Particle Coalescence (Sintering) in Polymer Processing and Beyond

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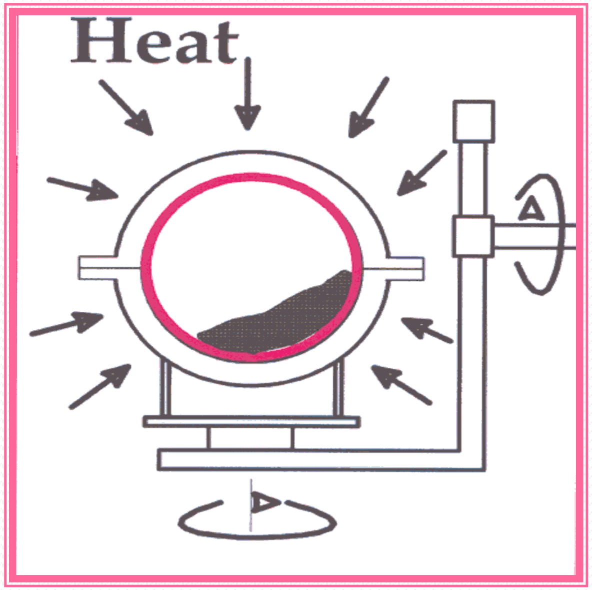
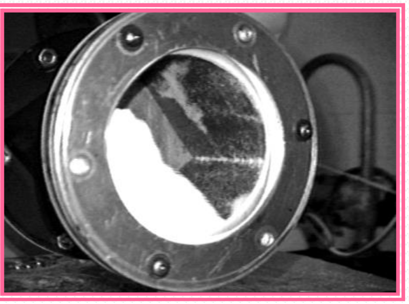
In honor of Zehev Tadmor
PPS2014, TEL AVIV, ISRAEL

