

Nucleation kinetics in closed systems

COST Action CM1402: From molecules to crystals – how do organic molecules form crystals?

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1 Introduction

2 Standard nucleation model

- Kinetic equations
- Work of formation of clusters

3 Selected Applications

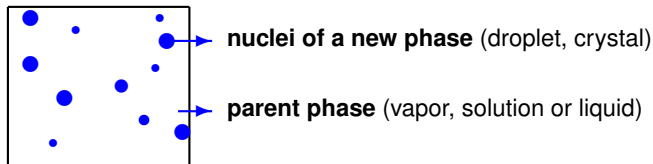
- Homogeneous nucleation
- Heterogeneous nucleation on active centers

4 Summary

Introduction

Nucleation

- process leading to the formation of a new phase (solid, liquid) within metastable original phase (undercooled melt, supersaturated vapor or solution)
- first step in crystallization process; plays a decisive role in determining the crystal structure and the size distribution of nuclei



- **homogeneous nucleation (HON)**
(at random sites in the bulk of a parent phase)
- **heterogeneous nucleation (HEN)**
(on foreign substrate, impurities, defects, active centres)

nucleus: ? the smallest observable “particle” ? (often $\approx 1\mu m$)

Clusters of a new phase are formed on **nucleation sites** due to fluctuations and after overcoming some critical size ($< 1\text{ nm}$) become **nuclei** (overcritical clusters).

Introduction

Critical supersaturation

Experimental data: H.R. Pruppacher: *A new look at homogeneous ice nucleation in supercooled water drops*, J. Atmospheric Sciences 52(11) (1995) 1924.

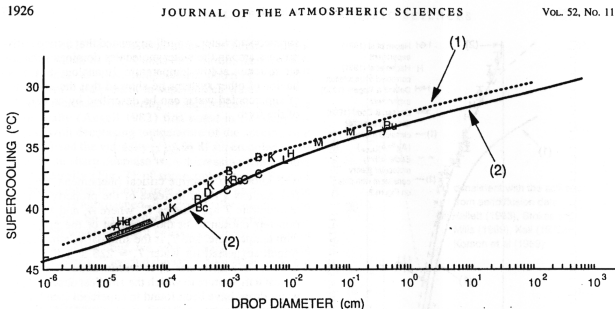


FIG. 2. Lowest temperatures at which extrapure water drops of given size and exposed to cooling rates between $1^{\circ}\text{C min}^{-1}$ and 1°C s^{-1} have been supercooled during laboratory experiments: H (Hoffer 1961), M (Mossop 1955), D (DeMott and Rogers 1990), B (Bigg 1953), P (Pruppacher and Neuberger 1963), L (Langham and Mason 1958), Ha (Hagen et al. 1981), Ru (Rouleau 1958), K (Kuhns and Mason 1968), Y (Bayardelle 1954), R (Rasmussen 1982), A (Anderson et al. 1980), Bs (Butorin and Skripov 1972), and Bc (Broto and Clause 1976). Lines 1 and 2: Temperature at which 99.99% of a population of uniform-sized water drops freezes when exposed to cooling rates of $1^{\circ}\text{C min}^{-1}$ and 1°C s^{-1} , respectively [from Eq. (7) with J values consistent with curve 2 in Fig. 3].

Supersaturation (supercooling) increases with volume decrease.

⇒ nucleation kinetics in confined volumes

Standard nucleation model

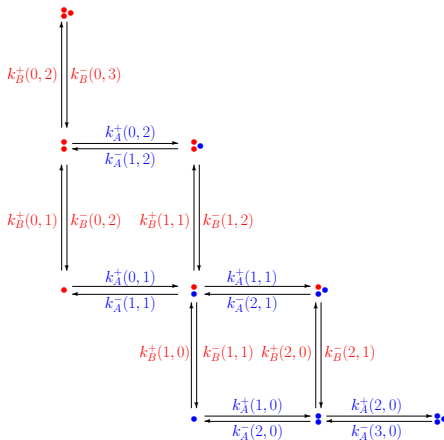
UNARY NUCLEATION

(single component system of a new phase)



BINARY NUCLEATION

(A, B components)



Standard nucleation model

Kinetic equations

k_i^+ (k_i^-) – attachment (detachment) frequencies of molecules

$$\frac{dF_i}{dt} = k_{i-1}^+ F_{i-1} - [k_i^+ + k_i^-] F_i + k_{i+1}^- F_{i+1} = J_{i-1}(t) - J_i(t) \quad (1)$$

$$J_i(t) = k_i^+ F_i(t) - k_{i+1}^- F_{i+1}(t) \quad (2)$$

F_i – number density of clusters of size i

J_i – cluster flux density (**nucleation rate** for i^*)

k_i^+ (k_i^-) – attachment (detachment) frequencies

Total number of nuclei greater than m : $Z_m(t) = \sum_{i>m} F_i(t) = \int_0^t J_m(t') dt'$

Local equilibrium:

$$J_i = 0 \Rightarrow k_i^+ F_i^0 = k_{i+1}^- F_{i+1}^0 \Rightarrow k_{i+1}^- = k_i^+ \frac{F_i^0}{F_{i+1}^0} = k_i^+ \exp\left(\frac{W_{i+1} - W_i}{k_B T}\right) \quad (3)$$

