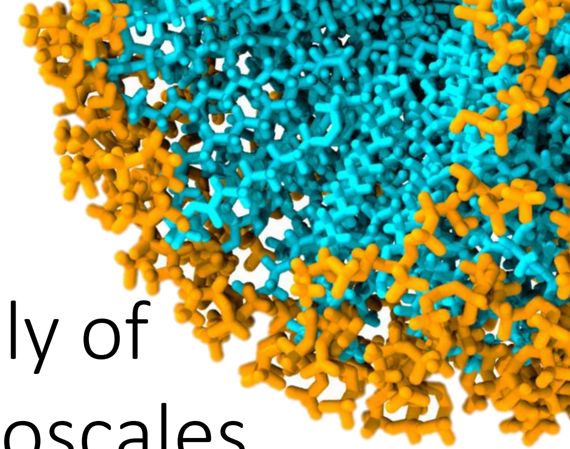
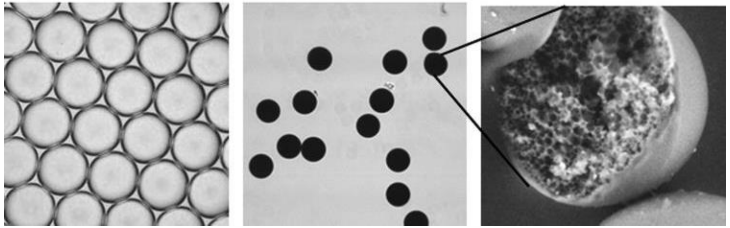
Imperial College London



Spontaneous and directed-assembly of polymers from the molecular to macroscales



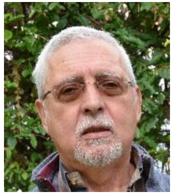
João T. Cabral
Department of Chemical Engineering, Imperial College London
j.cabral@ic.ac.uk

Colóquio de Física, IST 28 April 2021

a personal introduction…

TÉCNICO LISBOA

Dep Fisica
1992-1997


KTH VETENSKAP OCH KONST

Department of
Physics 1996

Orphée
Laboratoire Léon Brillouin

1997



SCIENTIA

Imperial College of Science
Technology & Medicine
PhD 1998-2002

NIST
National Institute of
Standards and Technology
U.S. Department of Commerce

Postdoc
2002-2005


Imperial College
London

2005-

MACROMOLECULAR SCIENCE 1958

復旦大學高分子科学系
DEPARTMENT OF
MACROMOLECULAR SCIENCE
FUDAN UNIVERSITY

2008

PRITZKER SCHOOL OF
MOLECULAR ENGINEERING
THE UNIVERSITY OF CHICAGO

2014-2015

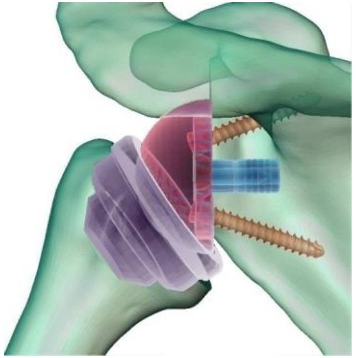
Imperial College London

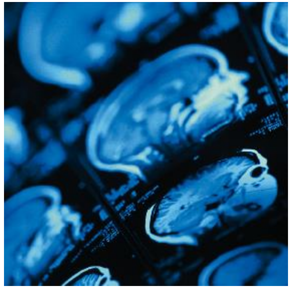
Imperial College London

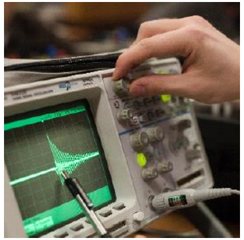
- Imperial is a **research-led** university specialised in:

- Engineering
  10 departments, incl Chemical Engineering
- Natural Sciences
  Physics, Chemistry, Maths, Biosciences
- Medicine
- Business

Humanities programme

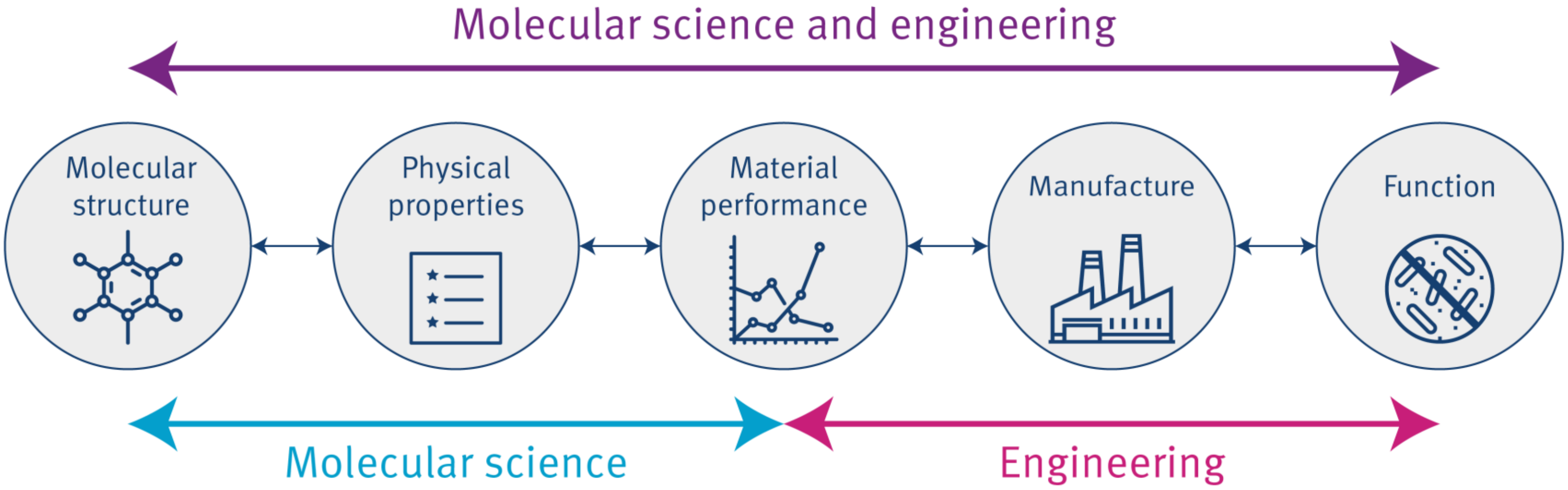






Imperial College London

Institute of Molecular science and engineering



imperial.ac.uk/imse

Outline

1. Polymer thermodynamics & demixing

Cahn-Hilliard theory & spinodal decomposition.

Membranes and photovoltaics

2. Particle and capsule formation

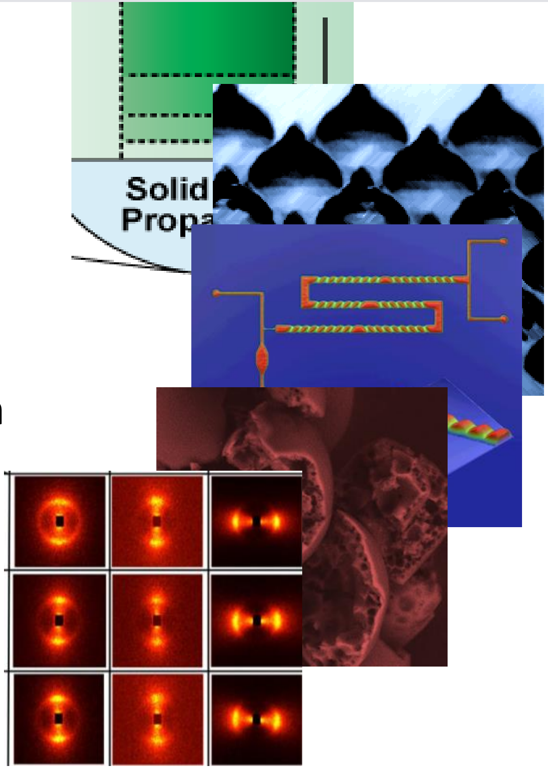
Levitation & microfluidics

Solution thermodynamics, phase inversion and solidification

Functional capsules with tunable, triggered release.

3. Waves of network formation

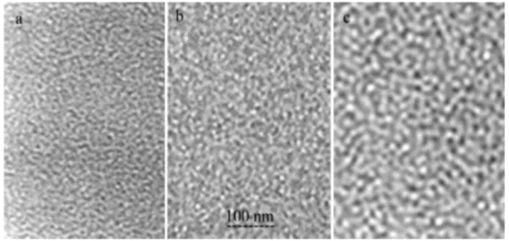
3D printing with light



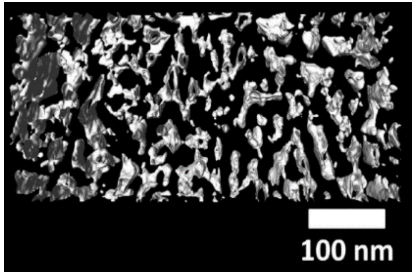
Functional polymeric spinodal nanostructures

(bicontinuous interpenetrating)

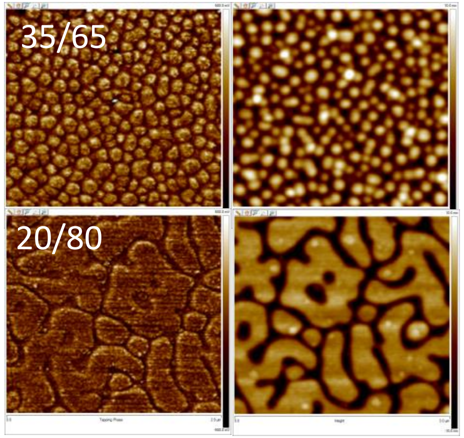
Organic photovoltaics (donor/acceptor)



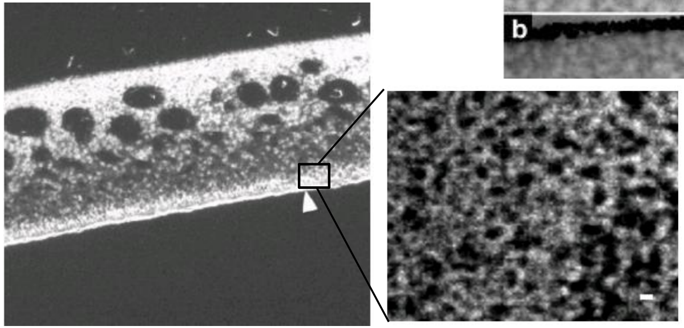
Heeger Adv Func Mater 2005 2012



PS/PCBM (S Pont)



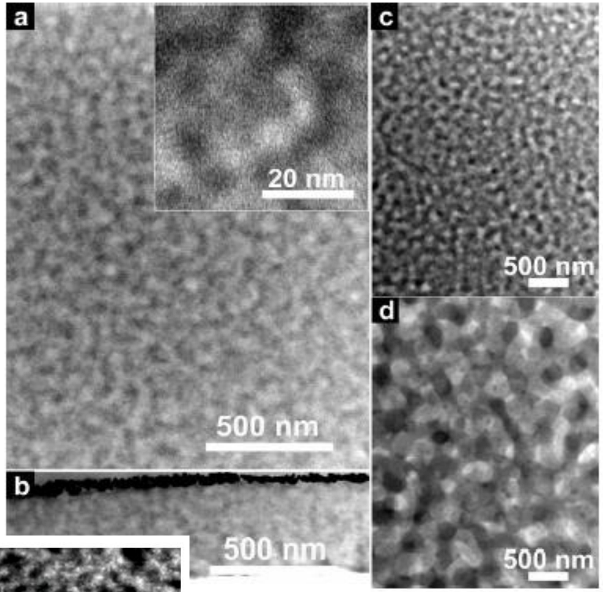
Membranes/separations



PVD, Liu JMS 2011

Phase inversion via ternary polymer/solvent/non-solvent quench

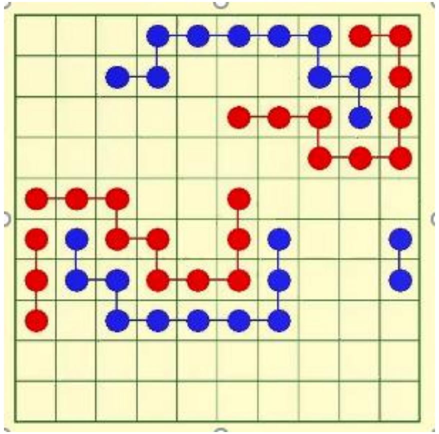
Reactive blending



T Russell 2012

Polymer miscibility & demixing

Flory-Huggins lattice



Binary mixture

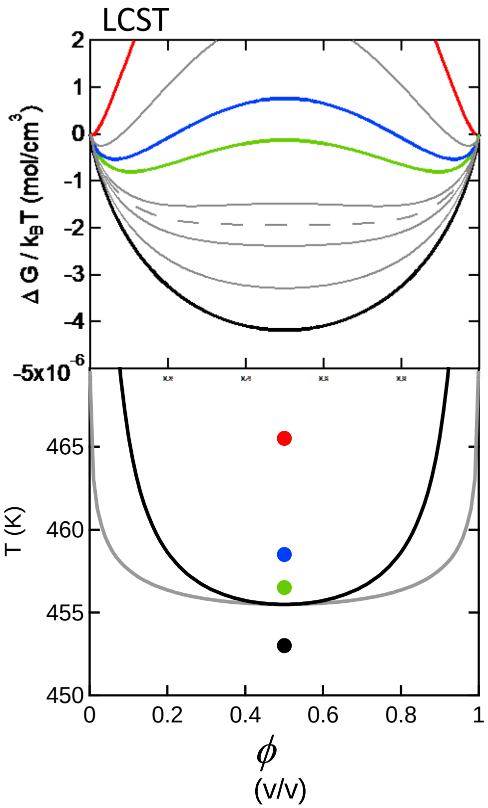
Thermodynamics $\Delta G_m = \Delta H_m - T\Delta S_m$

$$\frac{\Delta G_m}{k_B T} = \frac{\phi}{v_A N_A} \ln \phi + \frac{(1-\phi)}{v_B N_B} \ln(1-\phi) + \frac{\phi(1-\phi)}{v} \chi$$

Combinatorial entropy

Enthalpy

Polymer miscibility & demixing



Thermodynamics $\Delta G_m = \Delta H_m - T\Delta S_m$

$$\frac{\Delta G_m}{k_B T} = \frac{\phi}{v_A N_A}\ln\phi + \frac{(1-\phi)}{v_B N_B}\ln(1-\phi) + \frac{\phi(1-\phi)}{v}\chi$$

Combinatorial entropy

Enthalpy

Phase boundaries?

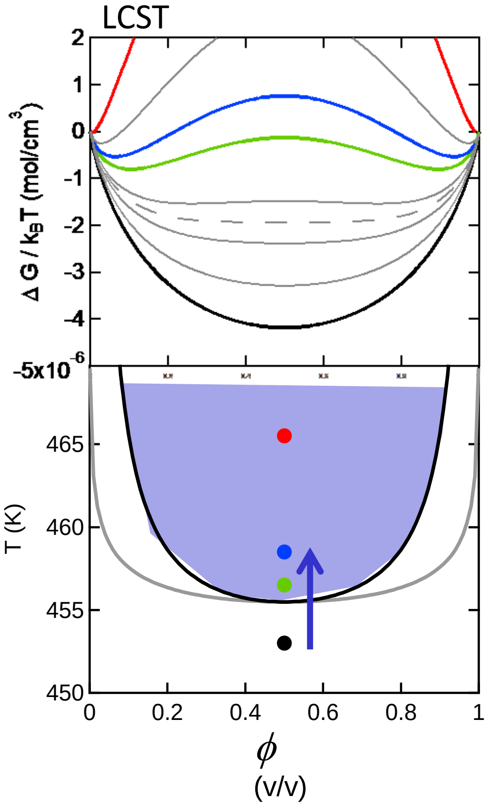
Binodal

$$\begin{cases} \dfrac{\partial \Delta G_m}{\partial \phi_{B1}} = \dfrac{\partial \Delta G_m}{\partial \phi_{B2}} \equiv \mu \\ \Delta G_m(\phi_{B1}) + \Delta G_m(\phi_{B2}) = \min \end{cases}$$

‘minima’

Spinodal $\dfrac{\partial^2 \Delta G_m}{\partial \phi^2} = 0$ inflection points

Polymer miscibility & demixing

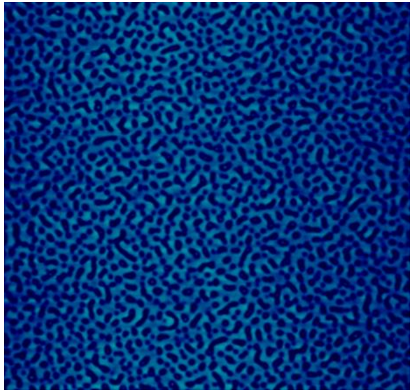


Thermodynamics $\Delta G_m = \Delta H_m - T\Delta S_m$

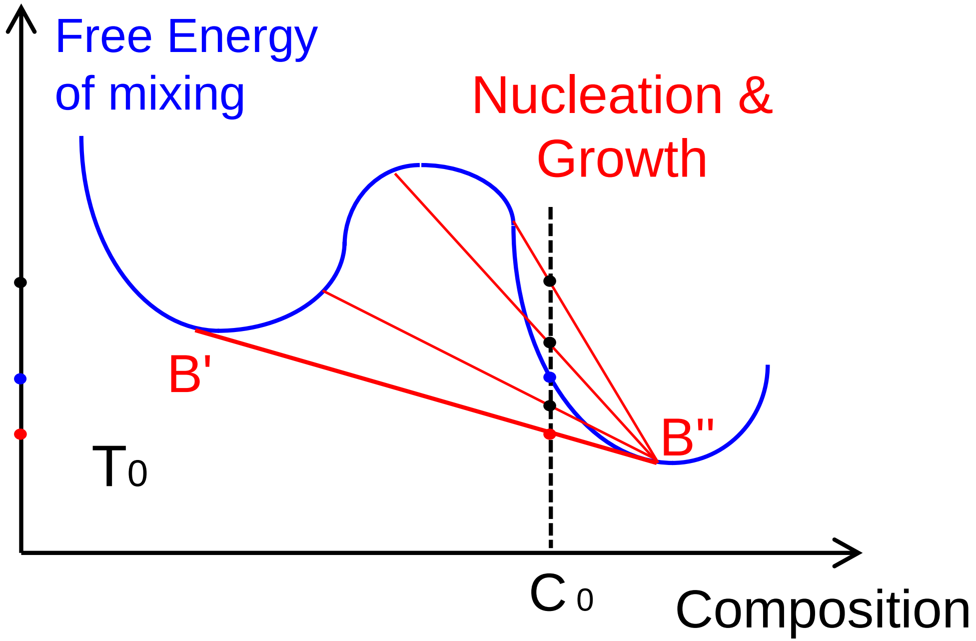
$$\frac{\Delta G_m}{k_B T} = \frac{\phi}{v_A N_A}\ln\phi + \frac{(1-\phi)}{v_B N_B}\ln(1-\phi) + \frac{\phi(1-\phi)}{v}\chi$$