ROTATIONAL MOLDING

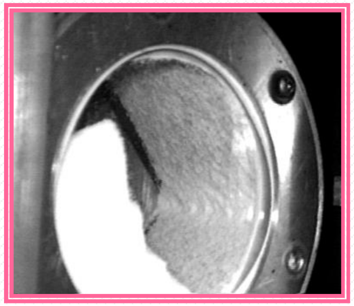


Virtually zero $\dot{\gamma}$, P

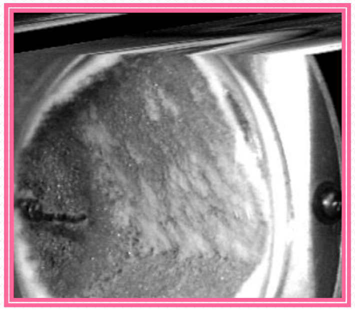
Induction



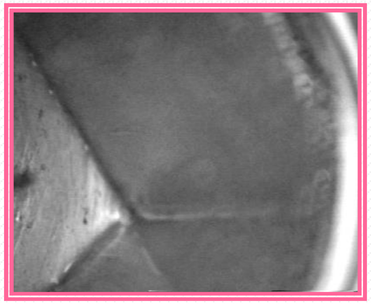
Adherence



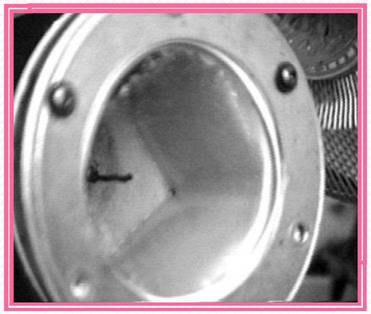
Coalescence

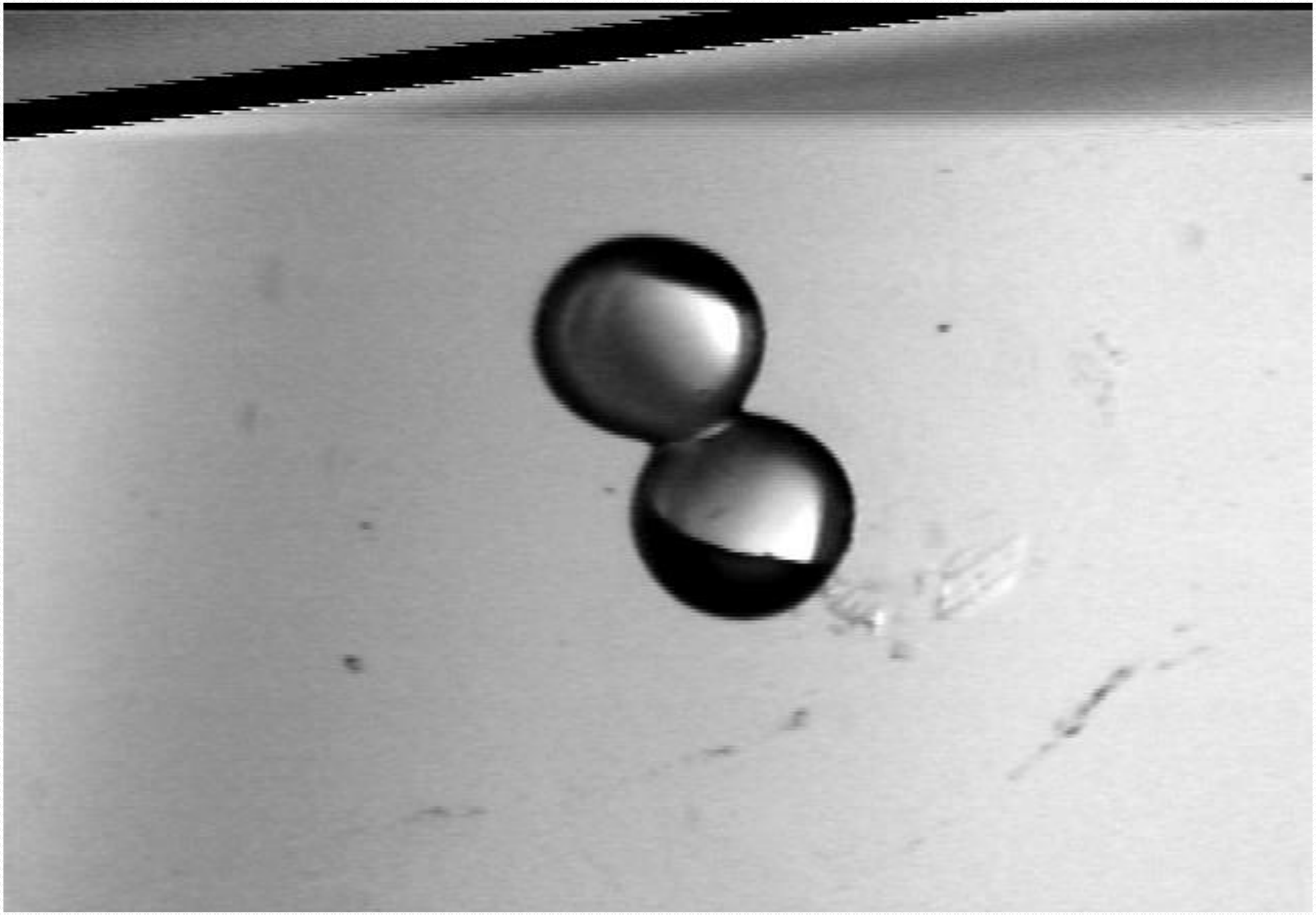


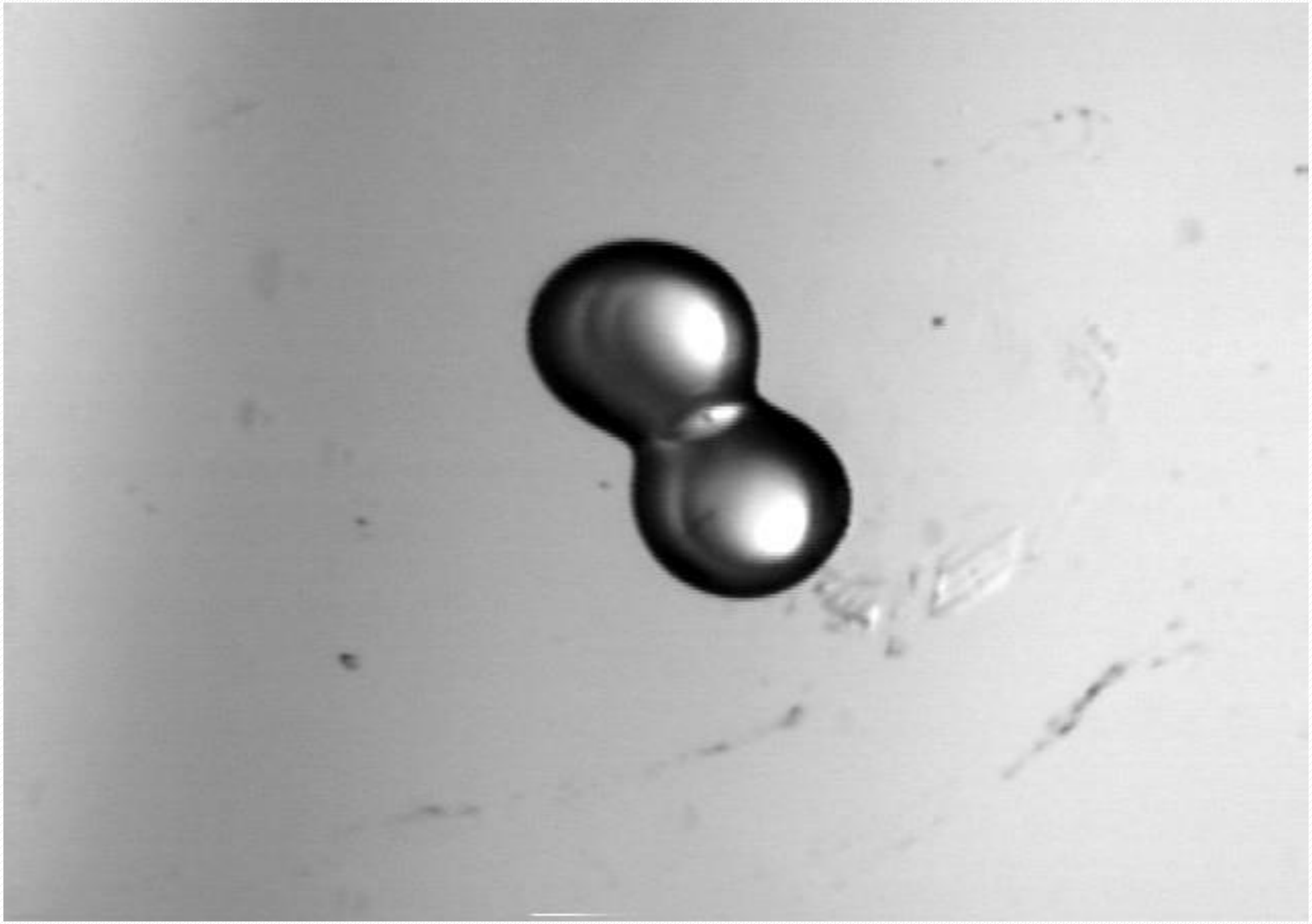