Kinetic equations

Equilibrium

$$J_i = 0 \Rightarrow k_i^+ F_i^0 = k_{i+1}^- F_{i+1}^0 \quad (4)$$

$$\Rightarrow F_i^0 = F_1^0 \frac{k_1^+ k_2^+ k_3^+ \dots k_{i-1}^+}{k_2^- k_3^- k_4^- \dots k_i^-}$$

F_i^0 – equilibrium number of cluster formed by i molecules It can be shown that

$$F_i^0 = B_2 \exp\left(-\frac{W_i}{kT}\right)$$

Homogeneous nucleation, self-consistent model: $B_2 = N_1 \exp\left(\frac{W_1}{kT}\right)$

N_1 – number of molecules within parent phase

Knowing F_i^0 and $k_i^+ \Rightarrow k_i^-$ from Eq. (4).

Standard nucleation model

Classical nucleation theory (CNT)

Initial and boundary conditions

N_1 - number of molecules (number of nucleation sites)

$$F_1(t=0) = N_1, \quad F_{i>1}(t=0) = 0$$

$$F_1(t) = N_1$$

CNT

$t \gg$ induction time \Rightarrow

Stationary nucleation (steady-state): $J_i(t) = J^S = \text{const.}$

$$J^S = \left(\sum_{i=1}^{\infty} \frac{1}{k_i^+ F_i^0} \right)^{-1} \quad \text{exact analytical formula}$$

$$J^S = k_{j^*}^+ z F_{j^*}^0, \quad \text{where Zeldovich factor: } z = \sqrt{\frac{1}{2\pi kT} \left(-\frac{d^2 W_i}{di^2} \right)_{i=j^*}}$$

$$F_i^0 = B \exp\left(-\frac{W_i}{kT}\right); \quad B = N_1 \exp\left(\frac{W_1}{kT}\right)$$

k_i^+ , $W_i = ?$; small clusters?

Standard nucleation model

Stationary nucleation (steady-state)

$J_i = J^S = \text{const.}$ for any cluster size i ($N_1 = \text{const.}!$) \Rightarrow

Boundary conditions:

$$F_i^S \rightarrow F_i^0 \quad \text{for } i \rightarrow 1; \quad F_i^S \rightarrow 0 \quad \text{for } i \rightarrow \infty$$

$$J^S = k_i^+ F_i^S - k_{i+1}^- F_{i+1}^S$$

Standard nucleation model

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$$\sum_{i=1}^{M-1} \frac{J^S}{k_i^+ F_i^0}$$

Standard nucleation model

Stationary nucleation (steady-state)

$J_i = J^S = \text{const.}$ for any cluster size i ($N_1 = \text{const.!$) \Rightarrow

Boundary conditions:

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$$\sum_{i=1}^{M-1} \frac{J^S}{k_i^+ F_i^0} = \left(\frac{F_1^S}{F_1^0} - \frac{F_2^S}{F_2^0} \right) + \left(\frac{F_2^S}{F_2^0} - \frac{F_3^S}{F_3^0} \right) + \left(\frac{F_3^S}{F_3^0} - \frac{F_4^S}{F_4^0} \right) + \dots$$

Standard nucleation model

Stationary nucleation (steady-state)

$J_i = J^S = \text{const.}$ for any cluster size i ($N_1 = \text{const.!$) \Rightarrow

Boundary conditions:

$$F_i^S \rightarrow F_i^0 \quad \text{for } i \rightarrow 1; \quad F_i^S \rightarrow 0 \quad \text{for } i \rightarrow \infty$$

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$$\sum_{i=1}^{M-1} \frac{J^S}{k_i^+ F_i^0} = \left(\frac{F_1^S}{F_1^0} - \frac{F_2^S}{F_2^0} \right) + \left(\frac{F_2^S}{F_2^0} - \frac{F_3^S}{F_3^0} \right) + \left(\frac{F_3^S}{F_3^0} - \frac{F_4^S}{F_4^0} \right) + \dots = 1 + \frac{F_M^S}{F_M^0} \rightarrow 1$$

for $M \rightarrow \infty$

Standard nucleation model

Stationary nucleation (steady-state)

$J_i = J^S = \text{const.}$ for any cluster size i ($N_i = \text{const.}!$) \Rightarrow

Boundary conditions:

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$$\sum_{i=1}^{M-1} \frac{J^S}{k_i^+ F_i^0} = \left(\frac{F_1^S}{F_1^0} - \frac{F_2^S}{F_2^0} \right) + \left(\frac{F_2^S}{F_2^0} - \frac{F_3^S}{F_3^0} \right) + \left(\frac{F_3^S}{F_3^0} - \frac{F_4^S}{F_4^0} \right) + \dots = 1 + \frac{F_M^S}{F_M^0} \rightarrow 1$$

for $M \rightarrow \infty$

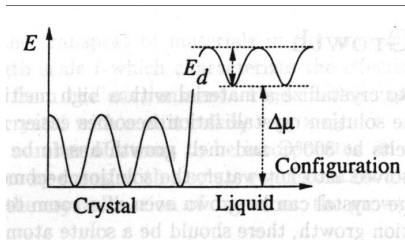
$$J^S = \left(\sum_{i=1}^{\infty} \frac{1}{k_i^+ F_i^0} \right)^{-1} \quad \text{exact analytical formula}$$

Standard nucleation model

k_i^+ - attachment frequency

k_i^- follows from the principle of local equilibrium (3)

Crystal nucleation



Crystal phase corresponds a stable phase, liquid a metastable phase, and in between is the diffusion activation energy.