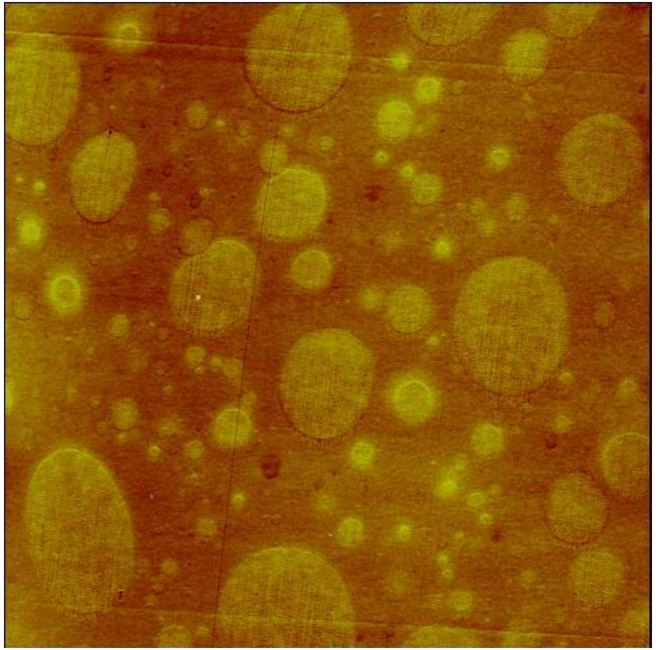
Combinatorial entropy

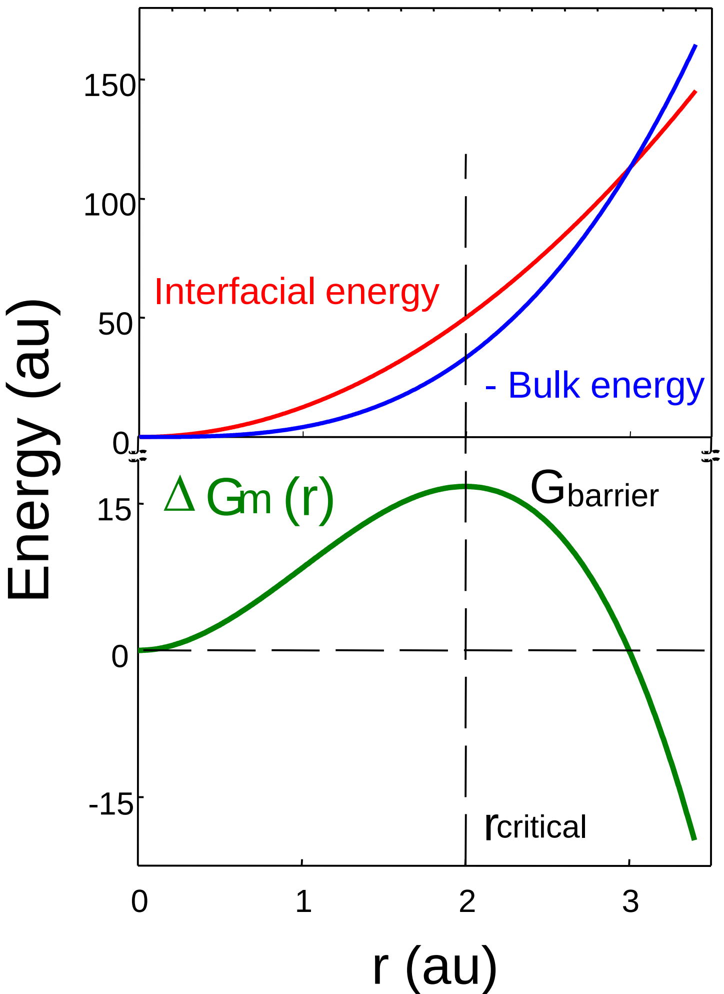
Enthalpy

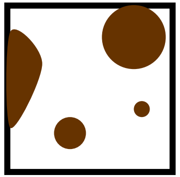


Nucleation and growth









Energy balance

$$\Delta G(r) = -\frac{4\pi}{3} r^3 \Delta g + 4\pi r^2 \sigma$$

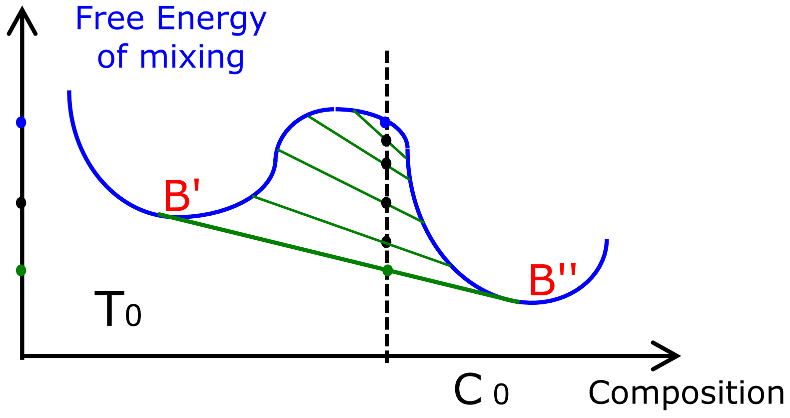
bulk interface

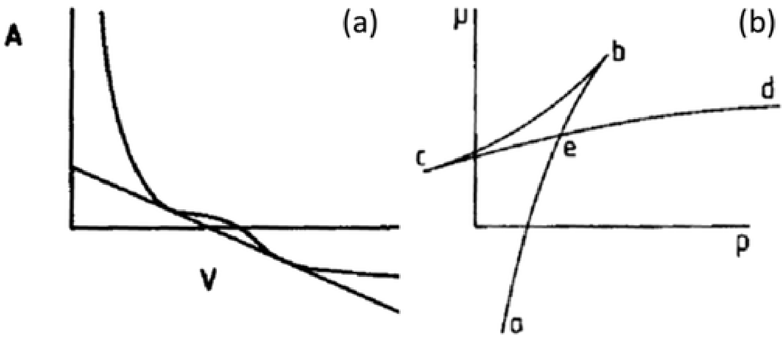
⟶ **Critical droplet**

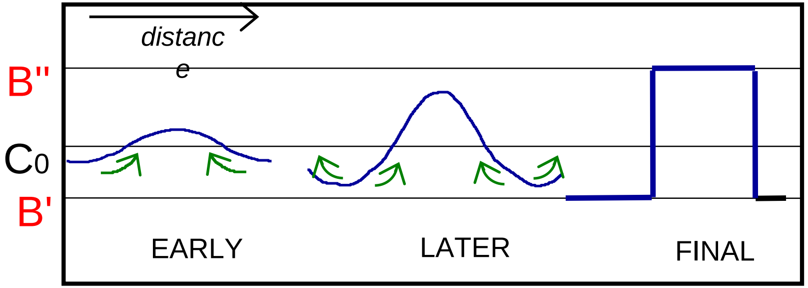
$$\Delta G_{barrier} = \frac{16\pi\sigma^3}{3\Delta g^2}$$

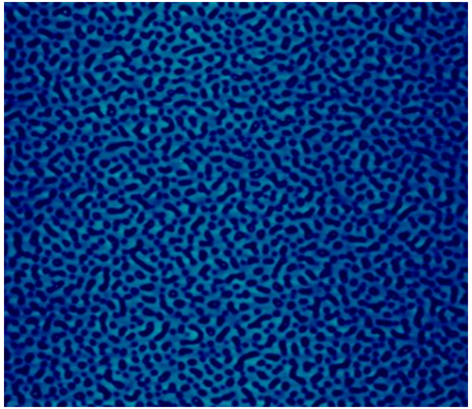
$r_c = 2\sigma/\Delta g$

Spinodal decomposition

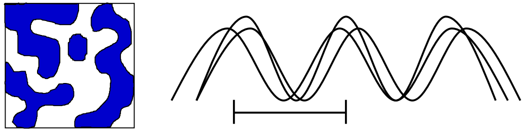








Cahn-Hilliard (Cook) linearised theory



$$d = \frac{2\pi}{q_m}$$

$$\phi = \phi_o + \tilde{\phi}$$

equation of motion
concentration fluctuations

d characteristic length of phase separation

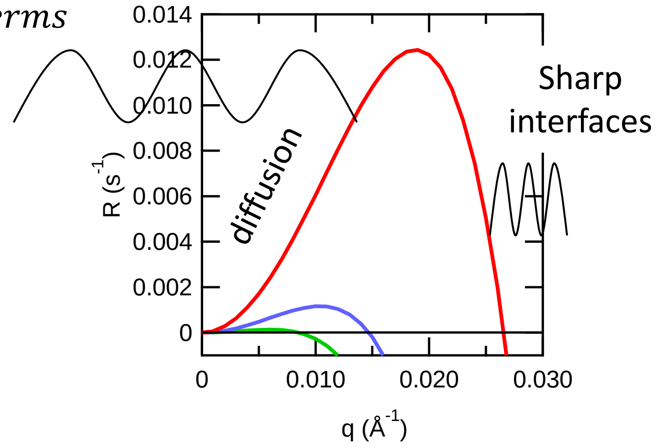
$$-\frac{\partial \phi}{\partial t} = MG''\nabla^2\phi - 2Mk\nabla^4\phi + non\ linear\ terms$$

$-D_{app}$

Growth rate of Fourier components

$$R(q) = -MG''q^2 - 2Mkq^4$$

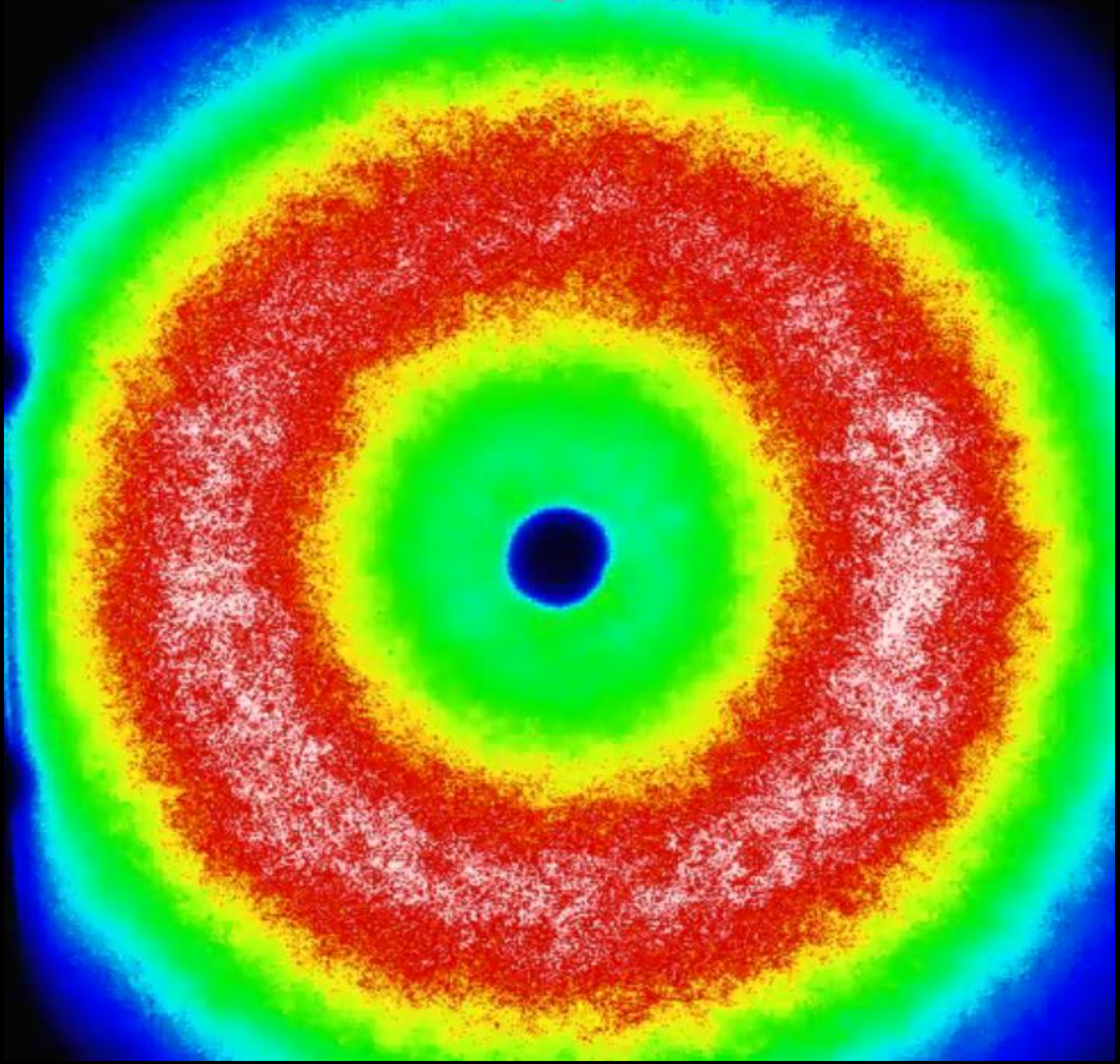
diffusion *sharp interfaces*



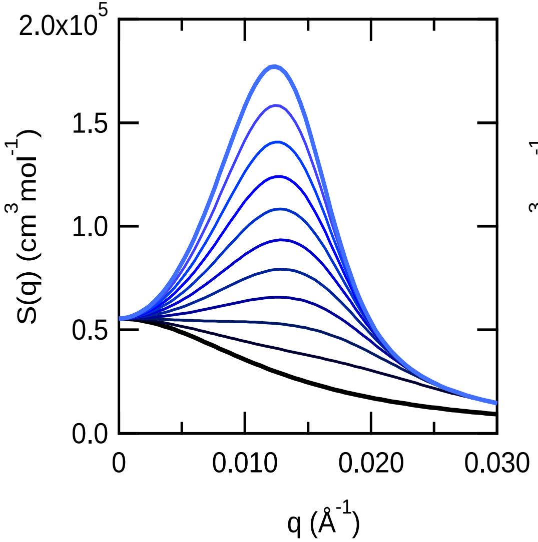
$$q_m = \sqrt{-\frac{G''}{4k}}$$ *dominant wavelength*

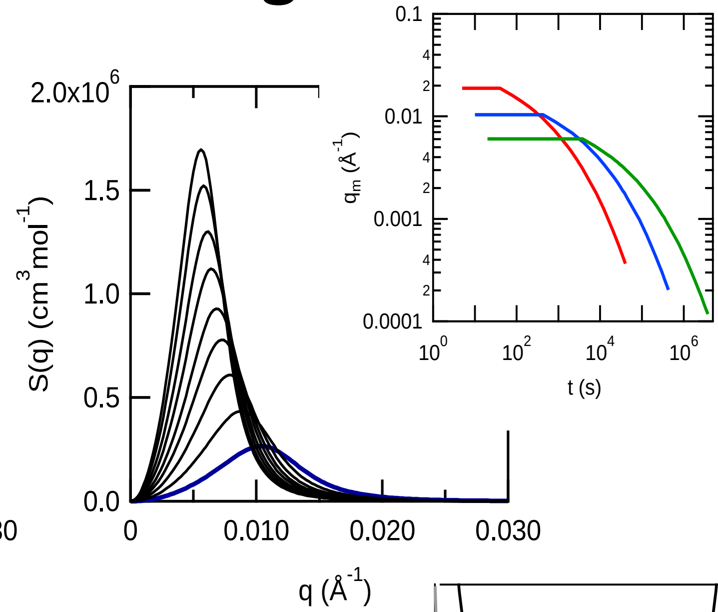
$$R(q_m) = \frac{MG''^2}{8k}$$

$$\tau_c \sim \left(\frac{MG''^2}{8k}\right)^{-1}$$ *duration of 'early stage'*

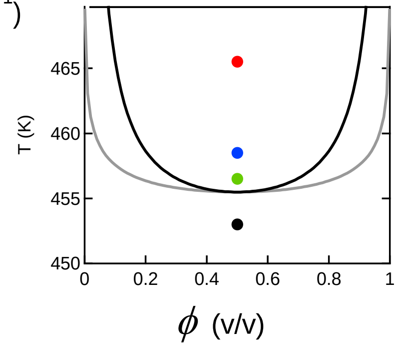


Early stages and coarsening





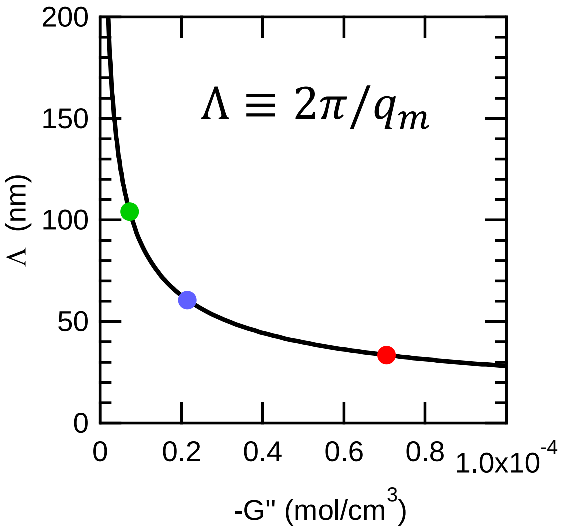
$$q_m = \sqrt{-\frac{G''}{4k}}$$



$\Delta T=2.5°C$, where $G''=1.8\ 10^{-5}$ mol/cm^3, and
$k=0.05$ Å^2 mol/cm^3, $M=10^6$ Å^2 s^{-1} cm^3 mol^{-1}

The dominant lengthscale

$$q_m = \sqrt{-\frac{G''}{4k}}$$



Second derivative of ΔG

$$G'' \equiv \frac{\partial^2 \left(\frac{\Delta G}{k_B T}\right)}{\partial \phi^2}$$

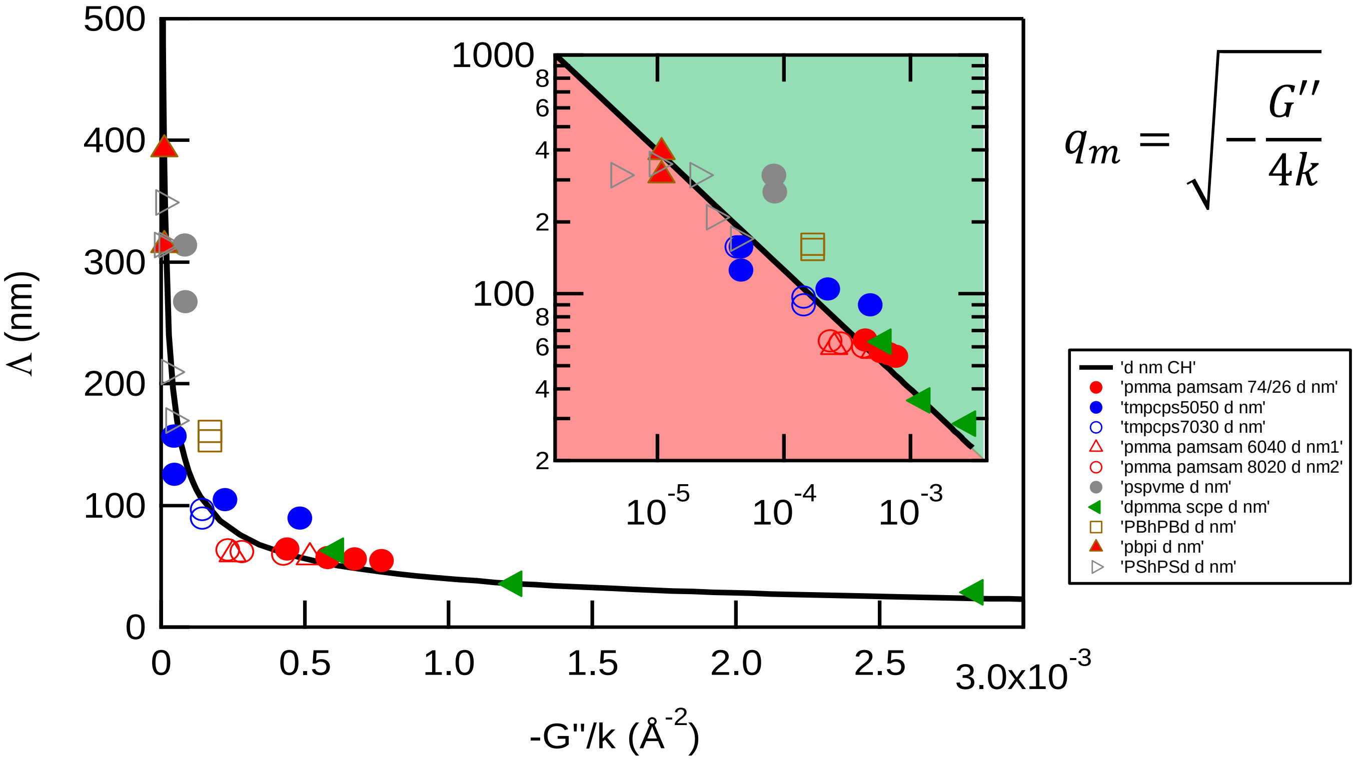
<u>if</u> we assume Flory-Huggins

$$G'' = \frac{1}{\phi_A v_A N_A} + \frac{1}{\phi_B v_B N_B} - 2\frac{\chi_{AB}(T)}{v}$$

Gradient coefficient (k=0.05 Å^2 mol/cm^3)

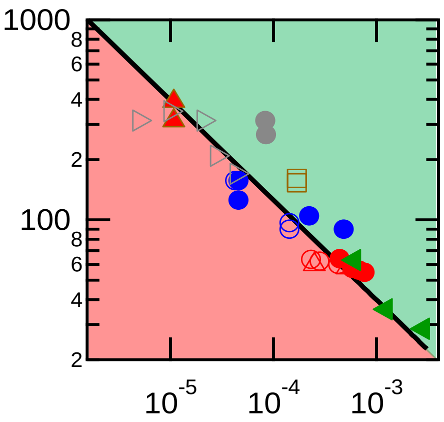
$$k = \frac{1}{6}\left(\frac{\langle R_{gA}^2\rangle_z}{\phi_A v_A \langle N_A\rangle_w} + \frac{\langle R_{gB}^2\rangle_z}{\phi_B v_B \langle N_B\rangle_w}\right) \approx k = \frac{1}{6}\left(\frac{b_A^2}{6\phi_A v_A} + \frac{b_B^2}{6\phi_B v_B}\right)$$