Densification

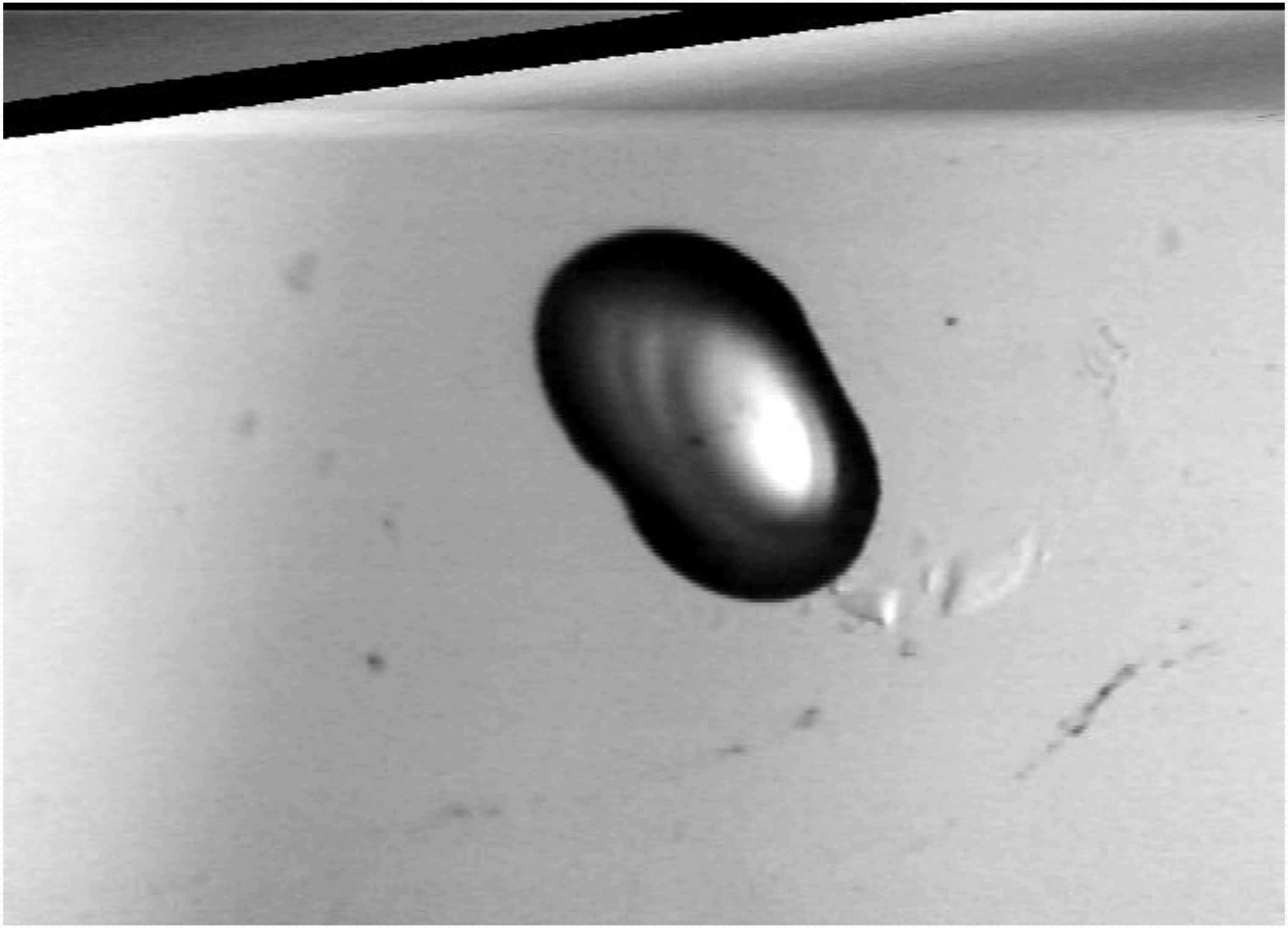


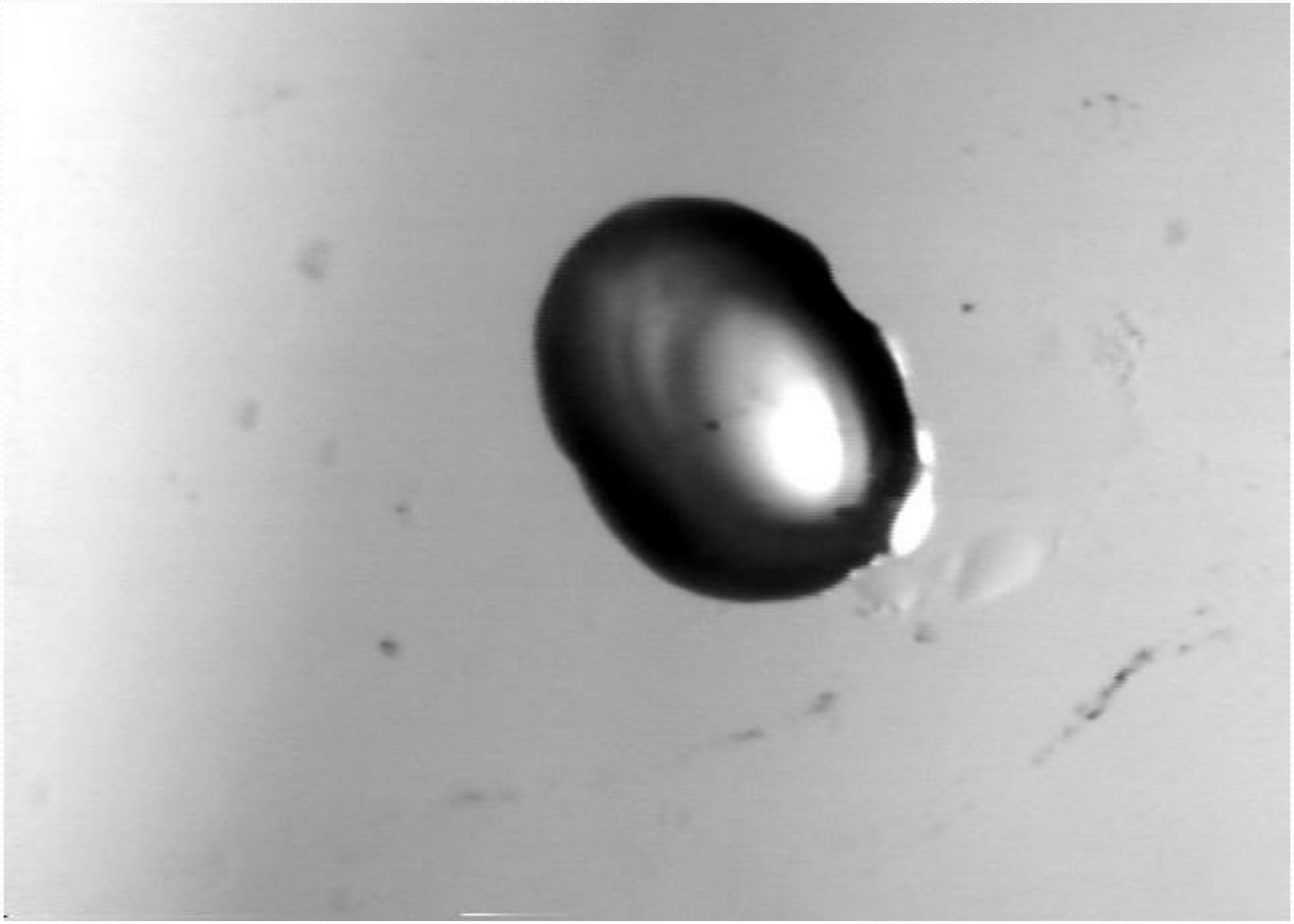
Cooling

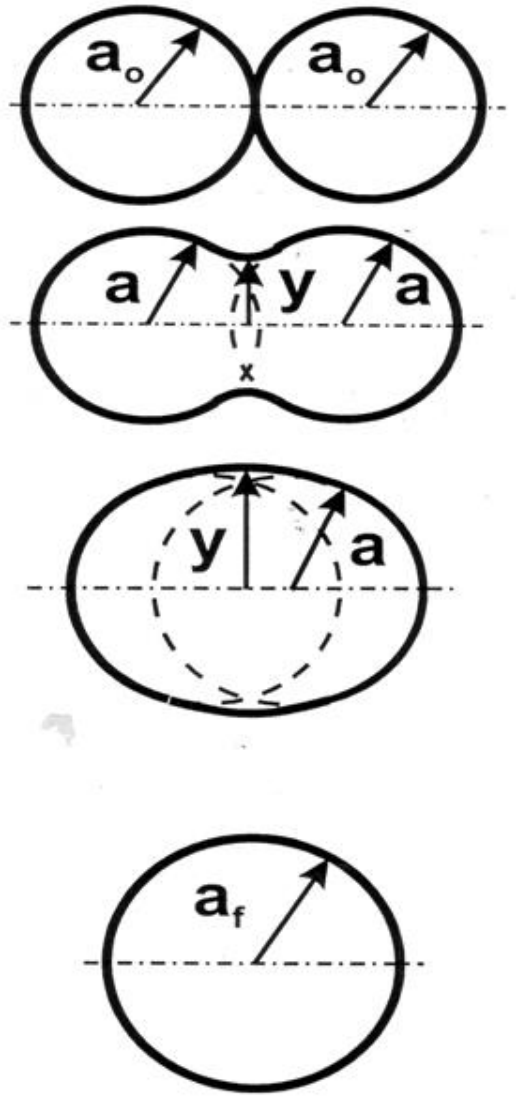