From: Yukio Saito, *Statistical Physics of Crystal Growth*, Word Scientific (1996).

$$k_i^+ = R_D A_i \exp\left(-\frac{E_D}{kT}\right) \exp\left(-\frac{q(W_{i+1} - W_i)}{kT}\right); \quad q = 0.5[1 + \text{sign}(W_{i+1} - W_i)]$$

$A_i = \gamma i^{2/3} = 4\pi r^2$ - surface area

R_D - mean number of molecules striking on unit nucleus surface

Standard nucleation model

k_i^+ - attachment frequency

Vapor \rightarrow crystal

$$R_D = \frac{P}{\sqrt{2\pi m_1 kT}} \quad (\text{deposition rate}); \quad P - \text{vapor pressure}; \quad m_1 - \text{molecular mass}$$

Melt \rightarrow crystal (unary parent phase)

D. Turnbull, J. Fisher, *Rate of nucleation in condensed systems*, J. Chem. Phys. 17 (1949) 145.

$$R_D = N_S \left(\frac{kT}{h} \right); \quad N_S = \rho_S A_i$$

N_S – number of nucleation sites on the nucleus surface; ρ_S – surface density of molecules

Solution \rightarrow crystal

HON: (A) Direct-impingement control / (B) Volume-diffusion control

$$R_D = CN_S \left(\frac{kT}{h} \right); \quad C - \text{concentration}; \quad (\text{A}) \text{ nucleation kinetics is restrictive}$$

R_D – incoming diffusion flux of monomers; (B) HON is controlled by volume diffusion

Standard nucleation model

Work of formation of clusters

Formation of phase interface is energetically disadvantageous

Homogeneous nucleation:

Capillarity approximation

$$W_i = -i\Delta\mu + \underbrace{\gamma i^{2/3}\sigma}_{W^S} = -\frac{\frac{4}{3}\pi r^3}{v_1}\Delta\mu + 4\pi r^2\sigma$$

$W^S = \sum_k A_k \sigma_k$ – surface energy

i – cluster size (number of molecules within cluster)

r – cluster radius; σ – interfacial energy; v_1 – molecular volume

$\Delta\mu$ – difference of chemical potentials

A_k – surface areas; σ_k – corresponding interfacial energies

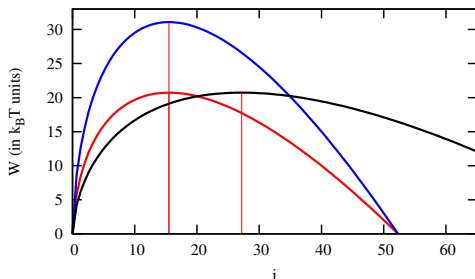
$$V_{n\varrho} = im_1 \Rightarrow r(i)$$

V_n - nucleus volume; ϱ – density of crystal phase; m_1 – molecular mass

Standard nucleation model

Work of formation of clusters

Homogeneous nucleation



$$\frac{\partial W_i}{\partial i} = 0 \quad \Rightarrow \quad i^* = \left(\frac{2\gamma\sigma}{3\Delta\mu} \right)^3; \quad i^* - \text{critical size}; \quad W^* = W_{i^*} - \text{nucleation barrier}$$

$$\text{melt} \rightarrow \text{crystal}: \Delta\mu = \frac{\Delta h_E}{N_A T_E} (T_E - T)$$

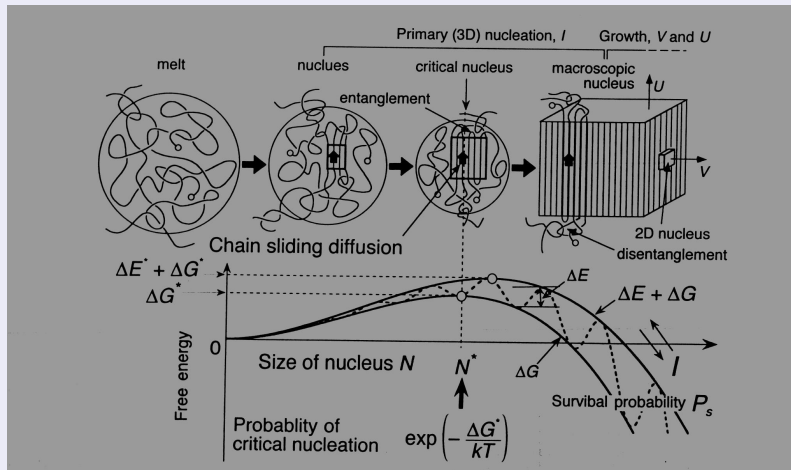
$$\text{solution} \rightarrow \text{crystal}: \Delta\mu = k_B T \ln S$$