Re-examining Cahn-Hilliard scale against (all?) early stage SD experiments



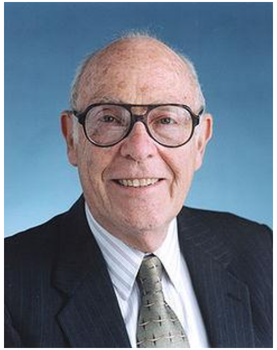
$$q_m = \sqrt{-\frac{G''}{4k}}$$

Perspective

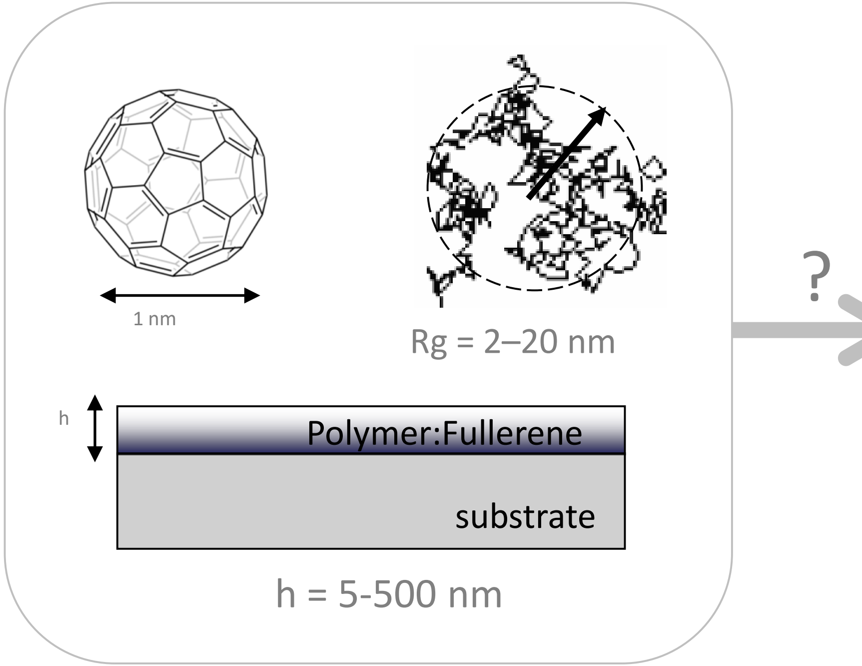


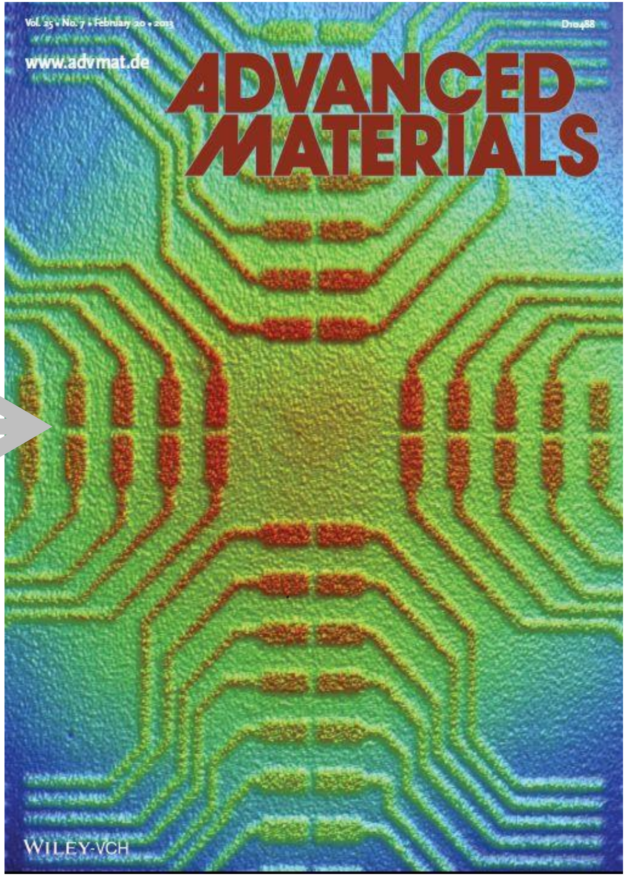
- C-H theory is an excellent predictor of initial S-D lengthscales
- Despite extensive χ(ϕ,T), F-H theory is not helpful for prediction of G" and thus behaviour in new blends.
- Remains great need for thermodynamic theory capable of correlating ΔG or G'' to molecular architecture to enable first principles material design by spinodal decomposition (LCT, Prism, LCL, …)

"Having been the father of this equation, it really is very similar to being a father, because it has a life of its own. I long ago lost the ability to keep guiding it. It's just going, and I'm very proud of it, *but it's on its own*."



Demixing in organic photovoltaics

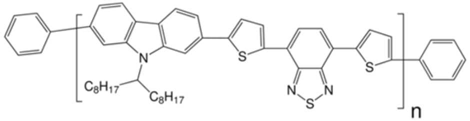




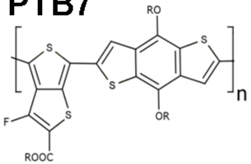
Organic photovoltaics

Morphology of efficient photovoltaics: *phase separation* on a length scale of the exciton diffusion length (~10 nm) in the active layer with interconnected phases and a thickness (~100 nm) optimised for light absorption…

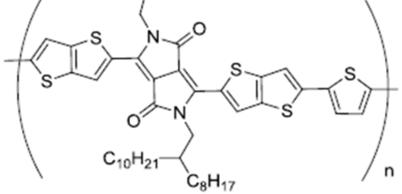
PCDTBT



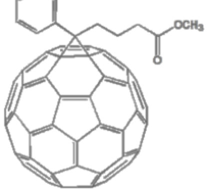
PTB7



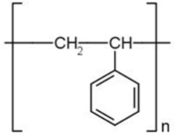
DPP-TT-T



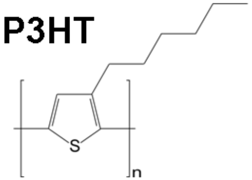
$PC_{60}BM$

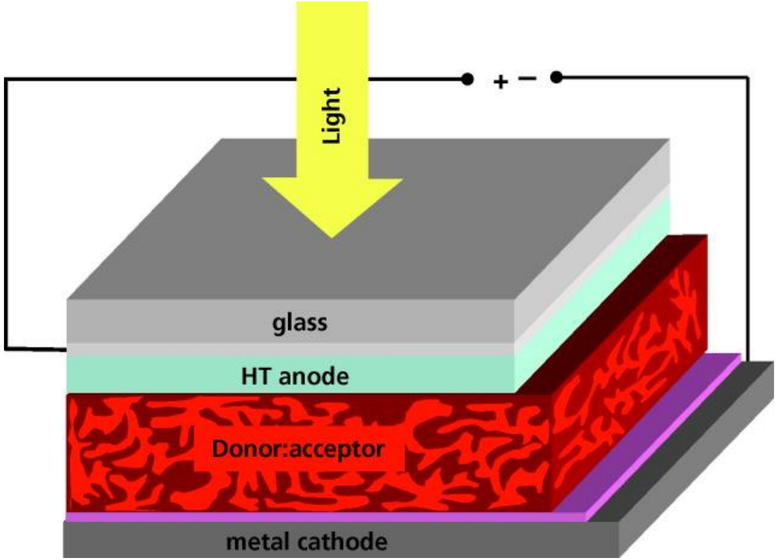


PS

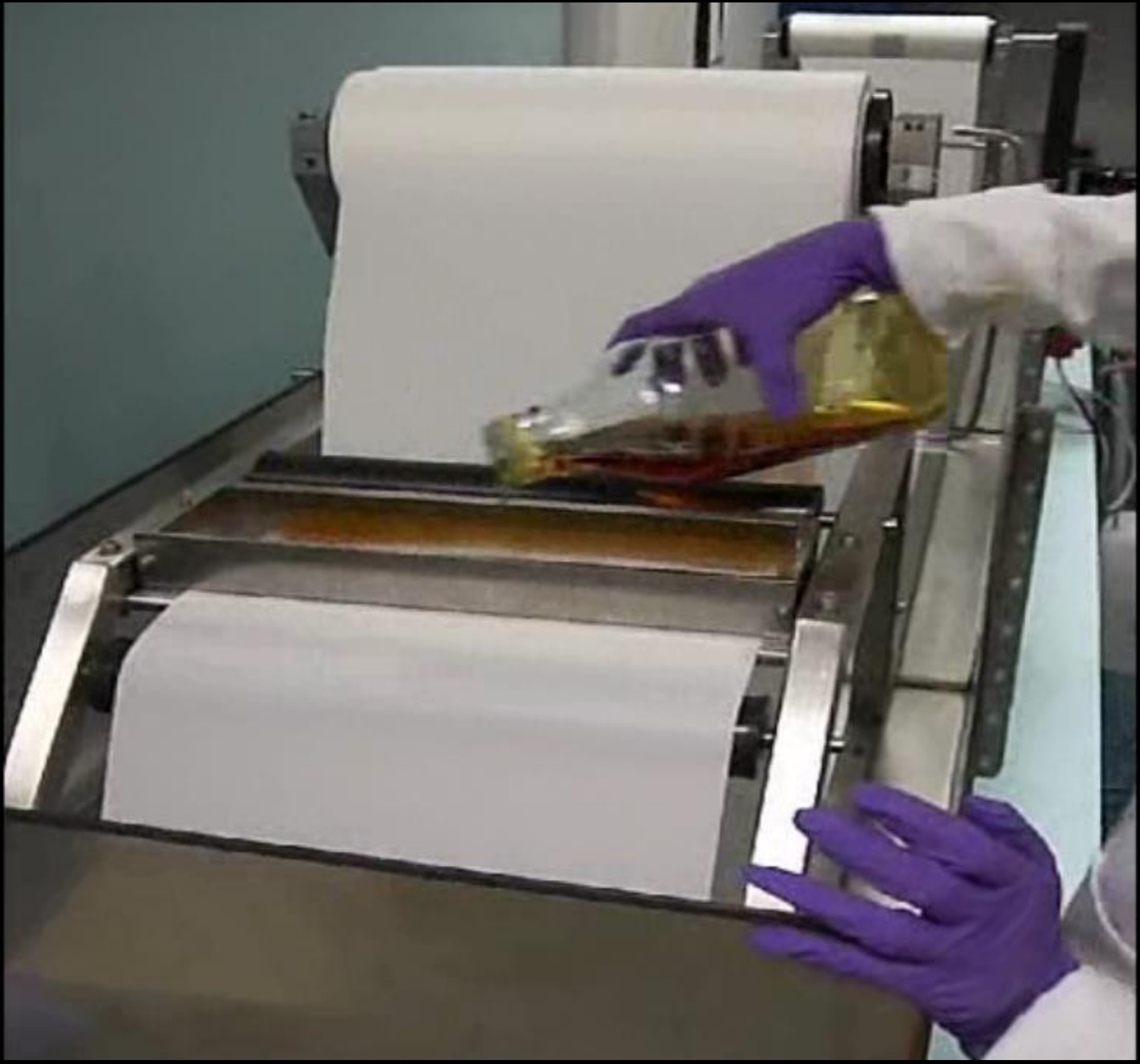


P3HT

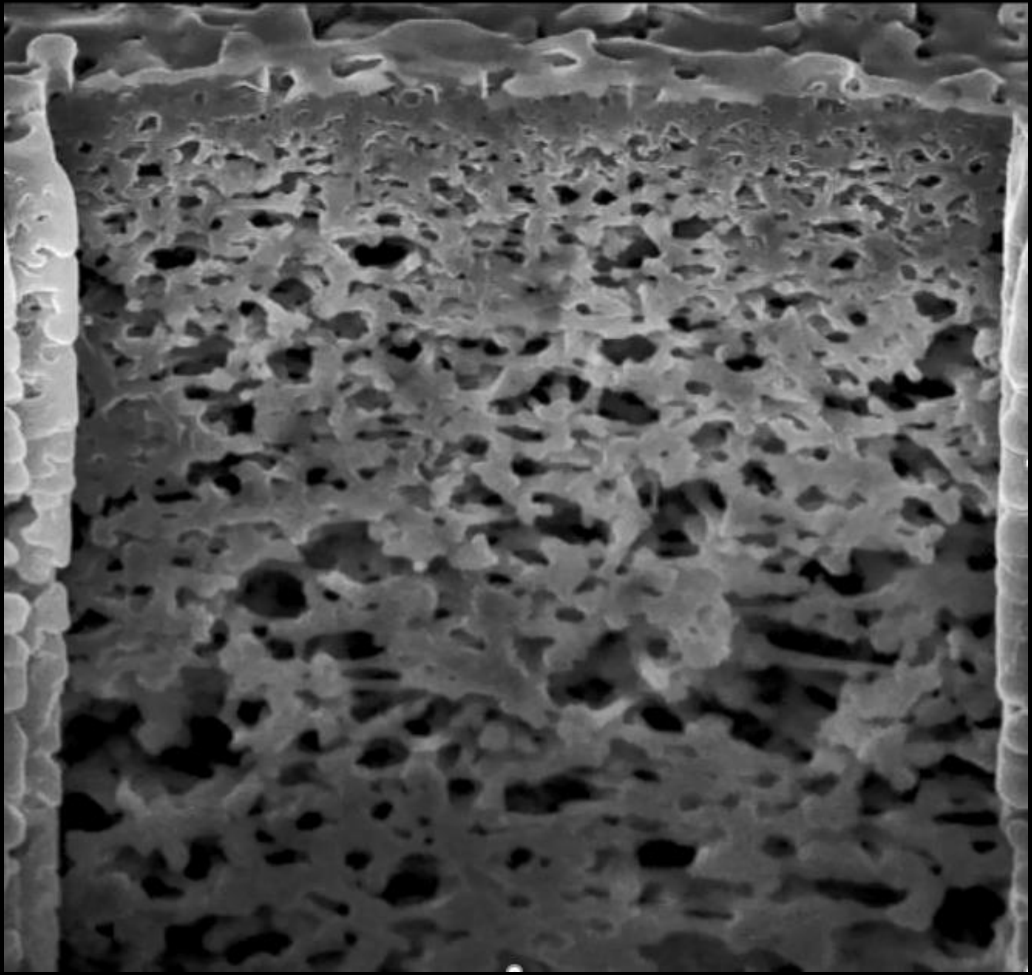




Nature Communications **4**, 2227 (2013) • *ACS Nano* **8**, 1297-1308 (2014)



Polymeric membranes for separations



Outline

1. Polymer thermodynamics & demixing

Cahn-Hilliard theory & spinodal decomposition.

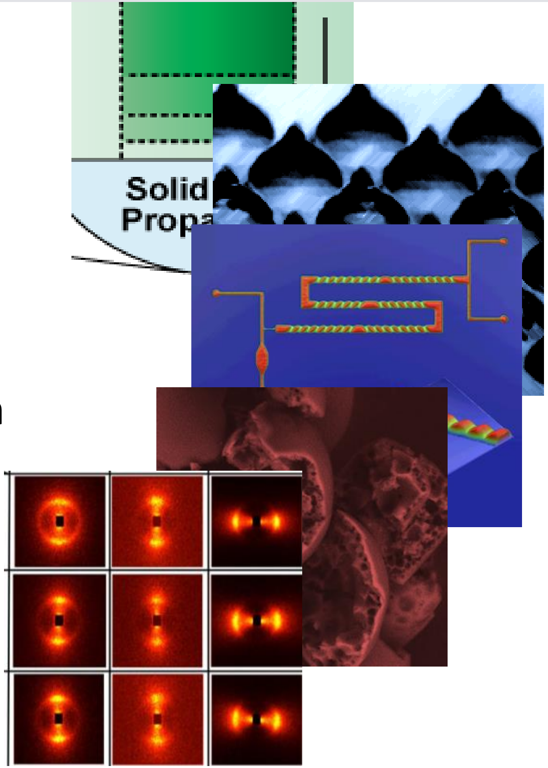
Membranes and photovoltaics

2. Particle and capsule formation

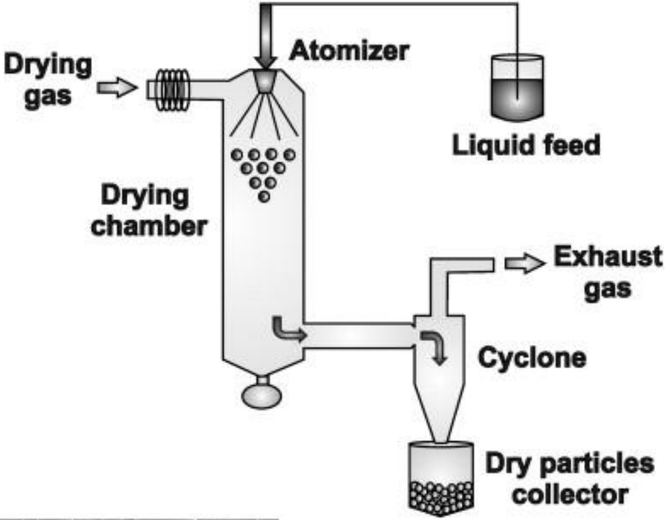
Levitation & microfluidics

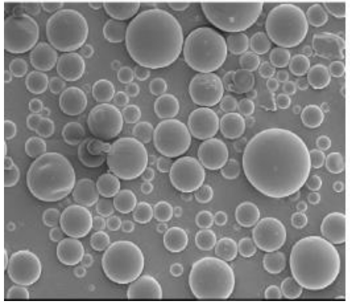
Solution thermodynamics, phase inversion and solidification

Functional capsules with tunable, triggered release.