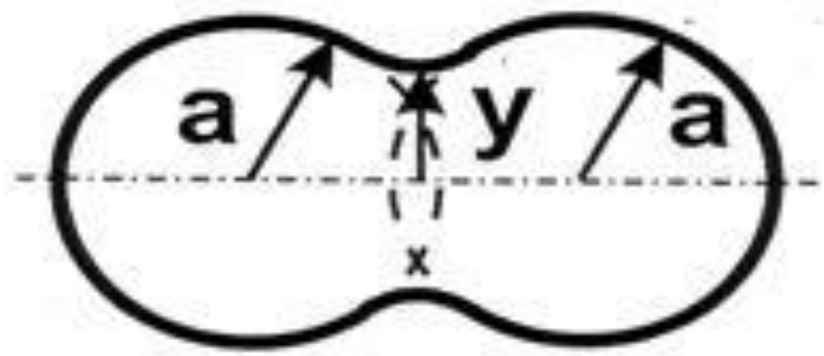




a_o
a_o
a
y
a
x
y
a
a_f

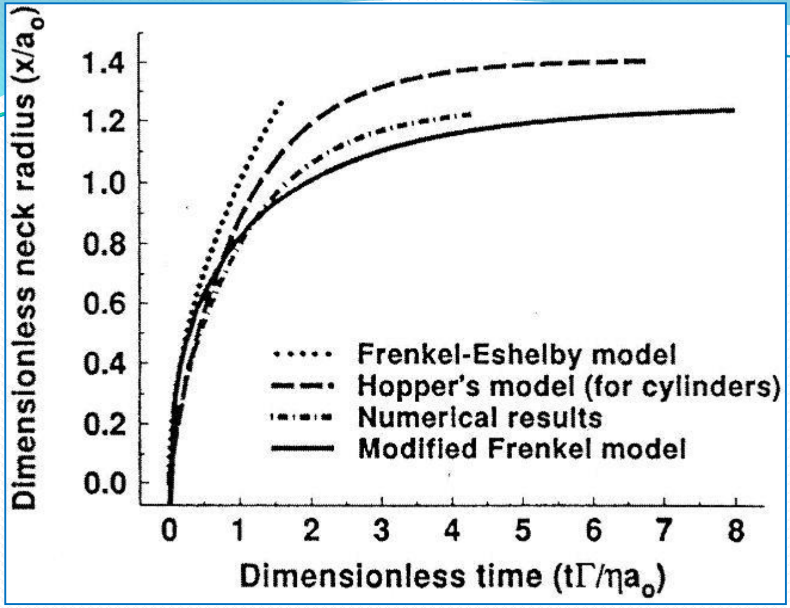
FRENKEL (1945) – ESHELBY corrected (1949) MODEL for the START of the process