Δh_E – heat of fusion; N_A – Avogadro constant; T_E – equilibrium temperature; T – temperature
 k_B – Boltzmann constant; S – supersaturation;

Standard nucleation model

Work of formation of clusters

Nucleation in polymer systems: thermodynamic aspects



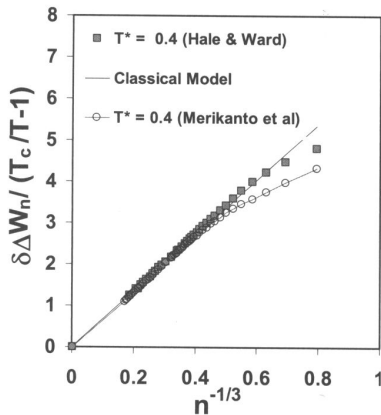
M. Nishi et al., Polymer Journal 31 (1999) 749.

Standard nucleation model

Classical nucleation theory

Classical nucleation theory (CNT): fails to explain exp. data ($W_i = ??$)

Argon Lennard-Jones nucleation – MC simulations



$$\delta\Delta W_n = W_n - W_{n-1}$$

\Rightarrow Down to very small cluster sizes, classical nucleation theory built on the liquid drop model can be used very **accurately** to describe the work required to add a monomer to the cluster!

However, erroneous absolute value for the cluster work of formation, W_i .

B. Hale, G. Wilemski, 18th ICNAA conference (2009) 593.

J. Merikanto et al., PRL 98 (2007) 145702.

Standard nucleation model

Confined systems

Initial and boundary conditions

$$F_i(t=0) = F_i^0 \quad \text{pro } i \leq i_0 \quad (\text{usually } i_0 \approx i^*/2)$$

F_i^0 - equilibrium distribution of nuclei

$$F_i(t=0) = 0 \quad \text{pro } i > i_0$$

$$F_1(t) = F_1^0 = N_n = \text{const.}$$

N_n - number of nucleation sites ($N_n = N_1$ for HON)

CNT model (HON+HEN)

$$N_n \gg \sum_{i>1} iF_i$$

Standard nucleation model

Confined systems

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N_n - number of nucleation sites ($N_n = N_1$ for HON)

CNT model (HON+HEN)

$$N_n \gg \sum_{i>1} iF_i$$

$$F_1(t) = N_1(t=0) - \sum_{i>1} iF_i(t)$$

confined system (HON)

$$F_1(t) = N_n(t=0) - \underbrace{\sum_{i>1} N_i^s(t)}$$

confined system (HEN)

free substrate surface ↓

number of nucleation sites occupied by nuclei

$$N_1(t) = N_T - \sum_{i>1} iF_i(t)$$

confined system (HEN)

volume of parent phase ↓

N_1 - number of molecules within parent phase

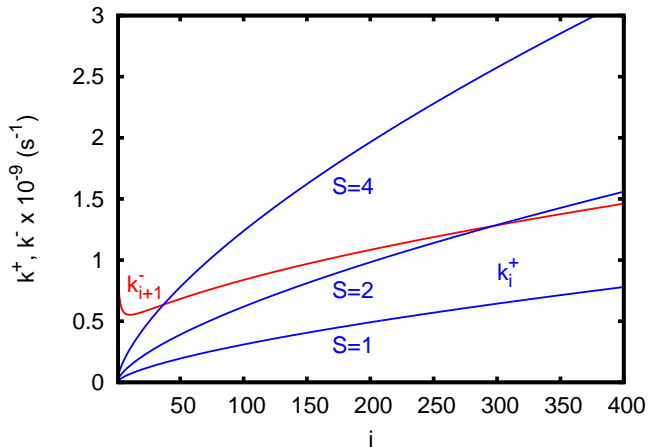
N_T - total number of molecules within system (liquid + solid phase)

Selected Applications

Homogeneous nucleation

HON: ethanol, V→L transition (T = 260 K)

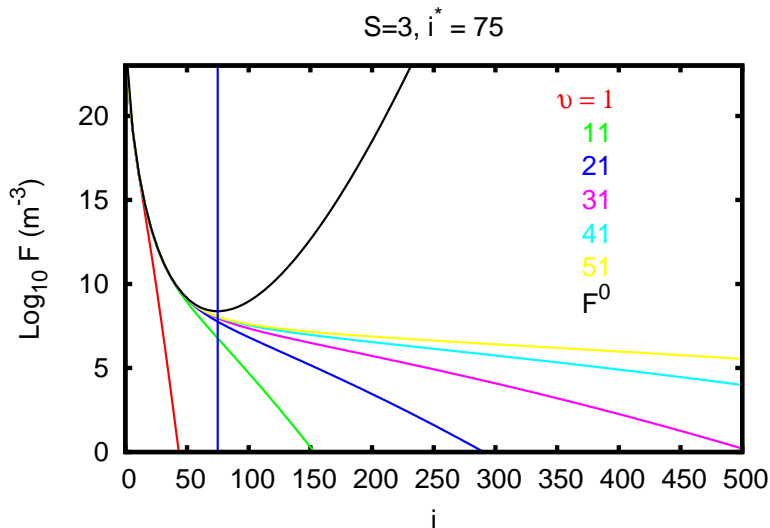
[Z. Kožíšek et al., J. Chem. Phys. 125 (2006) 114504]