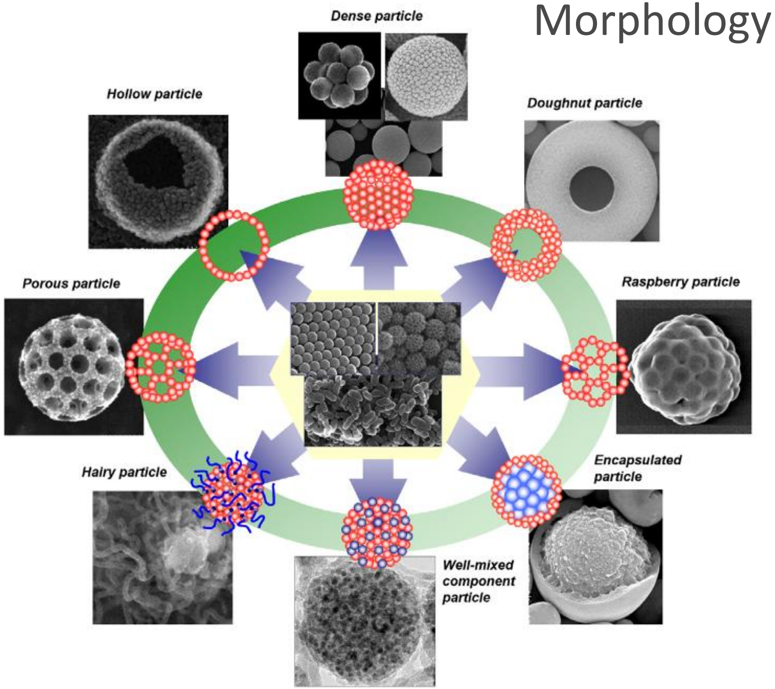


Precision ‘spray drying’

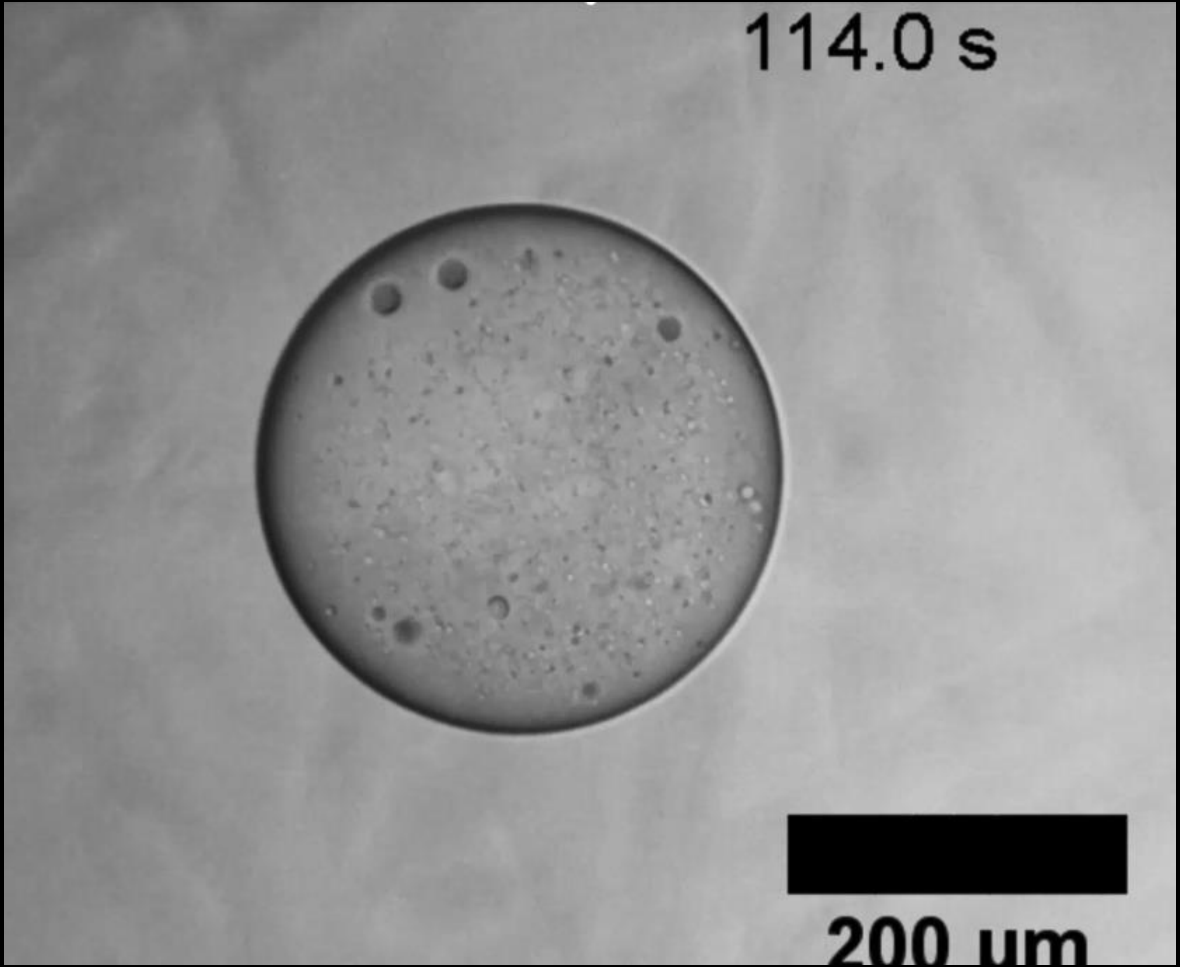




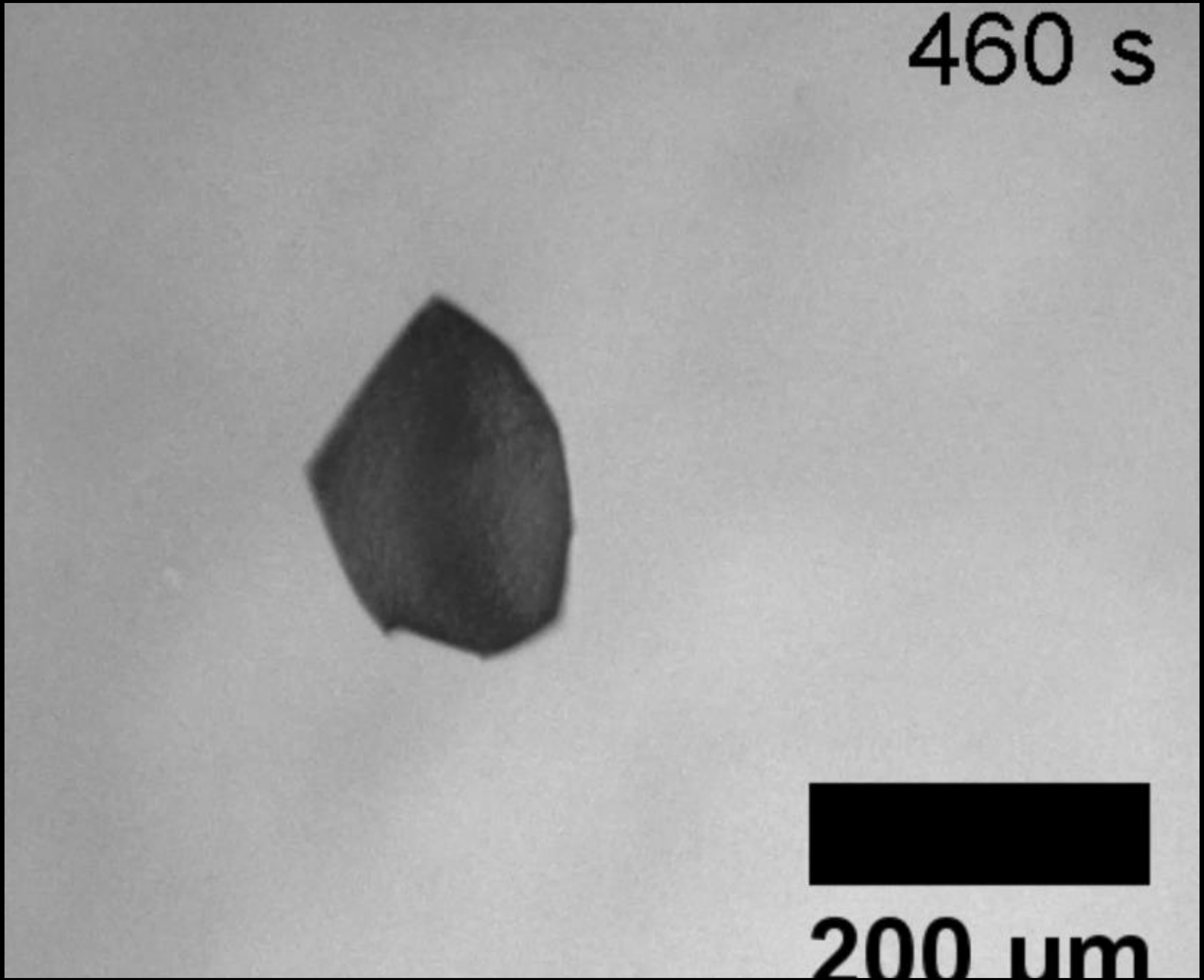
Morphology



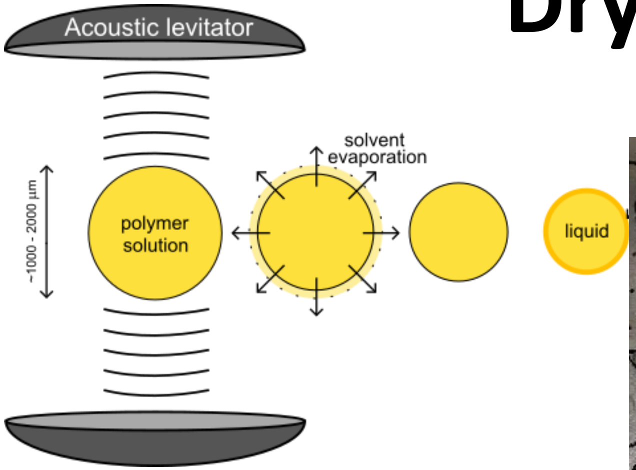
Sosnik and Seremeta, 2015; Lee et al. 2011; Nandiyanto and Okuyama, 2011