$$\frac{y}{a} = \left(\frac{t\Gamma}{\eta a_o} \right)^{1/2}$$



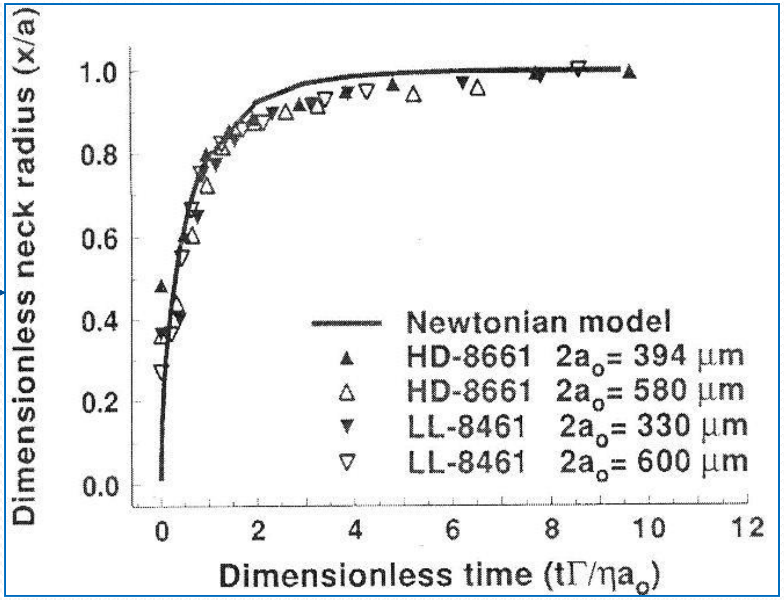
a= Particle radius
η = Viscosity
Γ = Surface tension

The model was developed by YAKOV ILICH FRENKEL (1894-1952). He was a brilliant theoretical physicist of the St. Petersburg Polytechnic Institute. His numerous contributions include defects in crystals (Frenkel defects), quantum theory of conductivity, cosmology, geophysics, geomagnetism, theory of vibrational - translational motion of molecules, fission of atomic nuclei, seismoelectric phenomena and more. He was given some recognition in Russia, but not the recognition he deserves around the world.

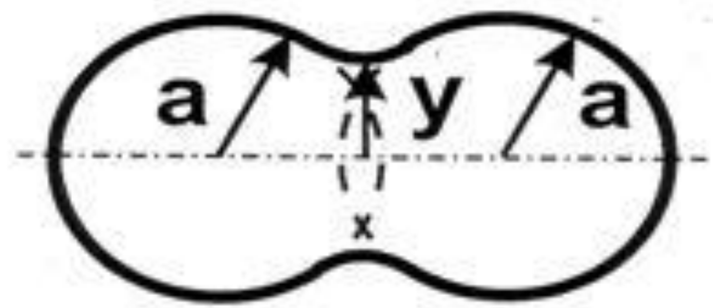


Model predictions by Polkluda , Bellehumeur and Vlachopoulos (1997), Frenkel – Eshelby (1949), Hopper (1984), and numerical results by Jagota and Dawson (1988).

Comparison of the modified Frenkel model predictions with experimental data obtained with rotational molding grade polyethylene resins (Bellehumeur et al. 1998).