Selected Applications

Homogeneous nucleation

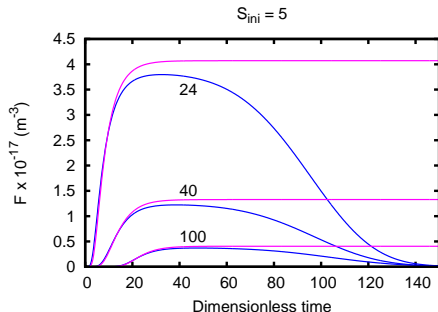
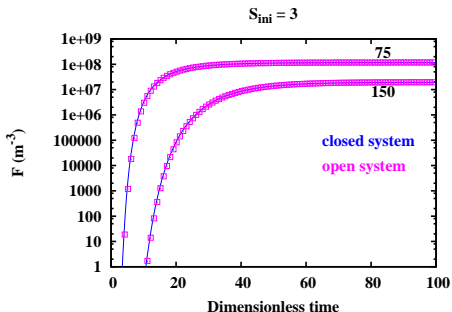
Size distribution of nuclei



Selected Applications

Homogeneous nucleation

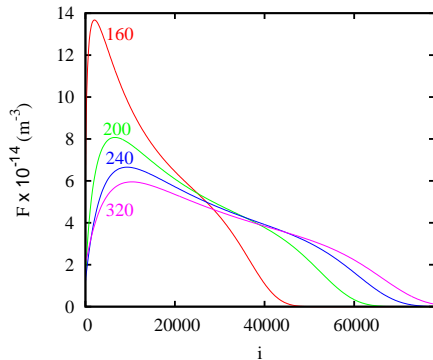
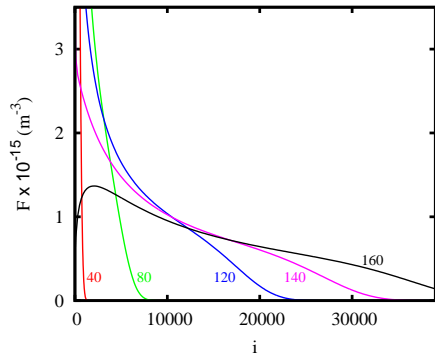
Distribution function - time dependence



Selected Applications

Homogeneous nucleation

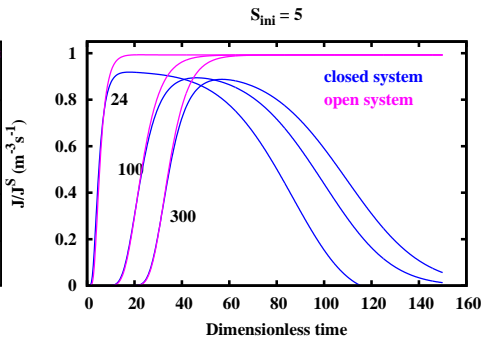
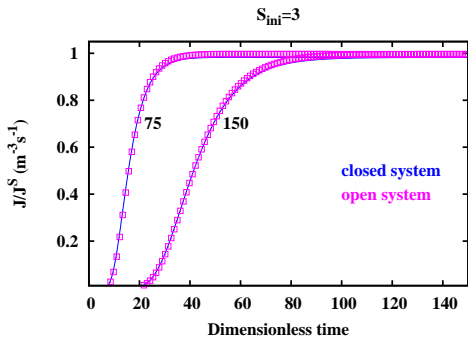
Distribution function - size dependence ($S_{ini} = 5$)



Selected Applications

Homogeneous nucleation

Nucleation rate - time dependence

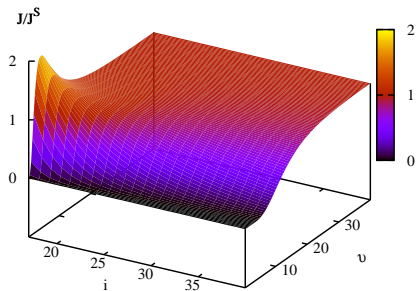


Selected Applications

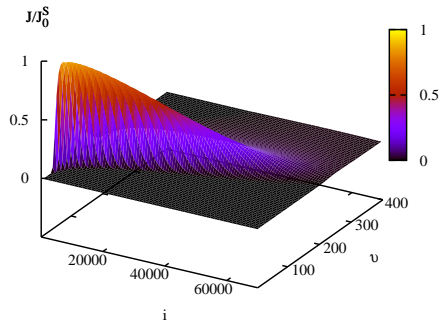
Homogeneous nucleation

Nucleation rate ($S_{ini} = 5, J_0^S = J^S$ at S_{ini})

Open system ($S_{ini} = const.$)



