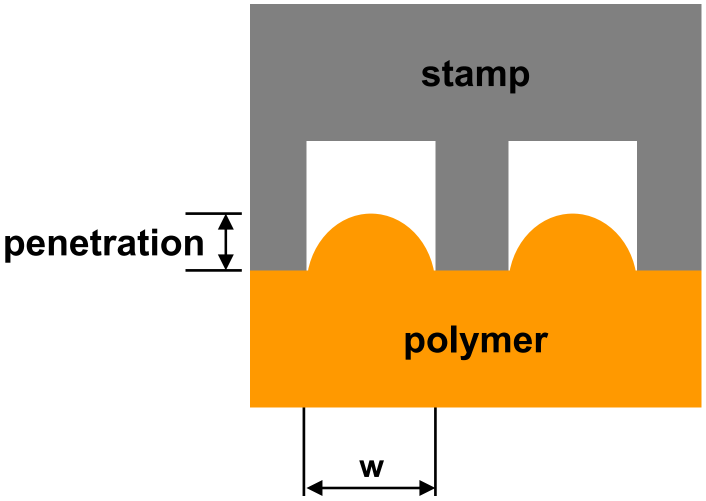


Simple estimates of strain rate:

$$\frac{\text{penetration}}{\frac{w}{2}\, t_{\text{hold}}} \left\{ \begin{array}{l} 10^{-3} \text{ to } 10^{-1} \text{ during loading} \\ \\ 10^{-4} \text{ to } 10^{-3} \text{ during hold} \end{array} \right.$$

Local contact pressure at feature corners > 8 MPa

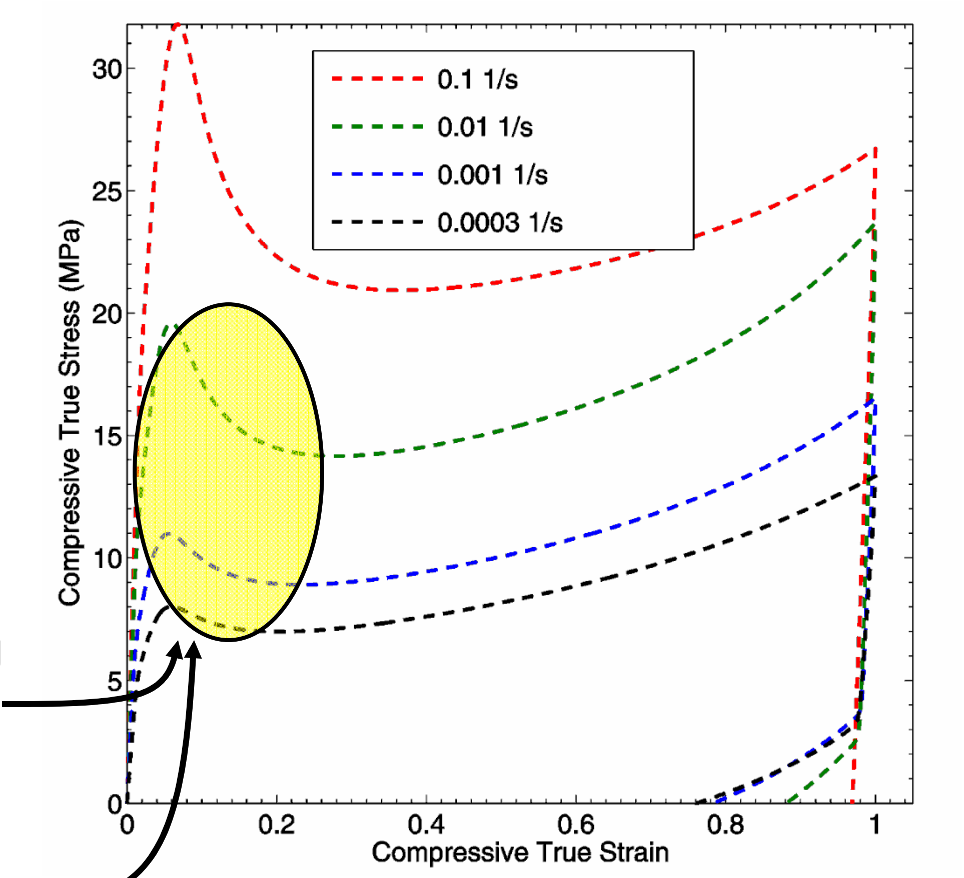
Yielding at 110 °C



Simple estimates of strain rate:

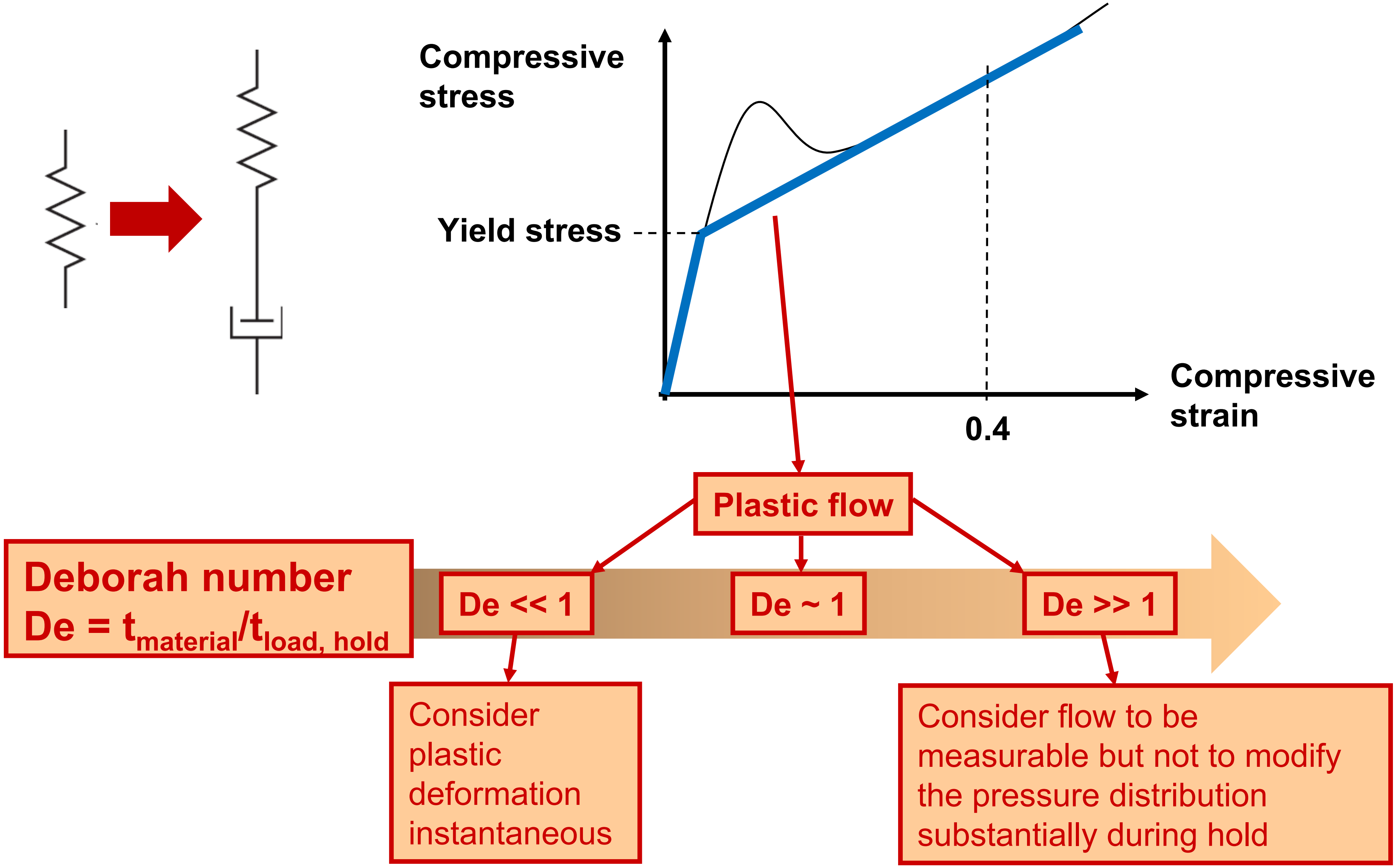
$$\frac{\text{penetration}}{\frac{w}{2}\,t_{\text{hold}}}\;\begin{cases}10^{-3}\text{ to }10^{-1}\text{ during loading}\\ 10^{-4}\text{ to }10^{-3}\text{ during hold}\end{cases}$$