$$\frac{y}{a} = \left(\frac{t\Gamma}{\eta a_o} \right)^{1/2}$$



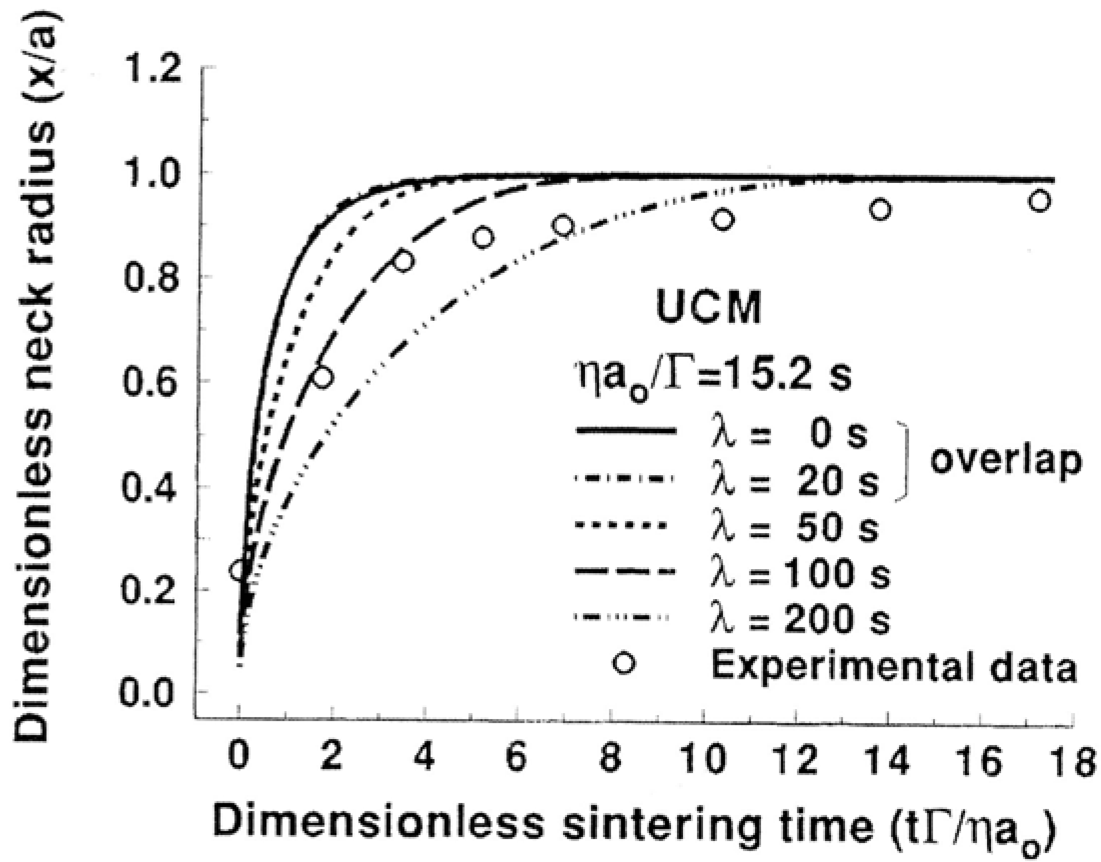
MODIFICATION OF FRENKEL'S MODEL (applicable for the start) TO COMPLETION (POKLUDA, BELLEHUMEUR, VLACHOPOULOS, AICHE J., 43, 3253 (1997))

$$a(t) = a_o \left(\frac{4}{(1+\cos(\theta(t)))^2 (2-\cos(\theta(t)))} \right)^{1/3}$$

$$\theta' = \frac{\Gamma}{\eta a_o} \frac{2^{-5/3} \cos(\theta)\sin(\theta)(2-\cos(\theta))^{1/3}}{(1-\cos(\theta))(1+\cos(\theta))^{1/3}}$$

$$\frac{y}{a} = \sin(\theta)$$

Upper Convected Maxwell quasi-steady-state



VISCOELASTIC MODELS

- **BELLEHUMEUR, KONTOPOULOU and VLACHOPOULOS (1998):** Quasi steady state Upper Convected Maxwell (UCM) explains qualitatively why more elastic resins coalesce SLOWER.

- **SCRIBBEN, BAIRD and WAPPEROM (2006):** Transient UCM predicts at short times INCREASE in coalescence rate.

VISCOELASTICITY

EXPERIMENTAL EVIDENCE:

- **MAZUR AND PLAZEK (1994):** resins with higher elasticity coalesce at a **FASTER RATE.**
- **MCMASTER group (1996-present):** resins with higher elasticity coalesce at a **SLOWER RATE.**
- **MULLER, BOUSMINA and MAAZOUZ (2008):** Elasticity **OPPOSES** coalescence.