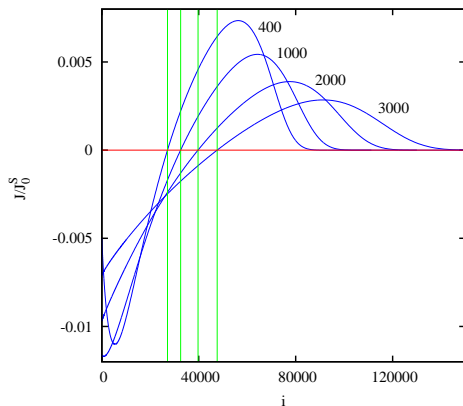
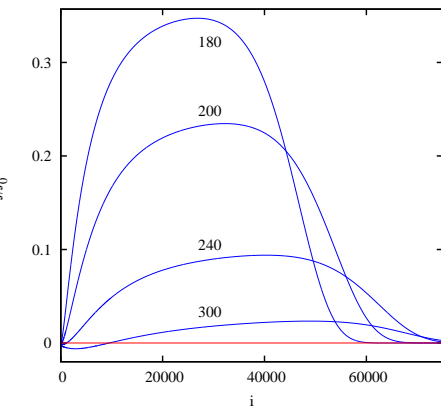
Closed system



Selected Applications

Homogeneous nucleation

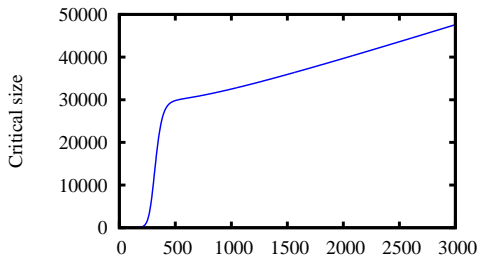
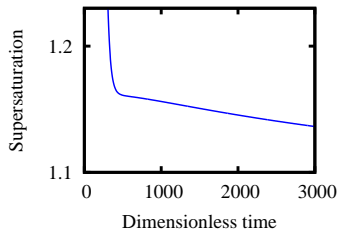
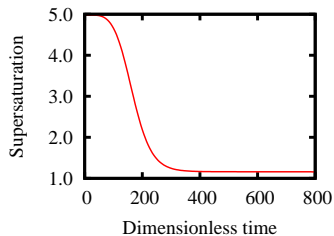
Nucleation rate ($S_{ini} = 5$)



Selected Applications

Homogeneous nucleation

Supersaturation



Selected Applications

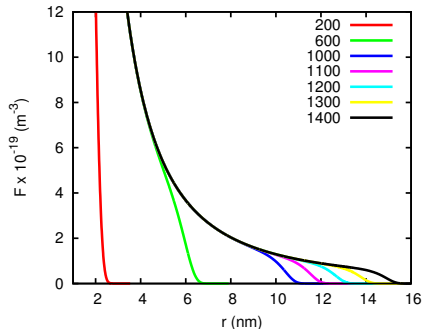
Homogeneous nucleation

HON: Liquid/Solution → Solid transition

Z. Kožíšek, CrystEngComm 15 (2013) 2269

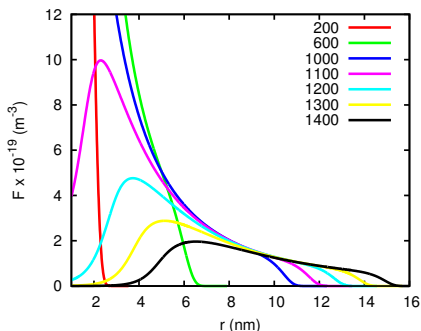
Size distribution of nuclei

CNT



$N_1(t) = \text{const.}$

Encapsulated system



N_1 decreases with time

Selected Applications

Homogeneous nucleation

Model system: nucleation of Ni melt

DSC experiments and MC simulations [J. Bokeloh et al., PRL 107 (2011) 145701
J. Bokeloh et al., Eur. Phys. J. Special Topics 223 (2014) 511]

J was obtained from a statistical evaluation of crystallization behavior during continuous cooling.
A single Ni sample was repeatedly heated up to 1773 K and subsequently cooled down to 1373 K.

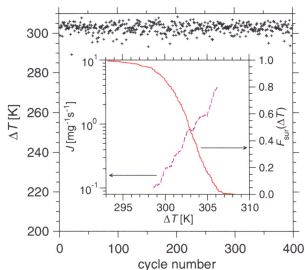


FIG. 1 (color online). Undercooling ΔT , as measured from 400 cycles of a 0.23 mg sample. The inset shows the survivorship function $F_{sur}(\Delta T)$ (right y axis) and nucleation rate J (left y axis).

sample masses: 23 μg – 63 mg

survivorship function:

$$F_{sur}(\Delta T) = 1 - \exp\left(-\int J(\Delta T) dt\right)$$

$$\Delta T \Rightarrow J = \Gamma \exp\left(-\frac{\Delta W^*}{k_B T}\right)$$

- **MC simulations** show a deviation of the energy of formation ΔW_i from **CNT**.
- However, the actual height of the energy barrier is in good agreement with **CNT**.