Local contact pressure at feature corners > 8 MPa



N.M. Ames, Ph.D. Thesis, MIT, 2007

Modelling combined elastic/plastic behavior



Plastic flow

Deborah number
De = $t_{material}/t_{load,\ hold}$

De << 1

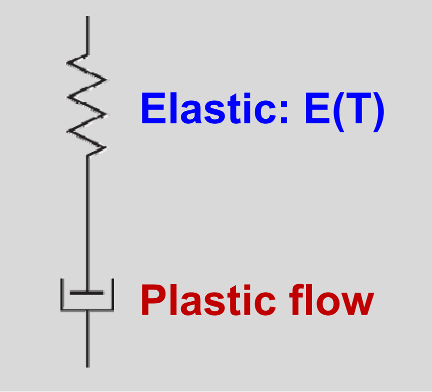
De ~ 1

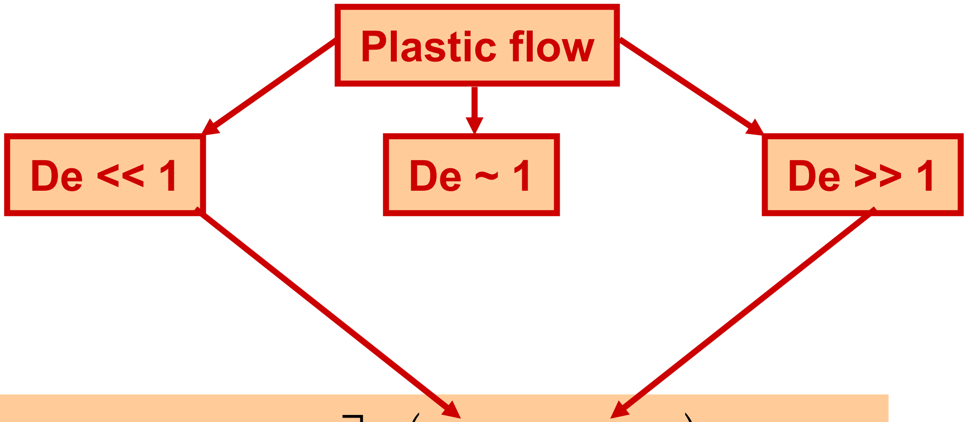
De >> 1

Consider plastic deformation instantaneous

Consider flow to be measurable but not to modify the pressure distribution substantially during hold

Modelling combined elastic/plastic behavior





Plastic flow

De << 1

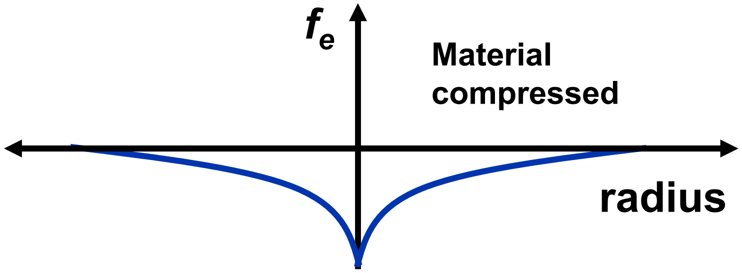
De ~ 1

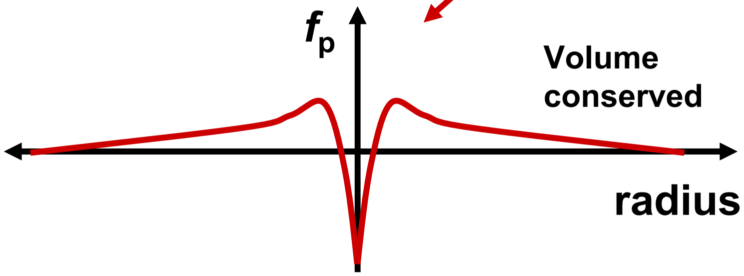
De >> 1

$$w(x,y) = p(x,y) * f_e(x,y) + \left[p(x,y) - p_{yield} \right] * \left(A + Bt_{hold} \right) f_p(x,y)$$

Existing linear-elastic component

Tuned to represent cases from capillary filling to non-slip Poiseuille flow





Summary and future directions

- The merits of a linear-elastic embossing polymer model have been probed
- This simulation approach completes an 800x800-element simulation in:
  - ~ 45 s (without filling)
  - ~ 4 min (with some filling)
- Our computational approach can be extended to capture yielding and plastic flow
- Is a single pressure distribution solution sufficient to model visco-elasto-plastic behaviour?
- Abstract further: mesh elements containing many features

Acknowledgements

**Nici Ames, Matthew Dirckx, David Hardt,
Yee Cheong Lam and Lallit Anand**

The Singapore-MIT Alliance