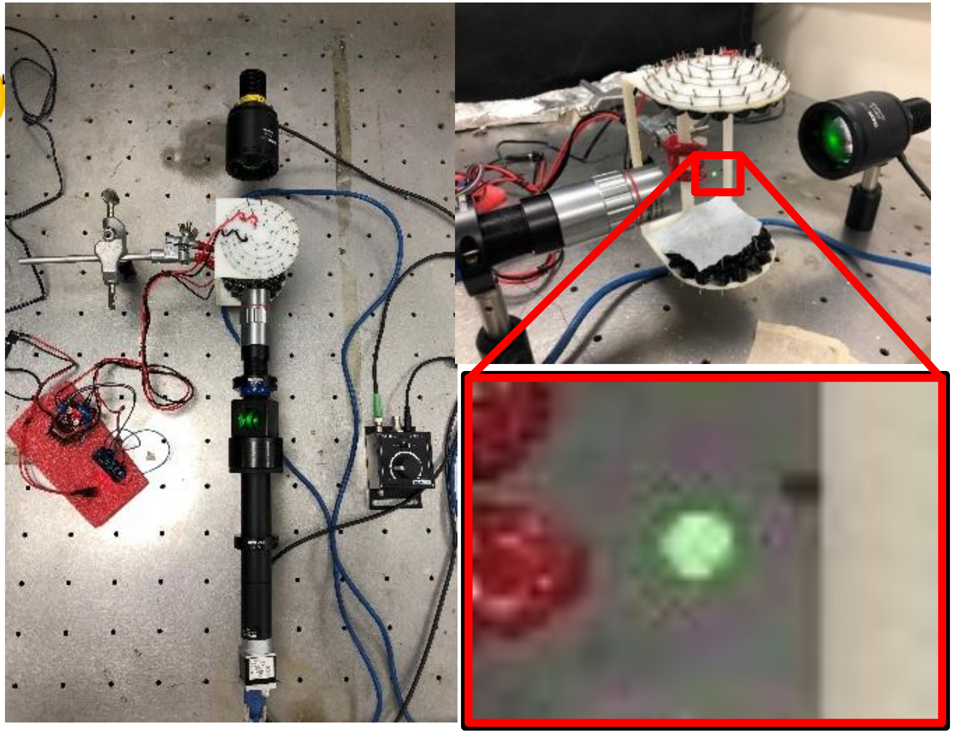


NaPSS

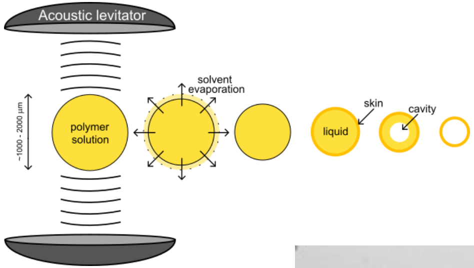

460 s
200 um

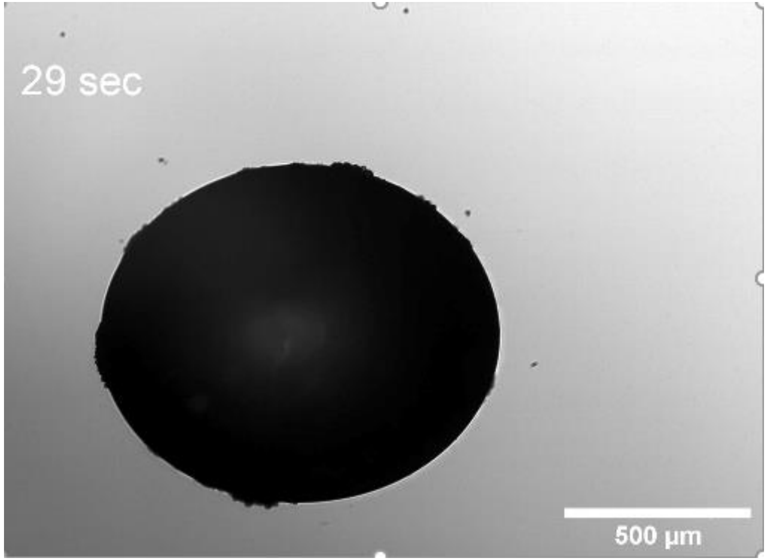
Drying in acoustic levitation



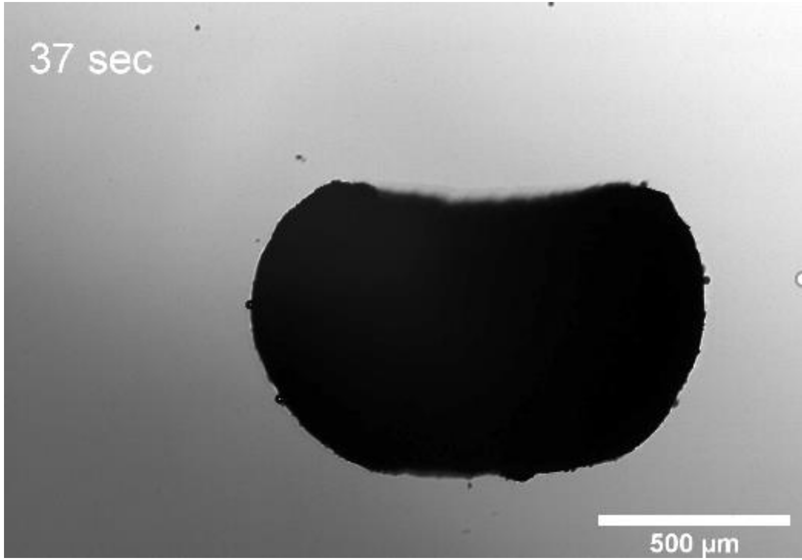


Drying in acoustic levitation



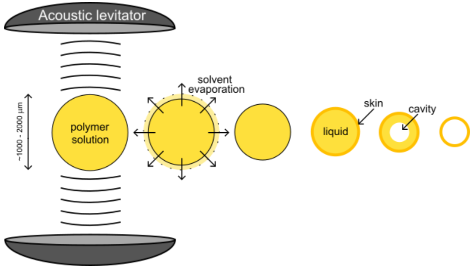


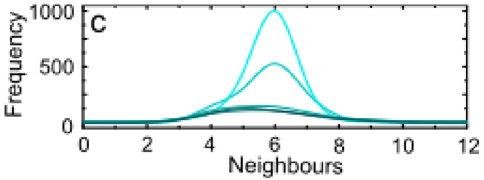
0.5 w/w%

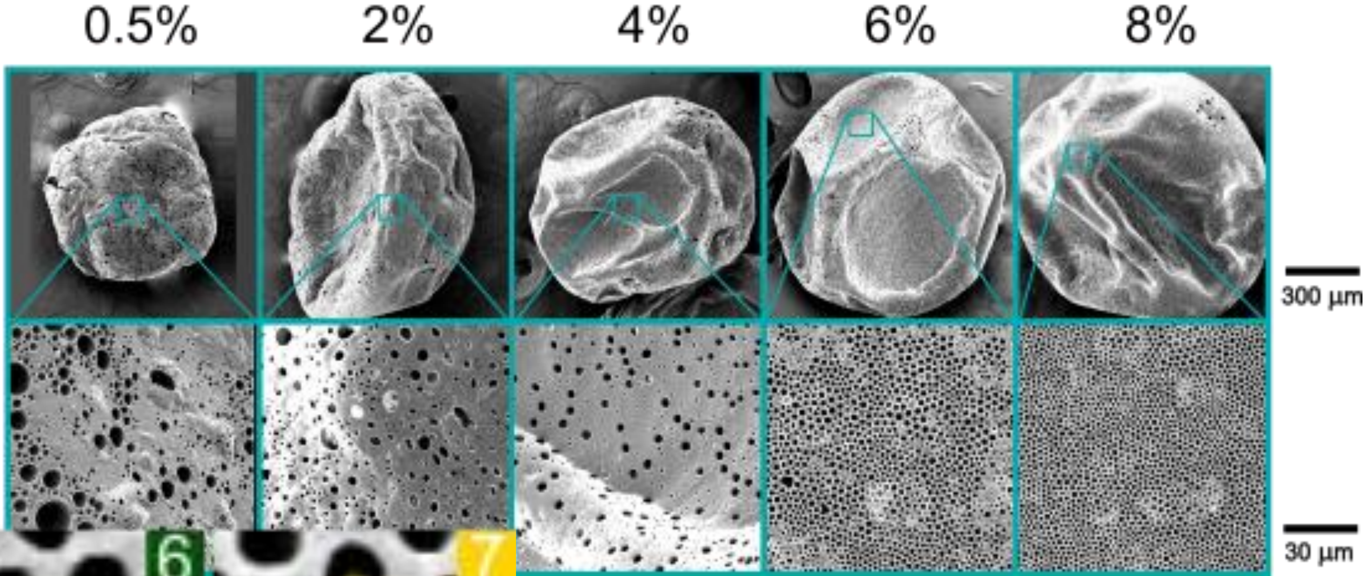


2 w/w%

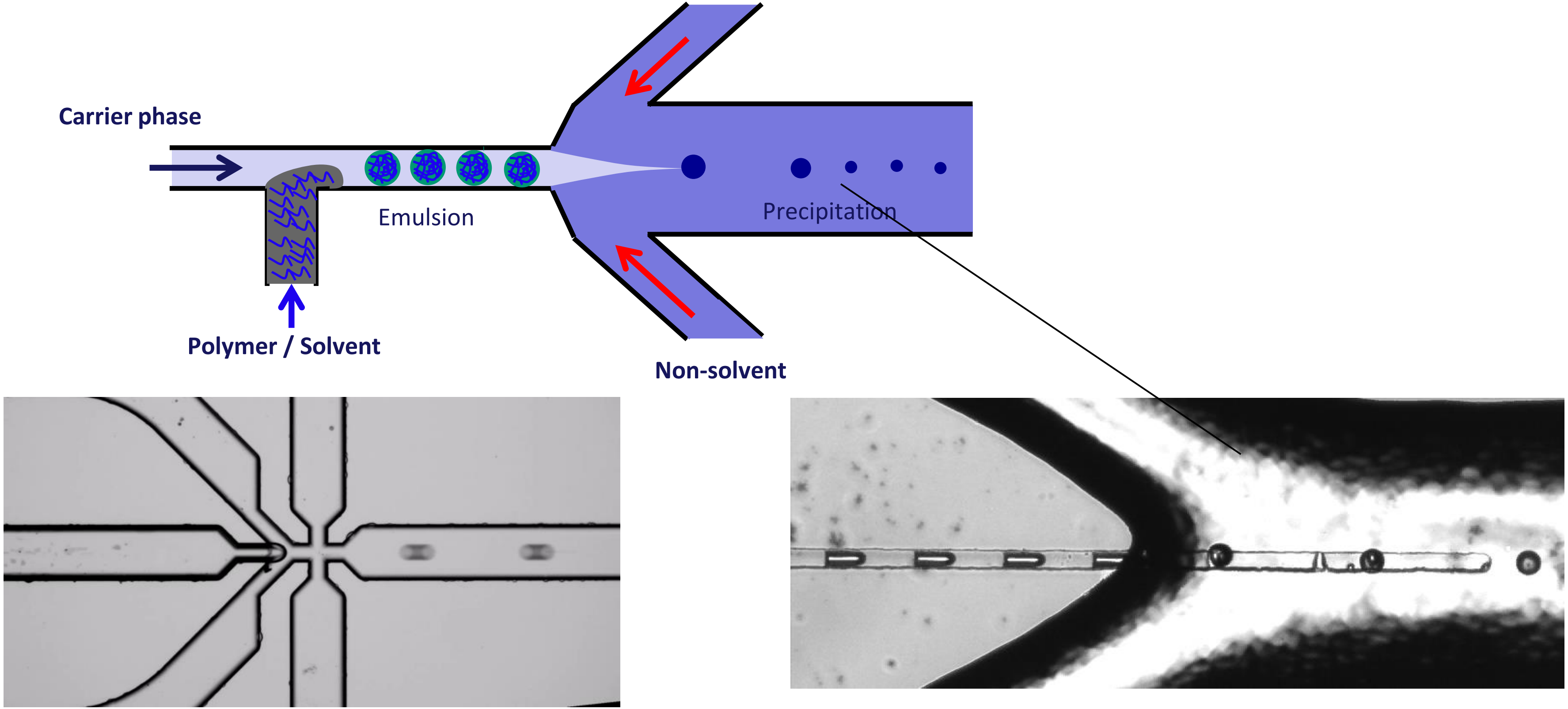
Drying in acoustic levitation



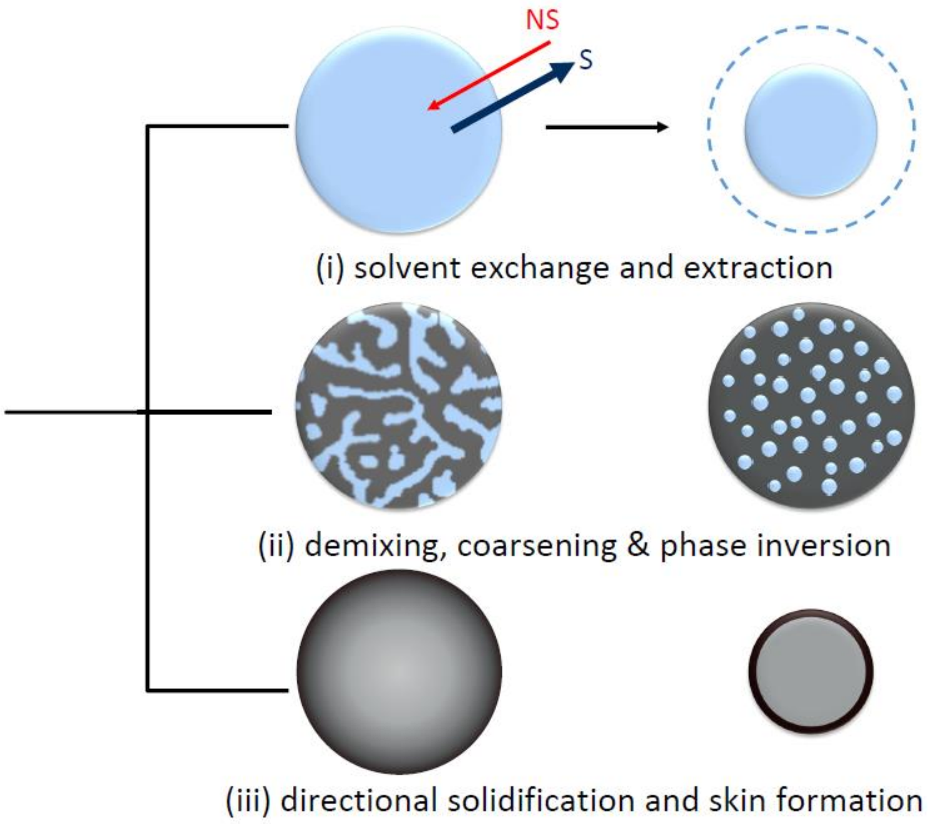




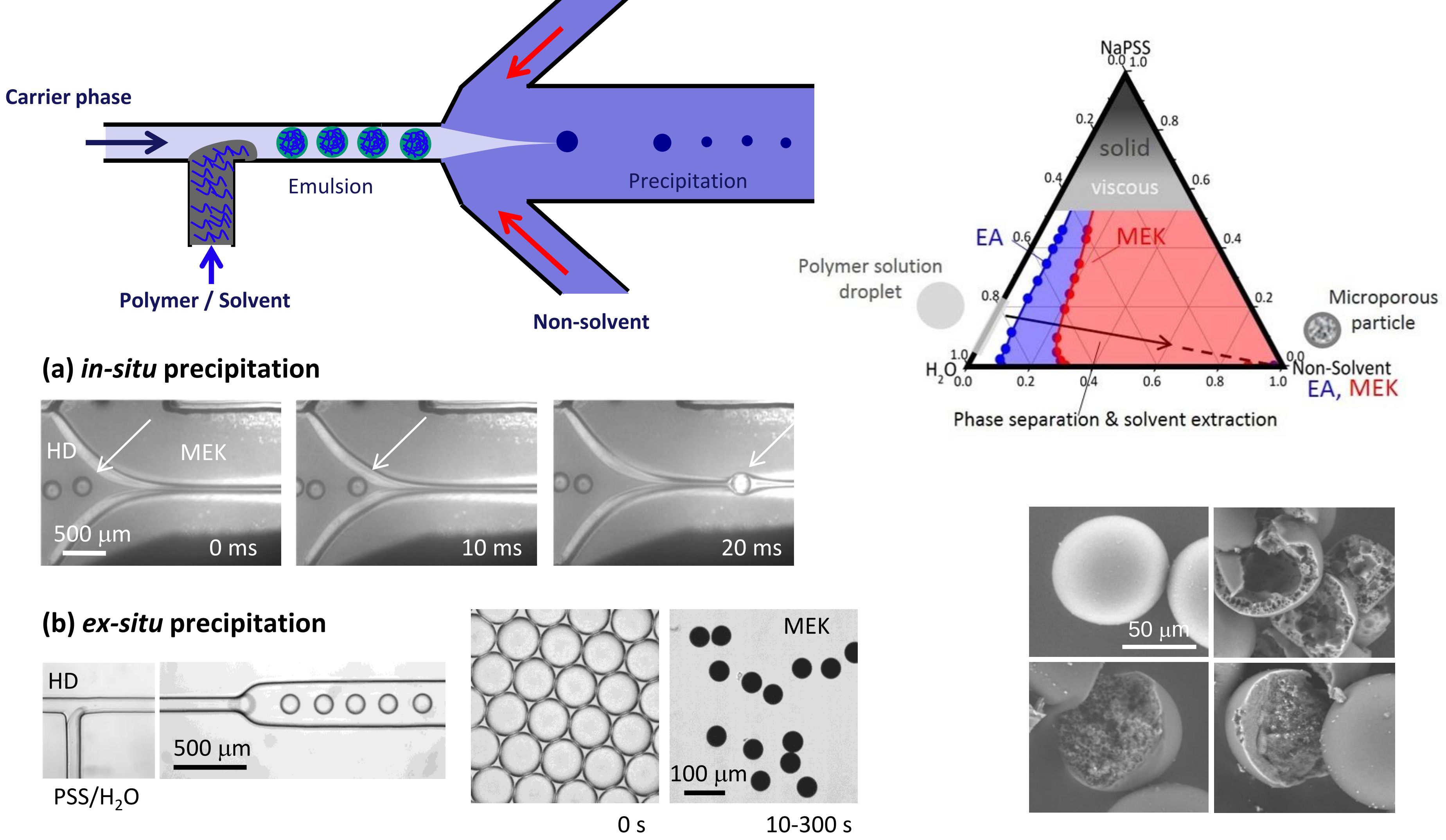
Microfluidic extraction



Coupling of mechanisms…

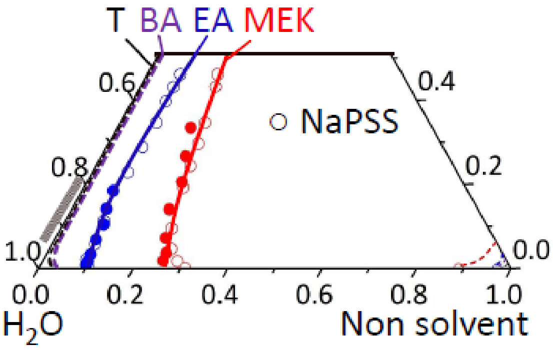


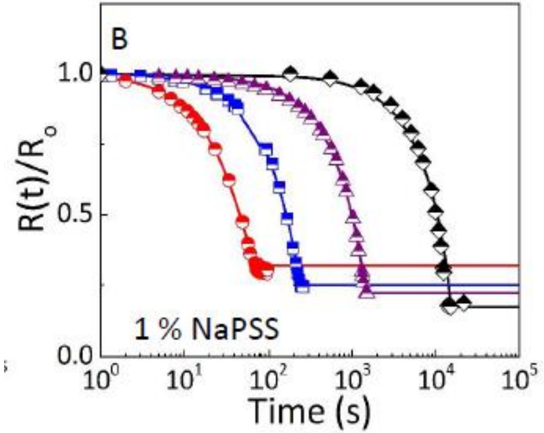
$$Pe = \frac{Ru}{D}$$

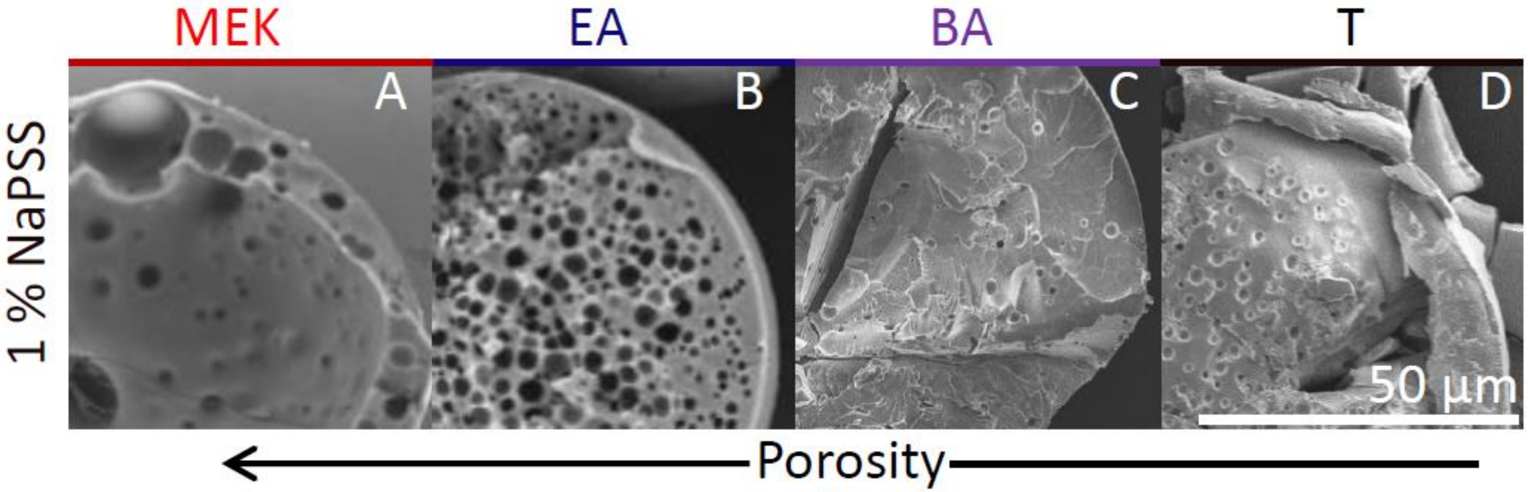


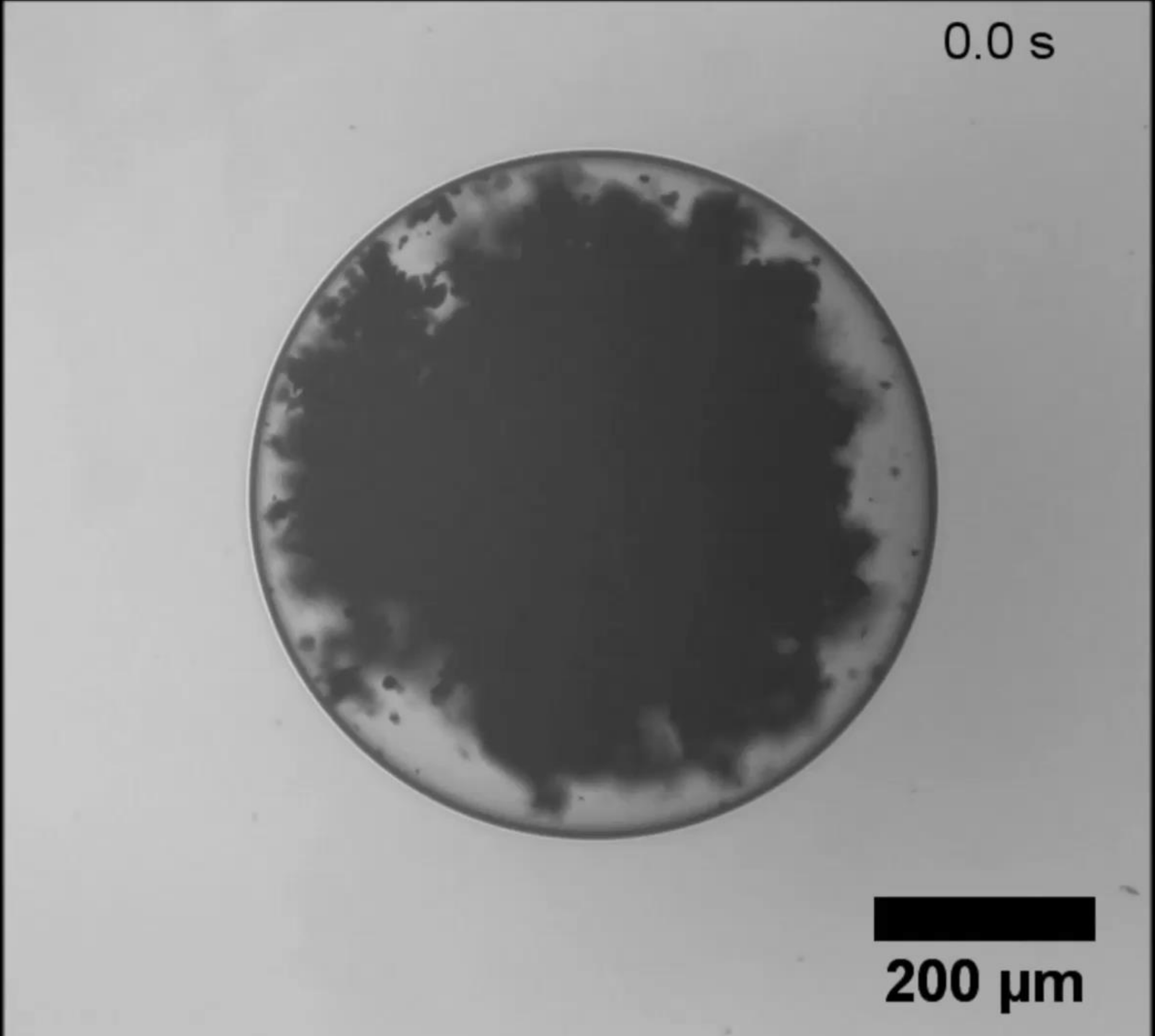
Carrier phase
Polymer / Solvent
Emulsion
Precipitation
Non-solvent
(a) in-situ precipitation
HD
MEK
500 μm
0 ms
10 ms
20 ms
(b) ex-situ precipitation
HD
PSS/H2O
500 μm
0 s
MEK
100 μm
10-300 s
NaPSS
solid
viscous
EA
MEK
Polymer solution droplet
Microporous particle
H2O
Non-Solvent
EA, MEK
Phase separation & solvent extraction
50 μm