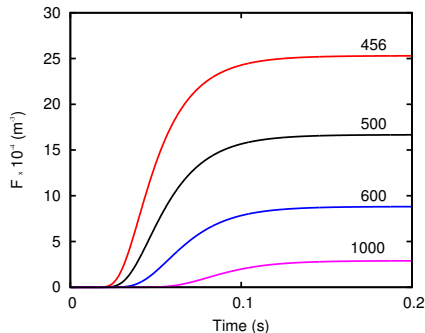
All system parameters are known \Rightarrow we can determine **the size distribution of nuclei F_i**

Selected Applications

Homogeneous nucleation

Ni melt: $\Delta h_E = 17.29 \text{ kJ mol}^{-1}$, $T_E = 1748 \text{ K}$, $\rho_S = 8357 \text{ kg m}^{-3}$, $\sigma = \sigma_m T / T_E$,
where $\sigma_m = 0.275 \text{ J m}^{-2}$, $E = 29.085 \text{ kJ mol}^{-1}$

$$T = 1449 \text{ K} \Rightarrow i^* = 456$$



$F_i V = 1$ – one i -sized nucleus is formed in V
 $F_{456}^S = 250000 \text{ m}^{-3} \Rightarrow V_1 = 1/F_{i^*}^S = 4 \text{ cm}^3$

sample masses: $23 \mu\text{g} - 63 \text{ mg}$
 $\Rightarrow V = 7.15 \times 10^{-9} \text{ m}^3 - 2.9 \times 10^{-12} \text{ m}^3$

In difference of experimental data, **no critical nuclei are formed** in Ni melt.

Solution: reduce the interfacial energy or take into account $\sigma(i)$ dependency \Rightarrow

lower nucleation barrier

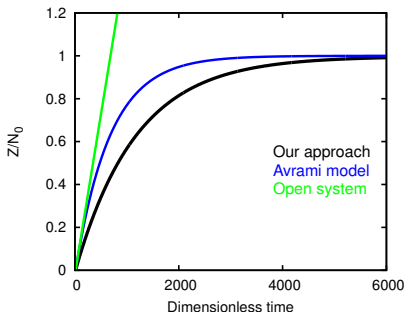
Maybe heterogeneous nucleation occurs ?

Selected Applications

Nucleation on active centers

CNT model of nucleation on active centers – one additional equation is needed

[S. Toshev, I. Gutzow, Krist. Tech. 7 (1972) 43; P. Ascarelli, S. Fontana: Diamond Rel. Mater. 2 (1993) 990-996; D. Kashchiev: *Nucleation, Butterworth-Heinemann Boston, 2000*]



Additional equation:

$$\frac{dZ(t)}{dt} = [N_0 - Z(t)]J^S(t)$$

$Z(t)$ - the total number of nuclei at time t

N_0 - the number of active sites;

J^S - time dependent nucleation frequency
(usually taken as fit <F8> parameter)

Our new model does not need additional equation!!

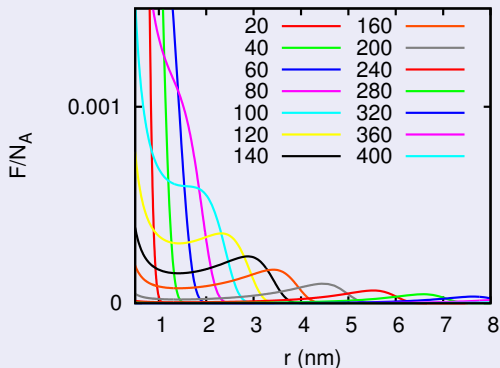
→ only modification of boundary conditions

Z. Kozisek et al., [Transient nucleation on inhomogeneous foreign substrate](#), J. Chem. Phys. 108 (1998) 9835; [Nucleation on active sites: evolution of size distribution](#), J. Cryst. Growth 209 (2000) 198-202.

Selected Applications

Nucleation on active centers

HEN: Vapor → **Solid transition**



Selected Applications

Nucleation on active centers

HEN: Vapor \rightarrow Solid transition

H. Kumomi, F.G. Shi: Phys. Rev. Lett. 82 (1999) 2717.

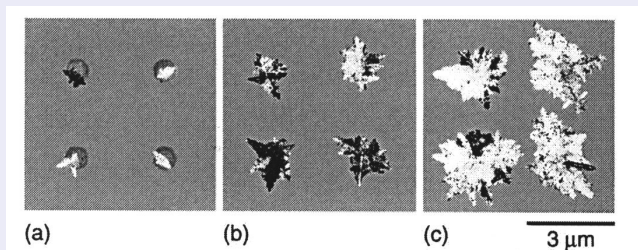


FIG. 1. Bright-field plan-view TEM images of *a*-Si thin films annealed at 873 K in nitrogen with the artificial nucleation sites, which show the evolution with the annealing time at (a) 2.0×10^4 s, (b) 3.6×10^4 s, and (c) 5.4×10^4 s. It is seen that a single dendritic crystallite grows at each artificial site, and no coalescence has occurred up to 5.4×10^4 s.