Particle Coalescence (Sintering) In Polymer Processing (PP)

- ❑ Rotational Molding
- ❑ Powder Coating
- ❑ Selective Laser Sintering

Beyond PP

- ❑ Tissue Engineering

Selective Laser Sintering (SLS)

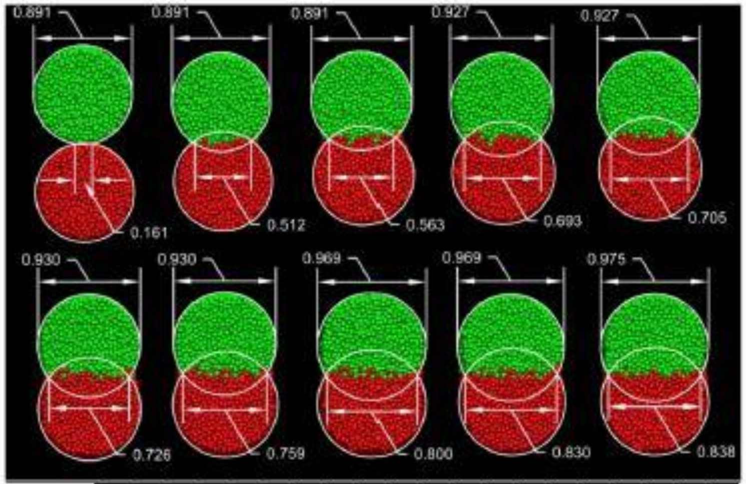
The objective is to built layer-by-layer using powdered materials, radiant heaters and a computer controlled laser.

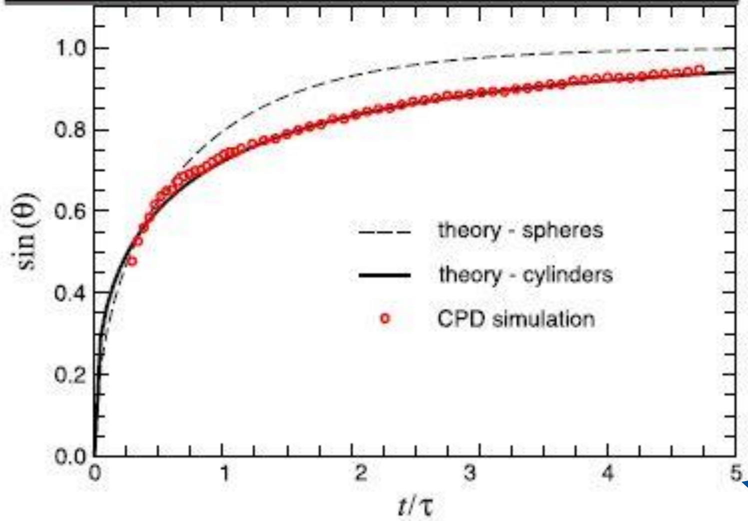
- **The starting point in modeling is Frenkel's model (1945) correction by Eshelby (1949) (for the initial stage sintering).**
- **Extension to completion with the help of my coworkers Pokluda, Bellehumeur and Kontopoulou (1997, 1998).**

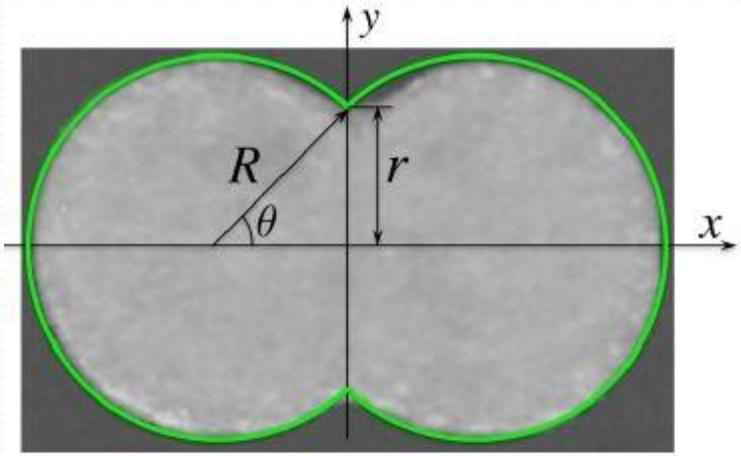
- **Tissue Engineering** aims at building functional tissues to improve or replace damaged ones.

- Modeling is based on Cellular Particle Dynamics (CPD) for prediction of shape evolution of multicellular systems that undergo shape-changing biomechanical relaxation (I. Kosztin et al, Rev. Mod. Phys. 84 1791, 2012).

Starting point is aggregate fusion







about 70 hours for Chinese hamster ovary cells, according to Kosztin et al (2012)

The centrality of Frenkel's model and its subsequent correction and extension is very well established in diverse areas of engineering.

This presentation would not have been possible without the efforts of my past and present coworkers:

- E. Soos Takács
- Dr. M. Emami
- A. Tinson
- D. D’Agostino
- D. Annechini
- Dr. M. Kontopoulou
- Dr. C.T. Bellehumeur
- Dr. M. Bisaria

THANK YOU

Q & A