non-solvent quality



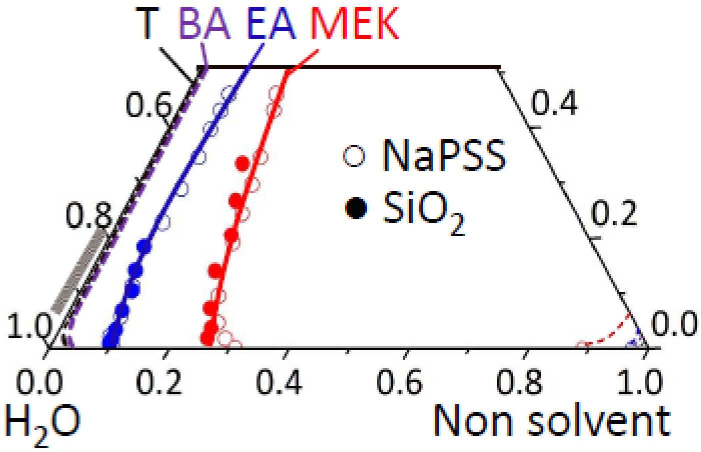


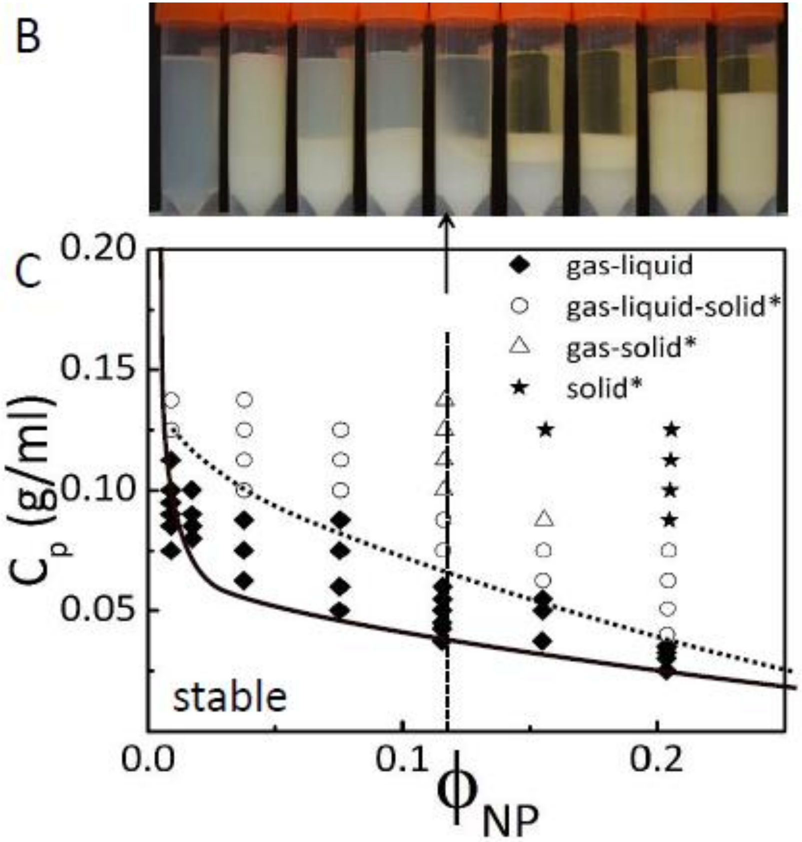


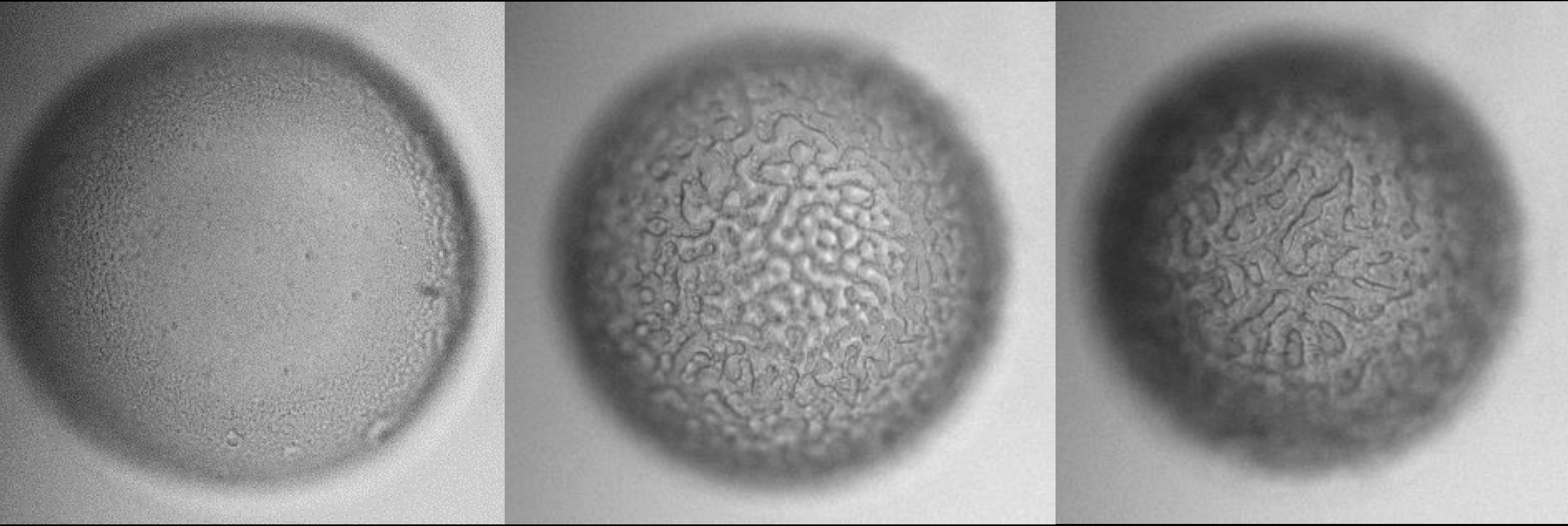


NaPSS/MWCNT/H_2O/MEK

Polymer-colloid thermodynamics

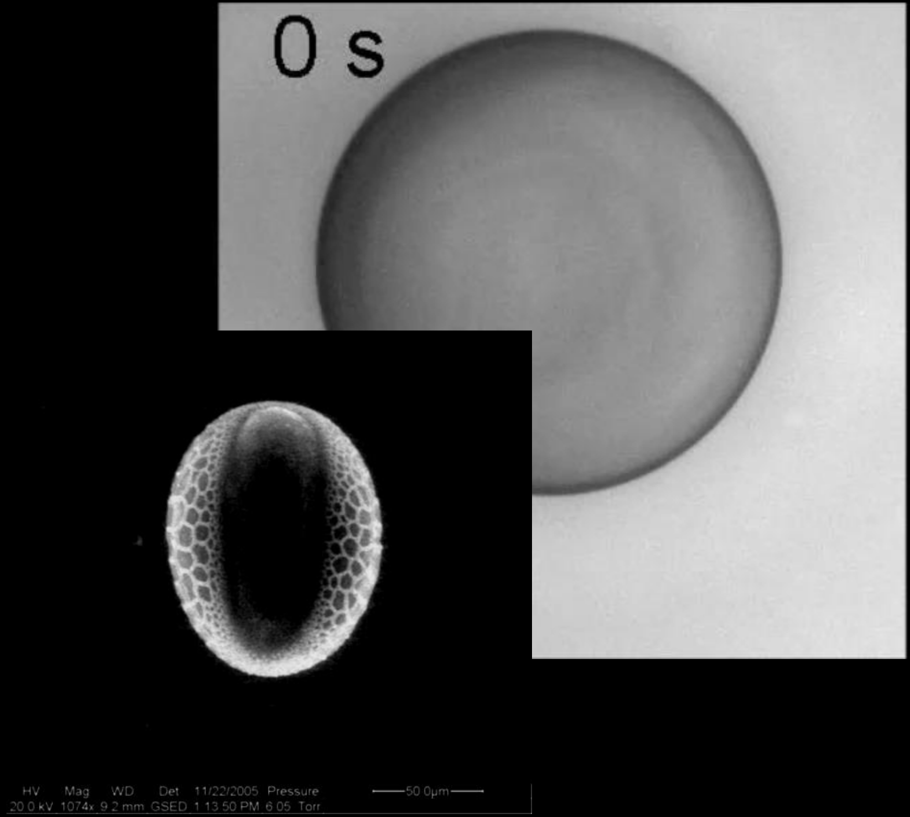


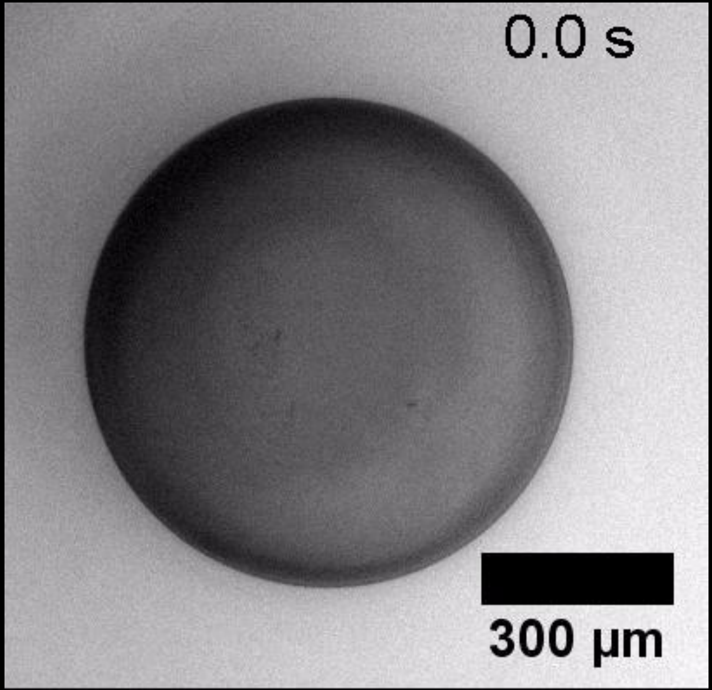




1% NaPSS, 2wt% SiO_2 22 nm/H_2O/ MEK

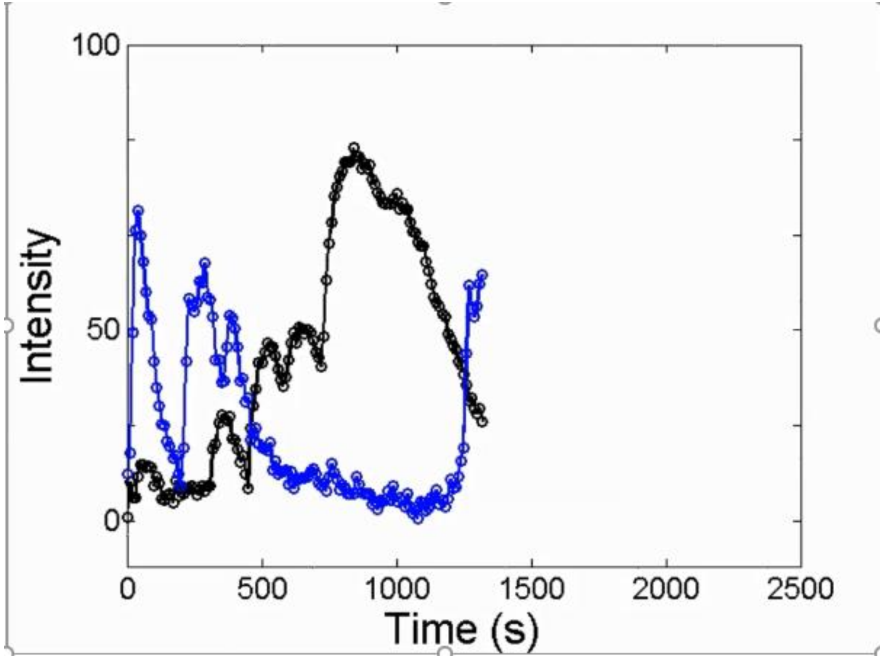
Polymer-nanoparticle capsules

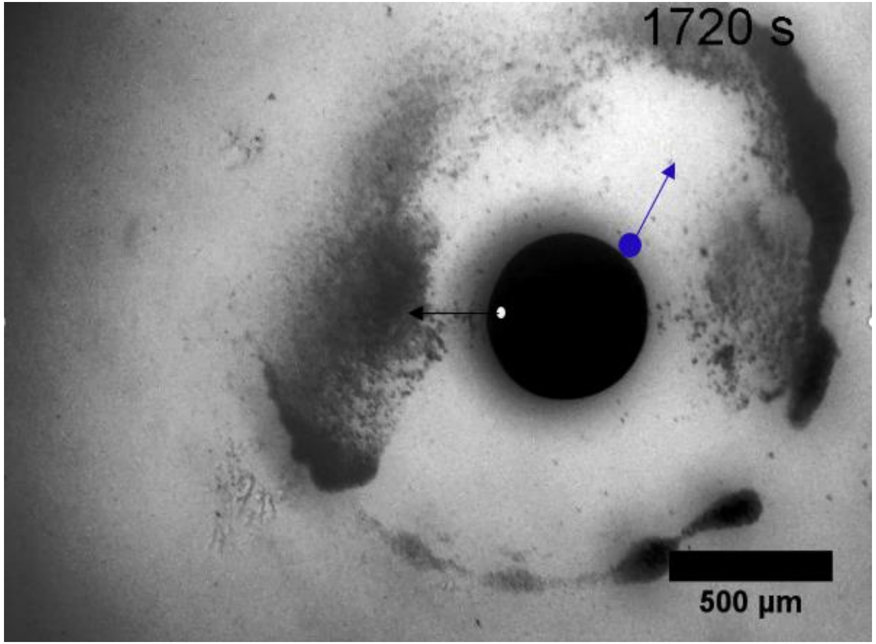




Pulsed, directional, triggered release

1 wt% P 10 wt% NP (DI H_2O)

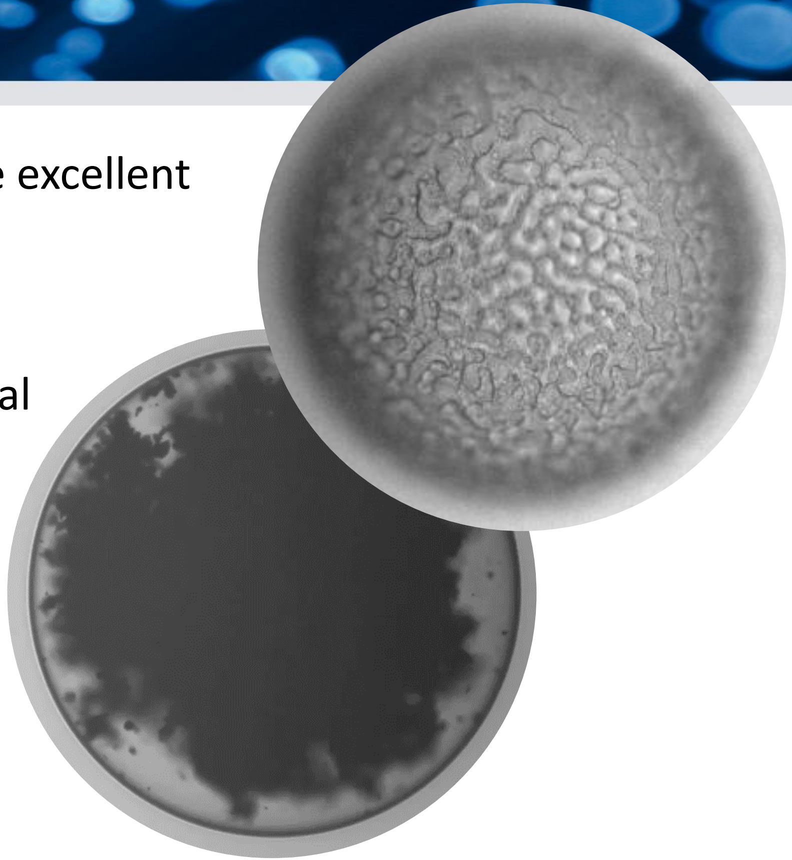




Udoh et al ScienceAdvances
AAAS's open-access journal

Perspective

- Levitation and microfluidic (osmotic) drying are excellent platforms to examine "spray drying"
- Solution thermodynamics, demixing and coarsening can de engineered to yield functional particles with unexpected performance
- Transformative predictive design requires molecular insight (eg scattering) and theory/simulation



Outline

1. Polymer thermodynamics & demixing

Cahn-Hilliard theory & spinodal decomposition.

Membranes and photovoltaics

2. Particle and capsule formation

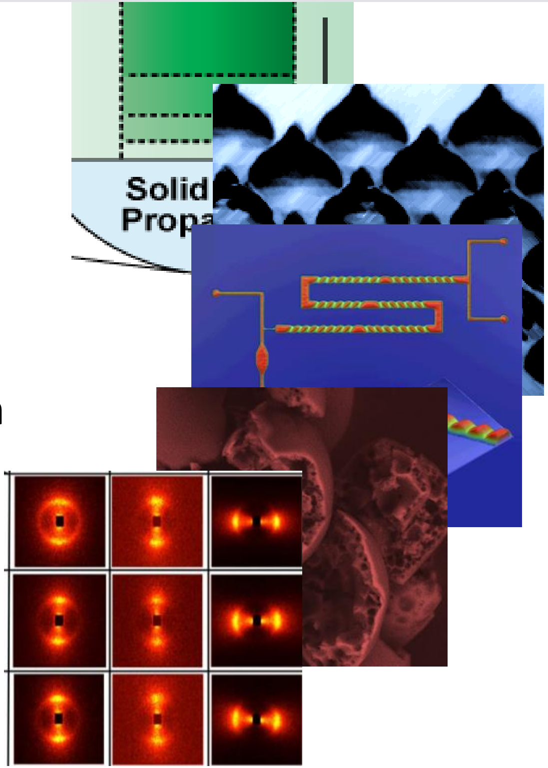
Levitation & microfluidics

Solution thermodynamics, phase inversion and solidification

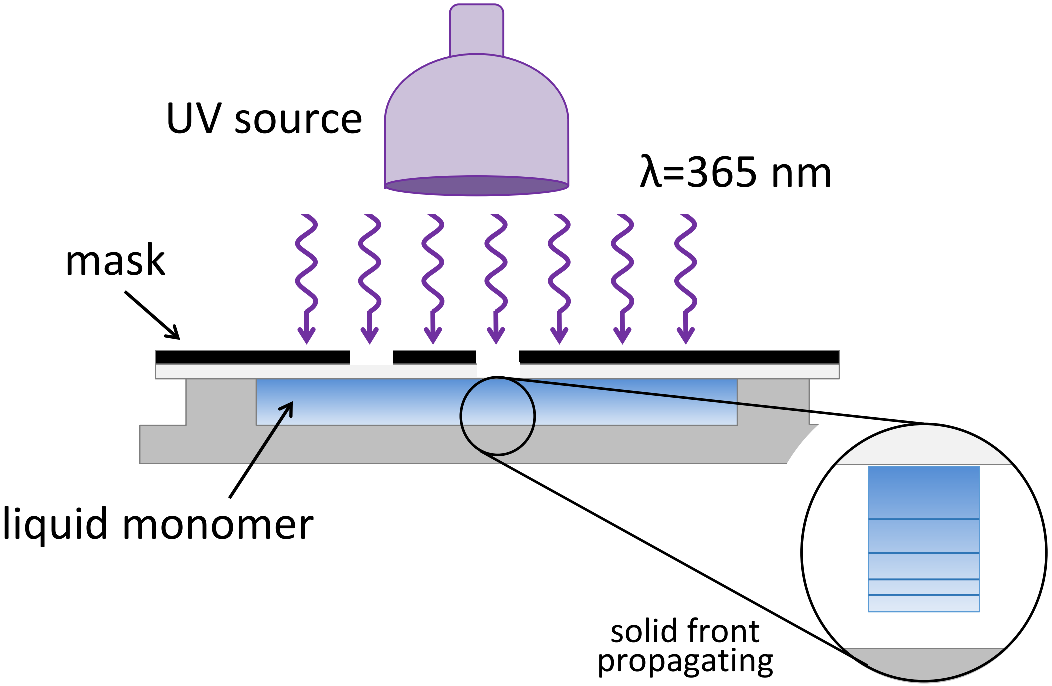
Functional capsules with tunable, triggered release.

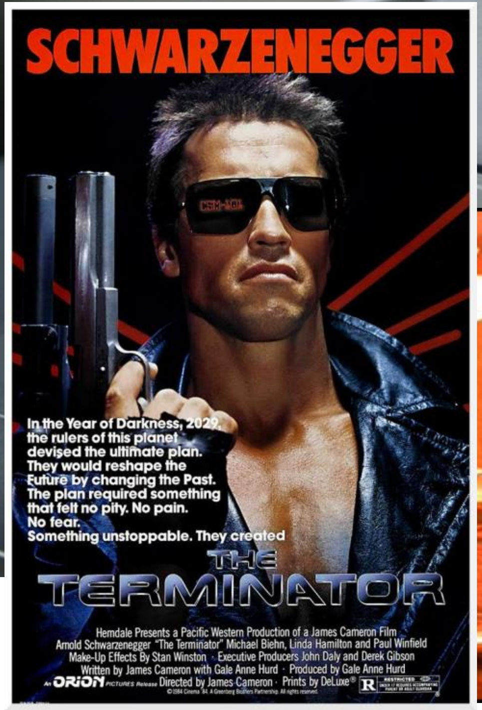
3. Waves of network formation

3D printing with light



Photopolymerisation & 3D printing




SCHWARZENEGGER
In the Year of Darkness, 2029,
the rulers of this planet
devised the ultimate plan.
They would reshape the
Future by changing the Past.
The plan required something
that felt no pity. No pain.
No fear.
Something unstoppable. They created
THE
TERMINATOR
Hemdale Presents a Pacific Western Production of a James Cameron Film
Arnold Schwarzenegger "The Terminator" Michael Biehn, Linda Hamilton and Paul Winfield
Make-Up Effects By Stan Winston · Executive Producers John Daly and Derek Gibson
Written by James Cameron with Gale Anne Hurd · Produced by Gale Anne Hurd
An ORION PICTURES Release Directed by James Cameron · Prints by DeLuxe®
R

Explicit photopolymerization models

Initiation

$$\mathsf{PI} \xrightarrow{\gamma} \dot{\mathsf{R}}$$

$$\dot{\mathsf{R}} + \mathsf{M} \xrightarrow{k_i} \dot{\mathsf{P}}_1$$

Propagation

$$\dot{\mathsf{P}}_n + \mathsf{M} \xrightarrow{k_p} \dot{\mathsf{P}}_{n+1}, \quad n = 1, 2, \ldots$$

Termination

$$\dot{\mathsf{P}}_n + \dot{\mathsf{P}}_m \xrightarrow{k_{tb}} \mathsf{P}_{n+m} \text{ or } \mathsf{P}_n + \mathsf{P}_m, \quad n, m = 1, 2, \ldots$$

$$\dot{\mathsf{P}}_n + \dot{\mathsf{R}} \xrightarrow{k_{tr}} \mathsf{P}_n, \quad n = 1, 2, \ldots$$

Inhibition

$$\dot{\mathsf{P}}_n + \mathsf{Z} \xrightarrow{k_z} \mathsf{P}_n\mathsf{Z}, \quad n = 1, 2, \ldots$$

Explicit photopolymerization models

$$\frac{\partial[\mathsf{PI}]}{\partial t} = -R_i,$$

$$\frac{\partial[\dot{\mathsf{R}}]}{\partial t} = R_i - k_i[\dot{\mathsf{R}}][\mathsf{M}] - k_{tr}[\dot{\mathsf{P}}][\dot{\mathsf{R}}],$$

$$\frac{\partial[\mathsf{M}]}{\partial t} = -k_i[\dot{\mathsf{R}}][\mathsf{M}] - k_p[\dot{\mathsf{P}}][\mathsf{M}],$$

$$\frac{\partial[\dot{\mathsf{P}}]}{\partial t} = k_i[\dot{\mathsf{R}}][\mathsf{M}] - k_{tb}[\dot{\mathsf{P}}]^2 - k_{tr}[\dot{\mathsf{P}}][\dot{\mathsf{R}}] - k_z[\dot{\mathsf{P}}][\mathsf{Z}],$$

$$\frac{\partial[\mathsf{Z}]}{\partial t} = -k_z[\dot{\mathsf{P}}][\mathsf{Z}],$$

$$\frac{\partial[\mathsf{P}]}{\partial t} = k_{tb}[\dot{\mathsf{P}}]^2 + k_{tr}[\dot{\mathsf{P}}][\dot{\mathsf{R}}]$$

$$\frac{\partial[\mathsf{PZ}]}{\partial t} = k_z[\dot{\mathsf{P}}][\mathsf{Z}].$$

Explicit photopolymerisation models

Parameter	Value	Units	Ref.	Remarks
$[M]_0$	8.2	mol/l		
MW_m	130.14	g/mol		
MW_s	92.09	g/mol		
R	4	l/mol	Goodner et al.	
α_M	0.0005	1/°C	Goodner et al.	
α_P	0.000075	1/°C	Goodner et al.	
α_S	0.0005	1/°C		Same as α_M
ρ_M	1.073	g/ml	Aldrich	
ρ_P	1.15	g/ml	Goodner et al.	
ρ_S	1.261	g/ml	Aldrich	
T_{gm}	213	K	Goodner et al.	
T_{gp}	328	K	Goodner et al.	
T_{gs}	173	K		Estimated
ϕ	0.6		Goodner et al.	
ε	150	l/mol c	Goodner et al.	
k_{p0}	1.6×10^{6}	l/mol s	Goodner et al.	
E_p	18.23×10^{3}	J/mol	Gao and Penlidis	For MMA
A_p	0.66		Goodner et al.	
f_{cp}	0.042		Goodner et al.	
k_{t0}	3.6×10^{6}	l/mol s	Goodner et al.	
E_t	2.94×10^{3}	J/mol	Gao and Penlidis	For MMA
A_t	1.2		Goodner et al.	
f_{ct}	0.060		Goodner et al.	
k_{10}	1.6×10^{6}	l/mol s		Same as k_{p0}
k_{20}	52.8×10^{9}	l/mol s	Odian	For O_2/MMA
k_{tp0}, k'_{t0}	0.0	l/mol s		Unless otherwise noted
E_1, E_2, E'_t	18.23×10^{3}	J/mol		Same as E_p
E_{tp}	2.94×10^{3}	J/mol		Same as E_t
A_1, A_{tp}, A'_t	0.66			Same as A_p
A_2	0.287			Calculated from diffusivity
f_{c1}, f_{ctp}, f'_{ct}	0.042		Goodner et al.	Same as f_{cp}
f_{c2}	0.010		Goodner et al.	Estimated
ΔH	-5.48×10^{4}	J/mol	Cook	From −13.1 kcal/mol
k	0.292	W/cm	Lide	For glycerine
ρc_p	1900	J/l K	Gao and Penlidis	Monomer/polymer average
D_{s0}	23.6×10^{-3}	cm^2/s	Lide	Small species in ethyl acetate
D_{m0}	23.6×10^{-3}	cm^2/s	Lide	Small species in ethyl acetate
D_{20}	49.1×10^{-3}	cm^2/s	Brandrup and Immergut	O_2 in ethyl methacrylate

Figure: Taken from Goodner & Bowman (2002)

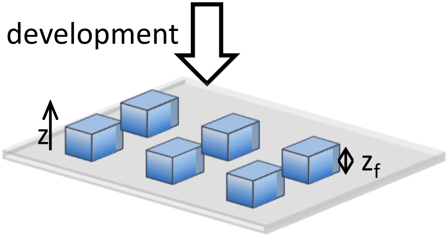
A 'minimal' FPP model

(Self-consistent & neglecting all chemical "details"!)