Selected Applications

Nucleation on active centers

HEN: Vapor \rightarrow Solid transition

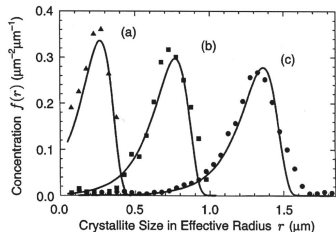
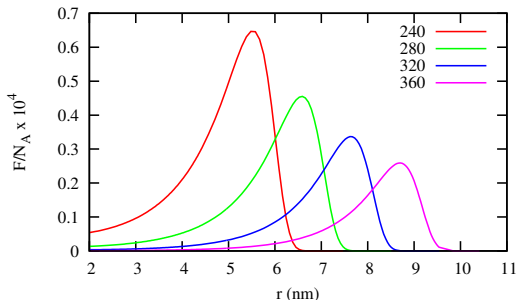
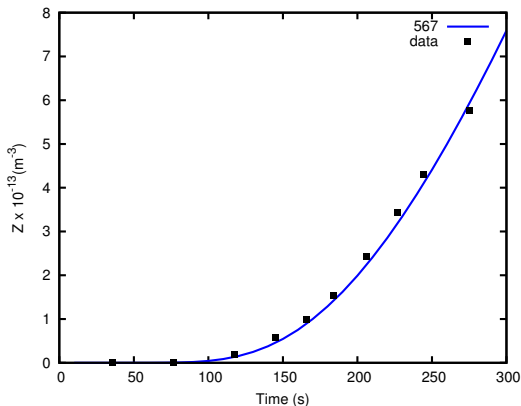


FIG. 2. Dynamic evolution of the CSD in the controlled solid-phase crystallization of *a*-Si thin films with artificial nucleation sites. Three CSDs marked with \blacktriangle , \blacksquare , and \bullet are observed in the samples shown by (a), (b), and (c) of Fig. 1, respectively. The solid lines are the theoretical predictions with the depletion of the nucleation sites taken into account.

Selected Applications

Nucleation on active centers

HEN: polymer nucleation from melt (polyethylene) $\Delta T = 10.4 K$



Z. Kožíšek et al. *Nucleation kinetics of folded chain crystals of polyethylene on active centers*, J. Chem. Phys. 121 (2004) 1587.

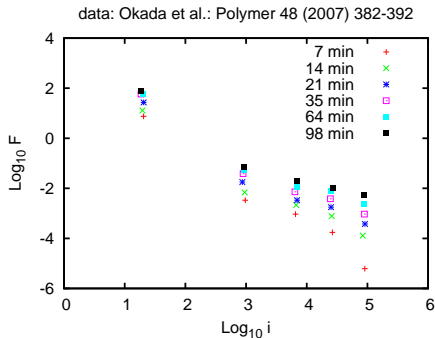
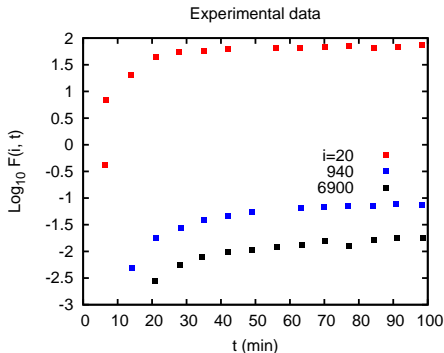
Z. Kožíšek et al. *Nucleation on active centers in confined volumes*, J. Chem. Phys. 134 (2011) 114904

Selected Applications

Nucleation on active centers

HEN: polymer nucleation from melt (polyethylene)

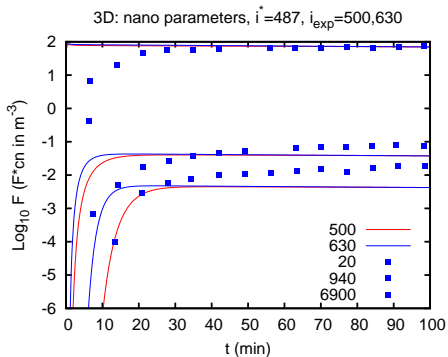
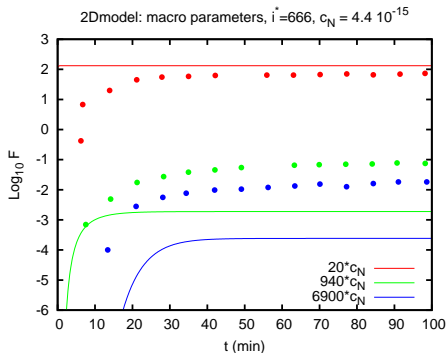
2007: K. Okada et al.: Polymer 48 (2007) 1116-1126.



σ_{nano} (instead of σ) introduced to fit $F_i^S \Rightarrow k^* = 9, l^* = 24.9, m^* = 4.5 \Rightarrow$ 3D model

Selected Applications

Polymer nucleation on active centers (polyethylene)



Z. Kožíšek, M. Hikosaka, K. Okada, P. Demo: J. Chem. Phys. 134 (2011) 114904 & 136 (2012) 164506

Summary

Advantages

- Relatively simple model enables to determine basic characteristics of nucleation in real time.
- Model takes into account depletion of the parent phase during phase transformation.
- Model includes exhaustion of active centres (new approach to heterogeneous nucleation).



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Thank you for your attention.

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