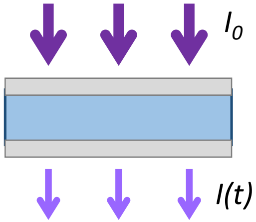
Physical observables :

- **pattern height**

(position of the solid/liquid front)



- **light transmission**



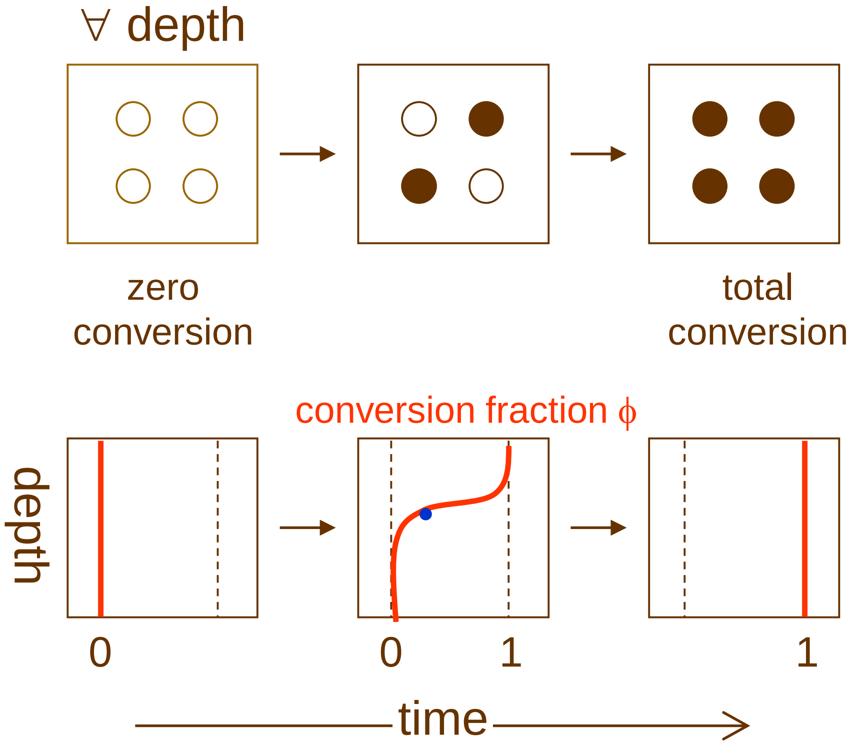
$$\begin{cases} \dfrac{\partial \phi(z,t)}{\partial t} = K[1-\phi(z,t)]I(z,t) \\ \dfrac{\partial I(z,t)}{\partial z} = -[\mu_0[1-\phi(z,t)] + \mu_\infty \phi(z,t)]I(z,t) \end{cases}$$

$$\phi(z,0) = 0, \qquad I(0,t) = 1$$

ϕ conversion fraction, I light intensity, μ_0 and μ_∞ initial and final attenuation coefficients, K conversion rate, ϕ_C solid threshold, z depth, t time.

A ‘minimal’ FPP model

(Self-consistent & neglecting all chemical “details”!)

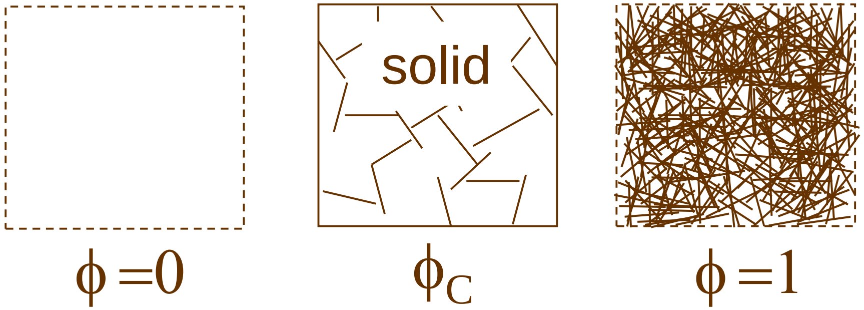


$$\begin{cases} \dfrac{\partial \phi(z,t)}{\partial t} = K[1-\phi(z,t)]I(z,t) \\ \dfrac{\partial I(z,t)}{\partial z} = -[\mu_0[1-\phi(z,t)] + \mu_\infty \phi(z,t)]I(z,t) \\ \phi(z,0)=0, \quad I(0,t)=1 \end{cases}$$

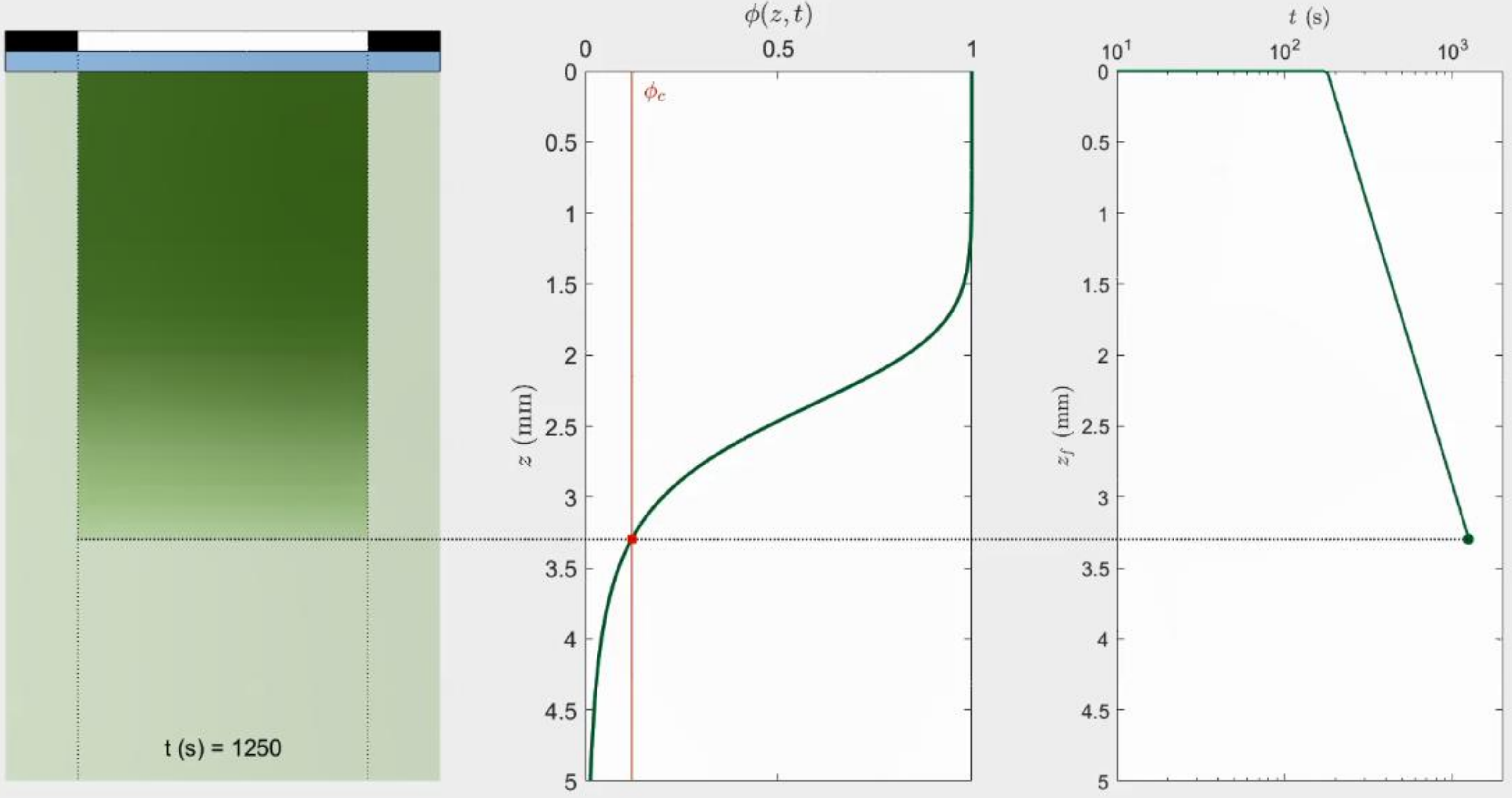
ϕ conversion fraction, I light intensity, μ_0 and μ_∞ initial and final attenuation coefficients, K conversion rate, ϕ_C solid threshold, z depth, t time.

Solid threshold

$$\begin{cases} \phi(x,t) > \phi_C, & solid \\ \phi(x,t) < \phi_C, & liquid \end{cases}$$



A ‘minimal’ FPP model



Traveling **fronts**

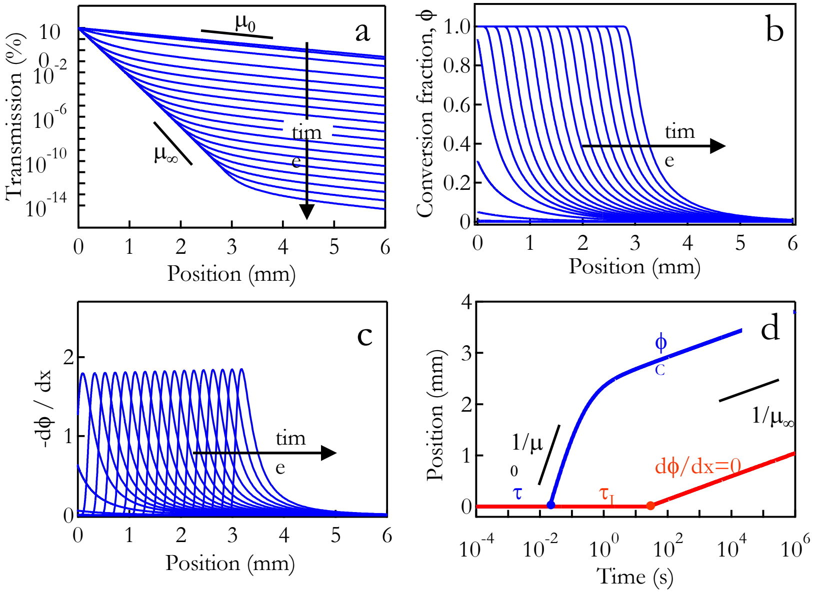
$$\begin{cases} \mu_0 > \mu_\infty (= 0) \\ \mu_0 = \mu_\infty \\ \mu_0 < \mu_\infty \end{cases}$$

Photobleaching (total)

↕

"Photodarkening"

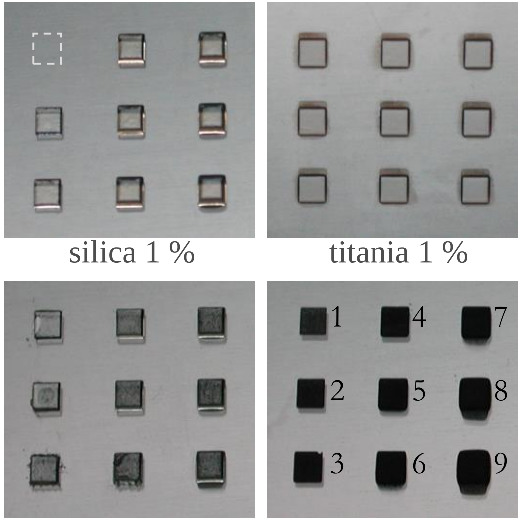
Considerable attenuation, negligible mass transfer



$$height = \frac{\ln(t/\tau)}{\bar{\mu}}$$

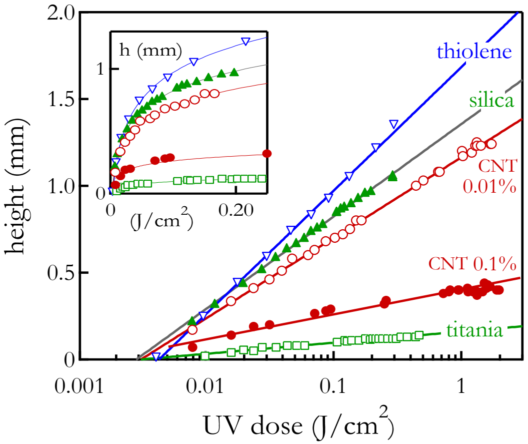
$$\textit{induction time} \equiv \frac{\ln\left[1/(1-\phi_C)\right]}{K}$$

FPP + nanofillers



silica 1 % titania 1 %

CNT 0.01 % CNT 0.1 %

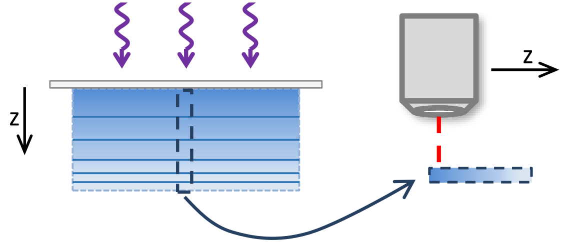


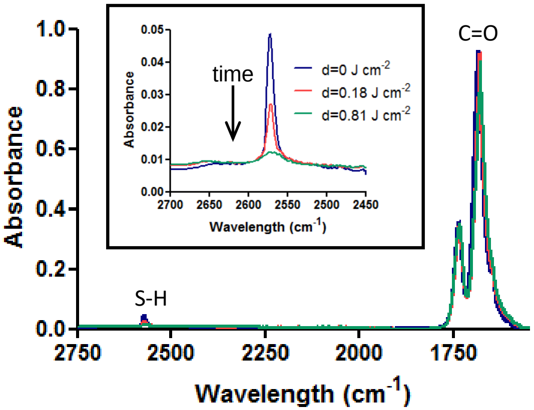
$$height = \frac{\ln(t/\tau)}{\bar{\mu}}$$

induction time $\equiv \dfrac{\ln[1/(1-\phi_C)]}{K}$

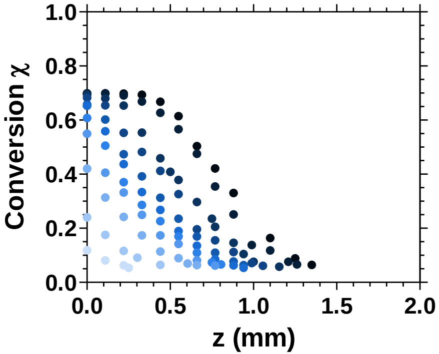
Sets the slope

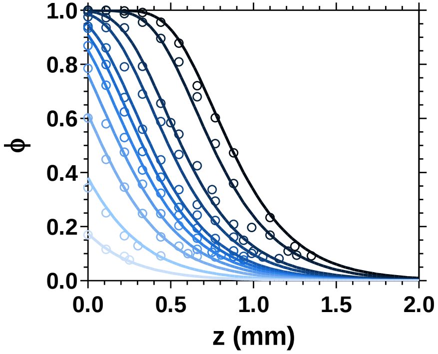
Spatio temporal conversion ϕ





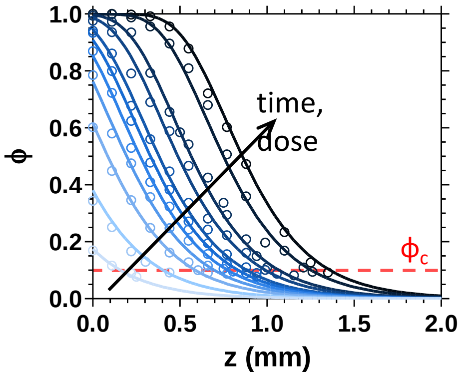
$$Conversion\ \chi \equiv 1 - \frac{A_{S-H}(t)/A_{C=O}(t)}{A_{S-H}(0)/A_{C=O}(0)}$$





Shape-invariant travelling waves

$$\phi(z,t) = 1 - \exp[-\mathrm{K}I_0 \exp(-\mu z)\, t]$$

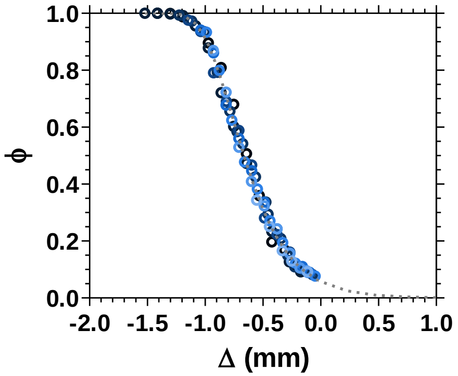


Thiol-ene 81

$\mu = 3.74 \pm 0.21\ \mathrm{mm}^{-1}$

$\mathrm{K}I_0 = 0.001598\ \mathrm{s}^{-1}$

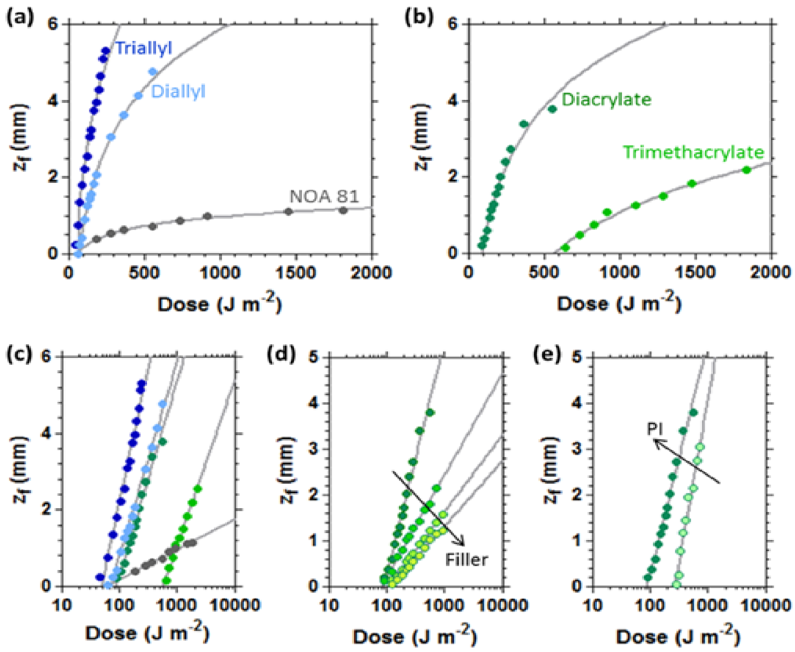
$\phi_C = 0.052 \pm 0.0021$

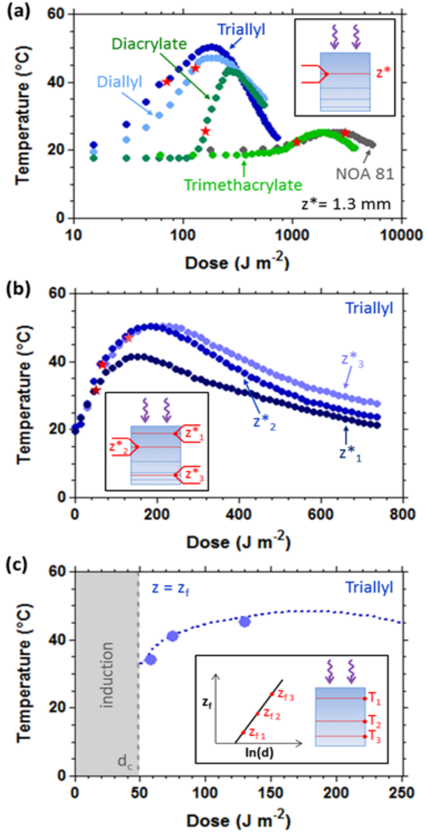


travelling frame

$$w = \left| \frac{\partial \phi(z_t(t), t)}{\partial z} \right|^{-1}$$

Thermal and mass diffusion





Vitale et al *Macromolecules* **48**, 198-205 (2015)

Thermal and mass diffusion

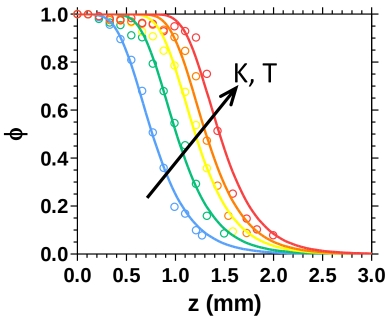
$$\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial z}\left(D(\phi)\frac{\partial \phi}{\partial z}\right) + K(T)(1-\phi)I$$

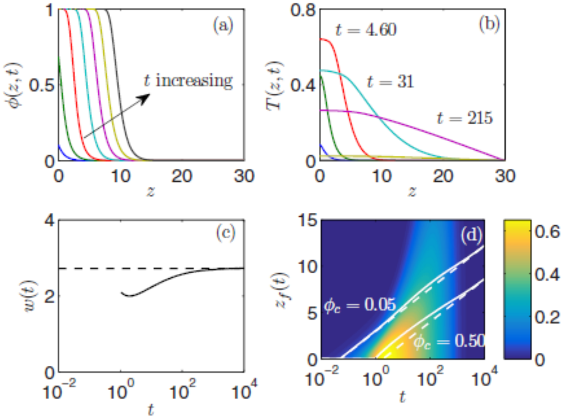
$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(k(T)\frac{\partial T}{\partial z}\right) + (\Delta H)\frac{\partial \phi}{\partial t}$$

$$\frac{\partial I}{\partial z} = -[\mu_\infty \phi + \mu_0(1-\phi)]I$$

$$K(T) = K_0 \exp\left(-\frac{E_a}{RT}\right)$$

ϕ conversion fraction, D diffusivity, K conversion rate, I light intensity, ρc_p volumetric heat capacity, k thermal conductivity, ΔH enthalpy of polymerization, μ_0 and μ_∞ initial and final absorption coefficients, E_a activation energy, R ideal gas constant, T temperature, z depth, t time

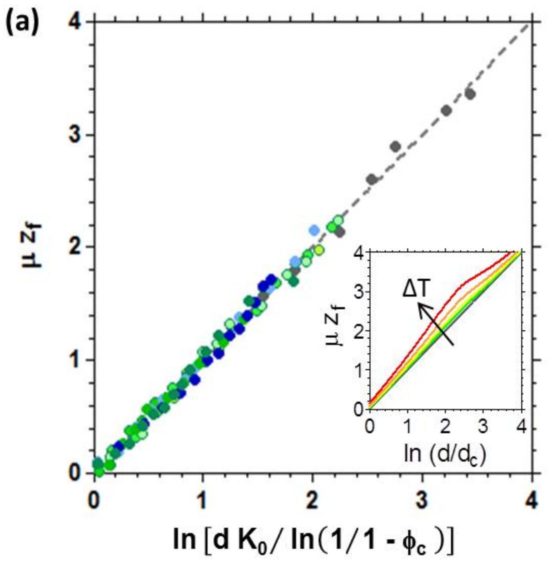


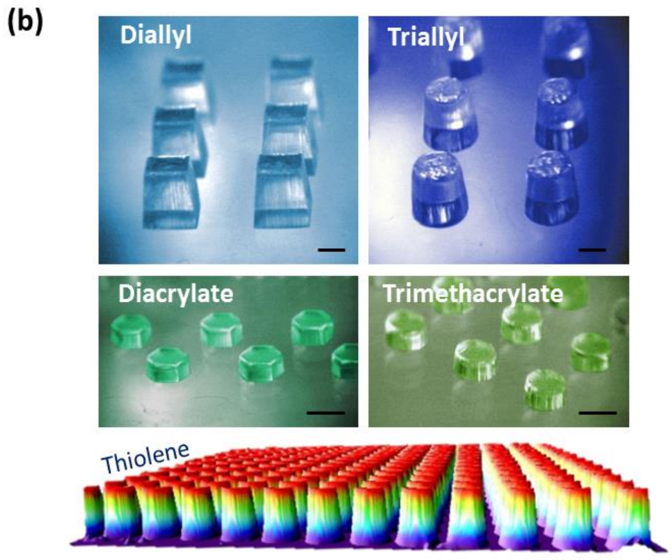


Hennessy et al PRE **91**, 062402 (2015); PRE **92**, 022403 (2015)

A unified FPP approach

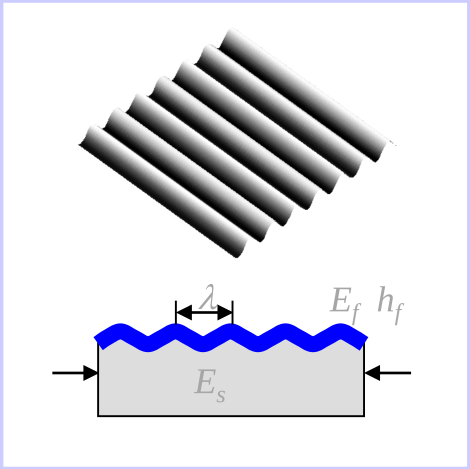
- photopolymerization conditions (irradiation time, incident light intensity)
- monomer chemistry (reactivity and diffusivity)
- temperature (both externally applied heat and heat generated by exothermic reactions)
- material absorbing properties





Adv. Mater. **27**, 6118–6124 (2015)

Mechanical instability of a bilayer



Deformation of the substrate disfavors wrinkling of long wavelengths and competes with bending to select an intermediate wavelength.

$$\lambda = 2\pi h_f \left(\frac{\bar{E}_f}{3\bar{E}_s} \right)^{1/3}$$

where $\bar{E}_x = \dfrac{E_x}{1-\nu_x^2}$

$$A = h_f \left(\frac{\varepsilon}{\varepsilon_c} - 1 \right)^{1/2}$$

: amplitude

where $\varepsilon_c = -\dfrac{1}{4}\left(\dfrac{3\bar{E}_s}{\bar{E}_f} \right)^{2/3}$: critical strain

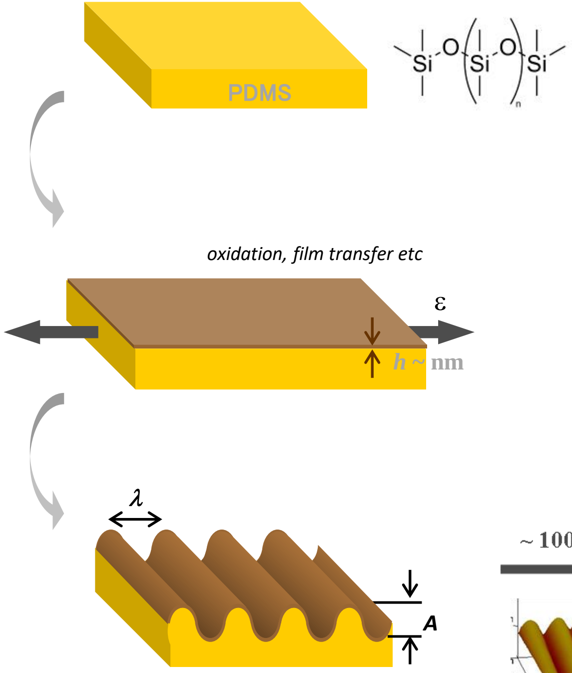
thick substrate ($h_s >> h_f$)

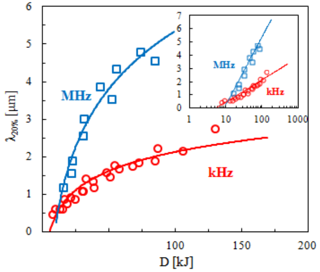
soft substrate ($E_s << E_f$)

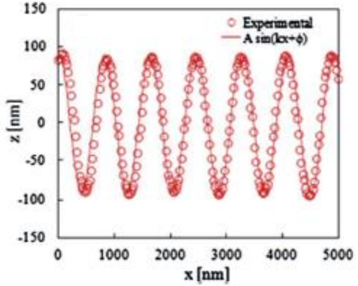
interface must be well-bonded (perfect adhesion, no slippage).

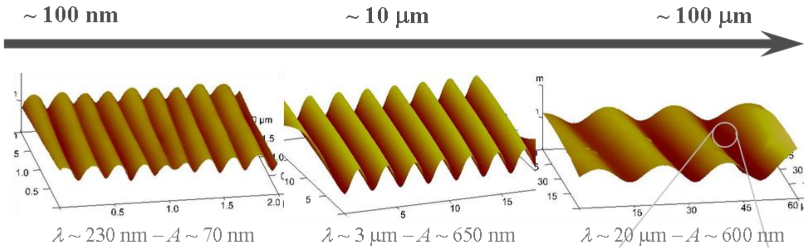
Mechanical instability of a bilayer

$$\lambda = 2\pi h_f \left(\frac{\bar{E}_f}{3\bar{E}_s} \right)^{1/3}$$

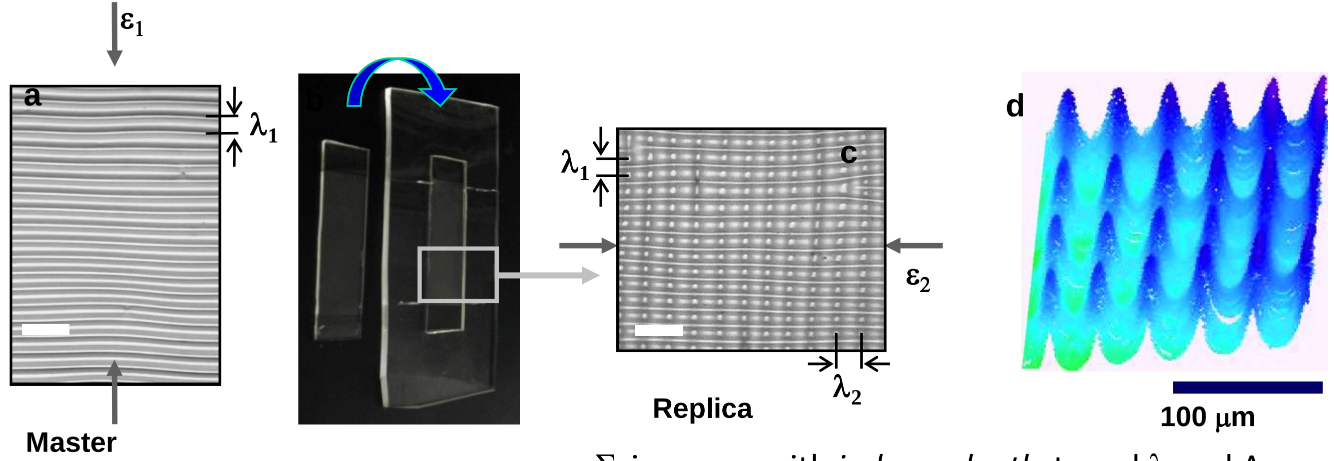




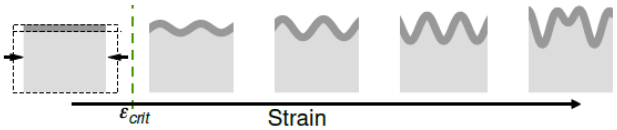


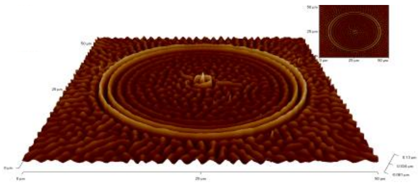


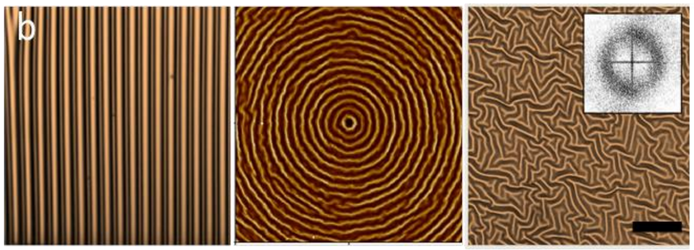
Multiaxial mechanical instabilities



Σsin waves with *independently* tuned λ and A

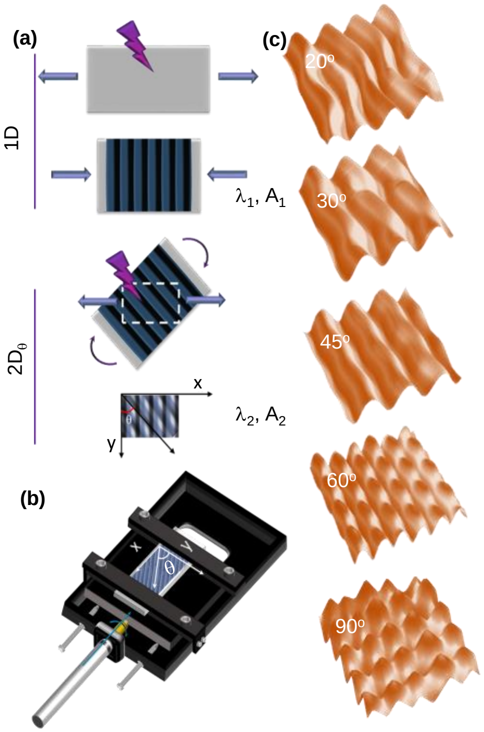


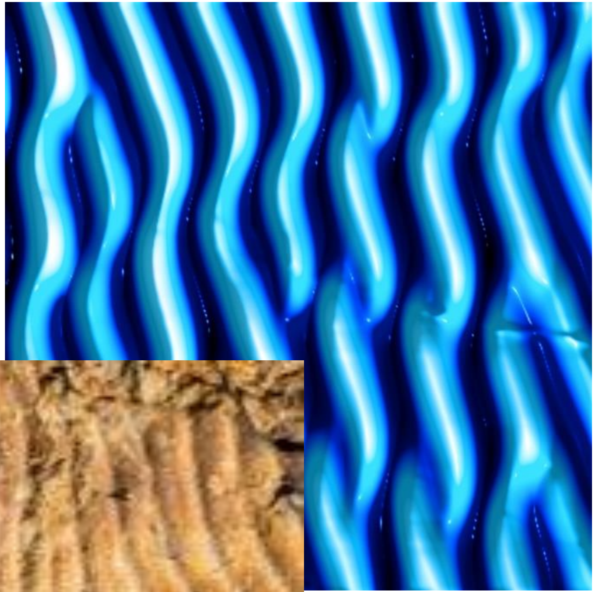




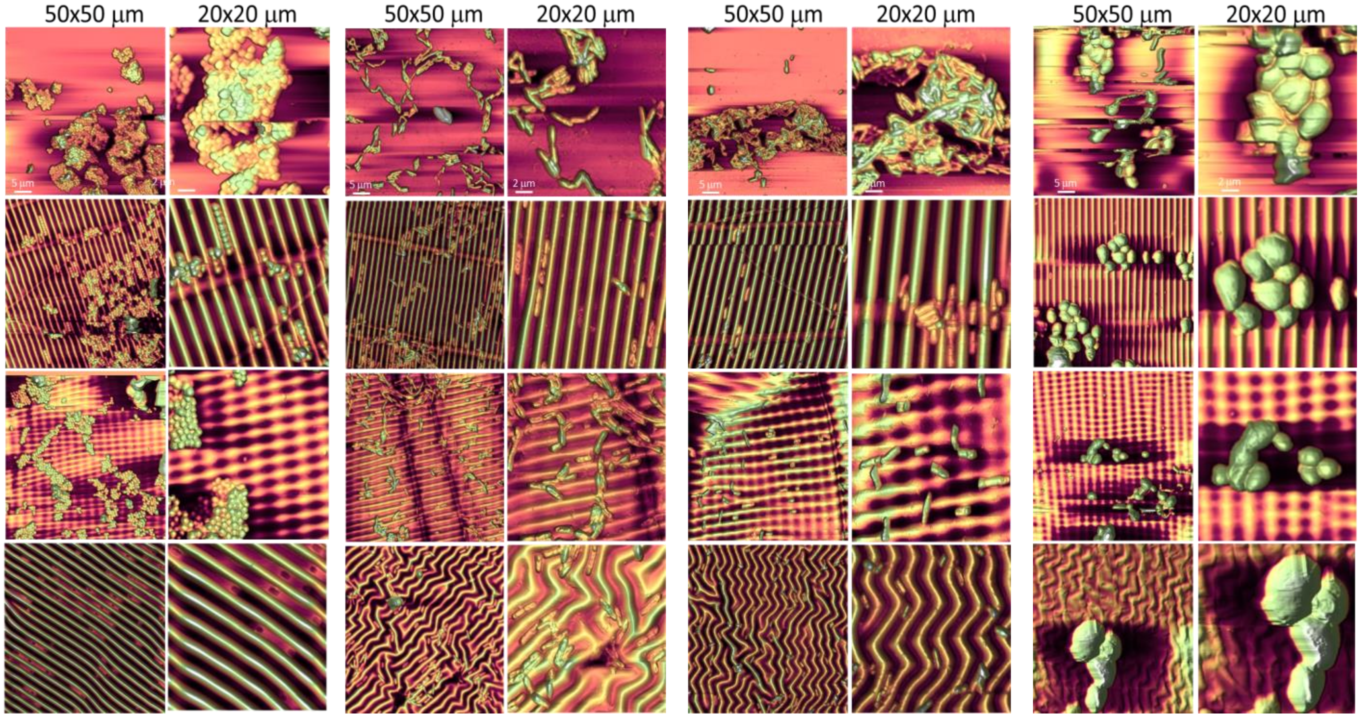
Soft Matter **4**, 2360 - 2364 (2008); **10**, 1155-1166 (2014); **11**, 3067-3075 (2015)

Fourier superposition... nearly

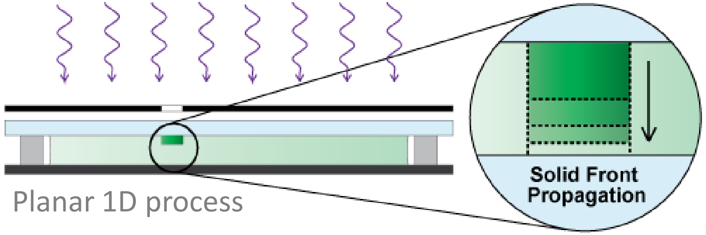


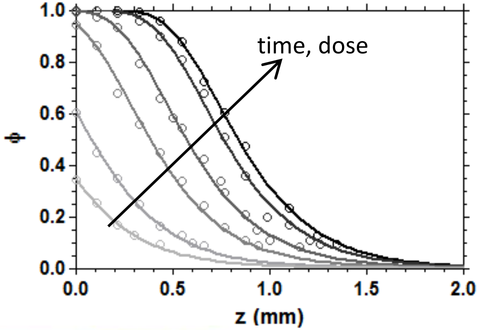


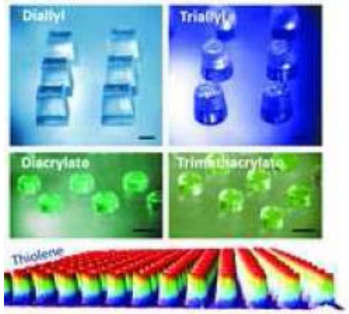
S. Aureus | P. Aeruginosa | E. Coli | C. Albicans



Summary: FPP1D and 3D







FPP1D

Spatio-temporal model

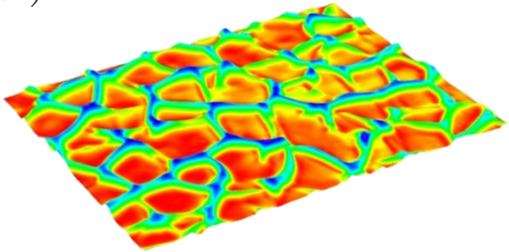
$$\frac{\partial \phi}{\partial t} = \frac{\partial}{\partial z}\left(D(\phi)\frac{\partial \phi}{\partial z}\right) + K(T)(1-\phi)I,$$

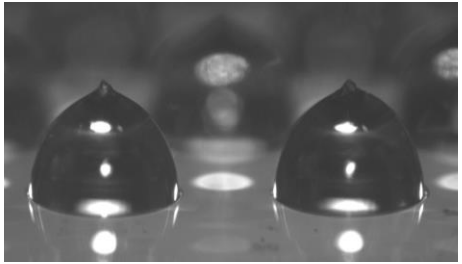
$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(k(T)\frac{\partial T}{\partial z}\right) + (\Delta H)\frac{\partial \phi}{\partial t},$$

$$\frac{\partial I}{\partial z} = -\left[\mu_\infty \phi + \mu_0(1-\phi)\right] I,$$

$$K(T) = K_0 \exp\left(-\frac{E_a}{RT}\right)$$

FPP3D





Thank you


Roisin O'Connell


Will Sharratt


Yutaka Aoki


Sepideh Khodaparast


Gunjan Tyagi

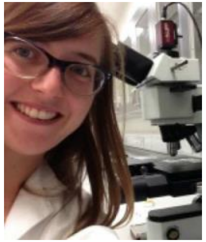

Marco Adamo


Christiana Udoh

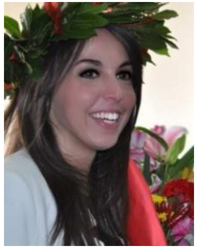

Carlos Gonzalez


Andreas Poulos


Haoyu Wang


Ale Vitale


Matt Hennessy


Manuela Nania

ROYAL ACADEMY OF ENGINEERING

NEUTRONS FOR SCIENCE® Institut Laue-Langevin

P&G

Castrol

THE ROYAL SOCIETY CELEBRATING 350 YEARS

bp

ACM EPSRC & SFI Centre for Doctoral Training in the Advanced Characterisation of Materials

ICAM International Centre for Advanced Materials

UKRI Engineering and Physical Sciences Research Council