2017/06/08

Dust formation theory in astronomical environments

Takaya Nozawa

(National Astronomical Observatory of Japan)

Contents:

1-1. Origin of cosmic dust grains

○ Cosmic dust grains

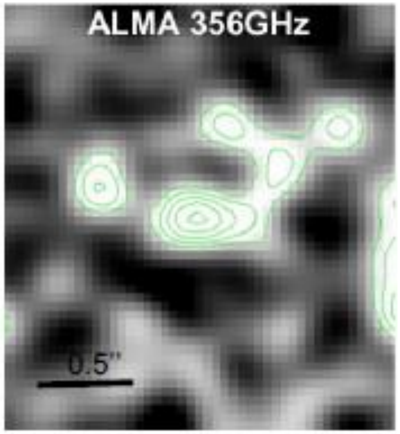
- universally exist in the universe
- cause various astrophysical phenomena

  extinction, scattering, polarization, IR emission,
  molecular formation on the surface, formation of planets …

The origin of dust remains to be clarified !!

○ Massive dust at z > 5 discovered

in the early universe, CCSNe must play dominant roles in the enrichment of ISM with dust



~10^6 M_{sun} of dust in a galaxy at z = 8.4
Laporte+2017

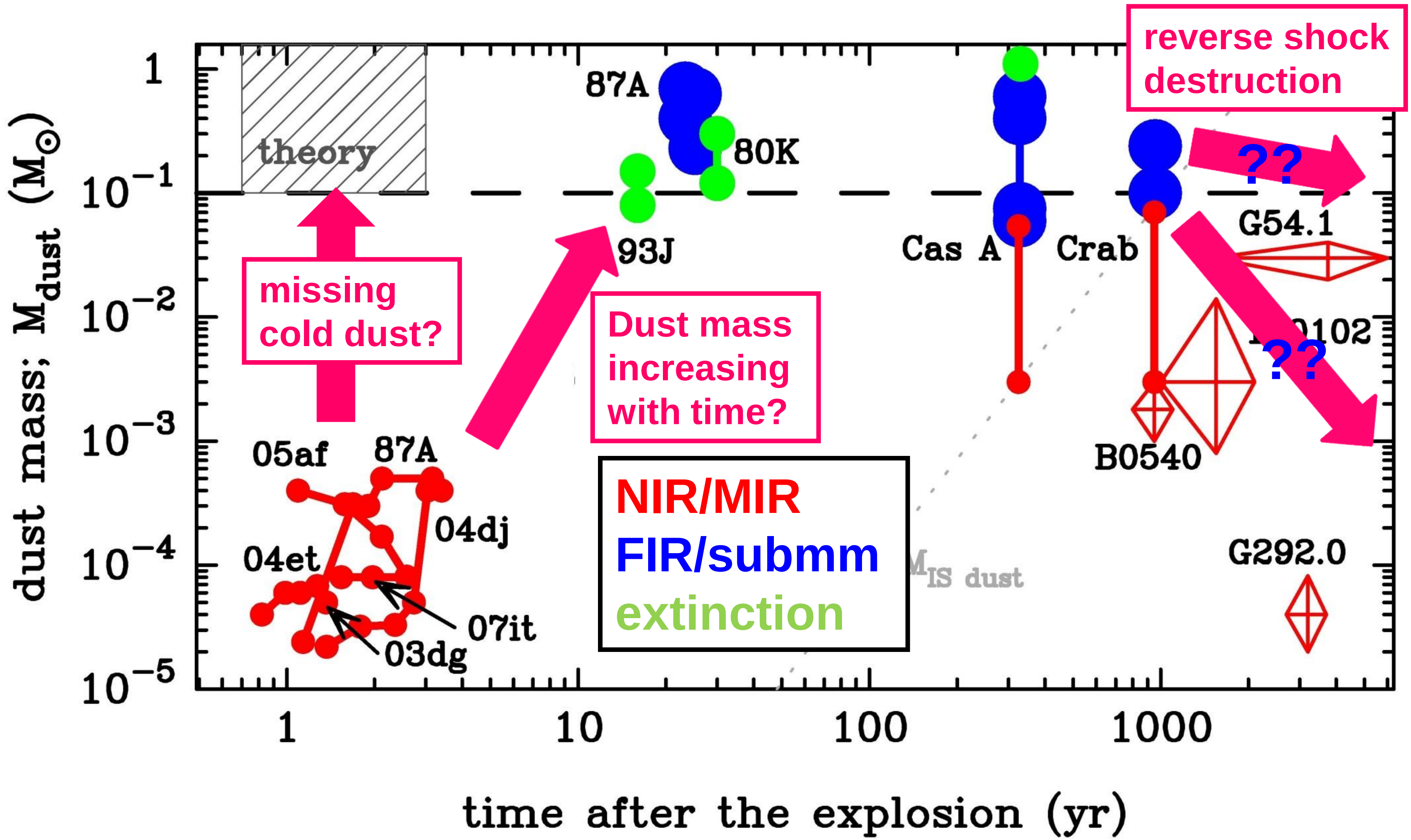
1-2. Key questions for dust formation

1. How much dust grains form?

2. What is the size distribution of dust?

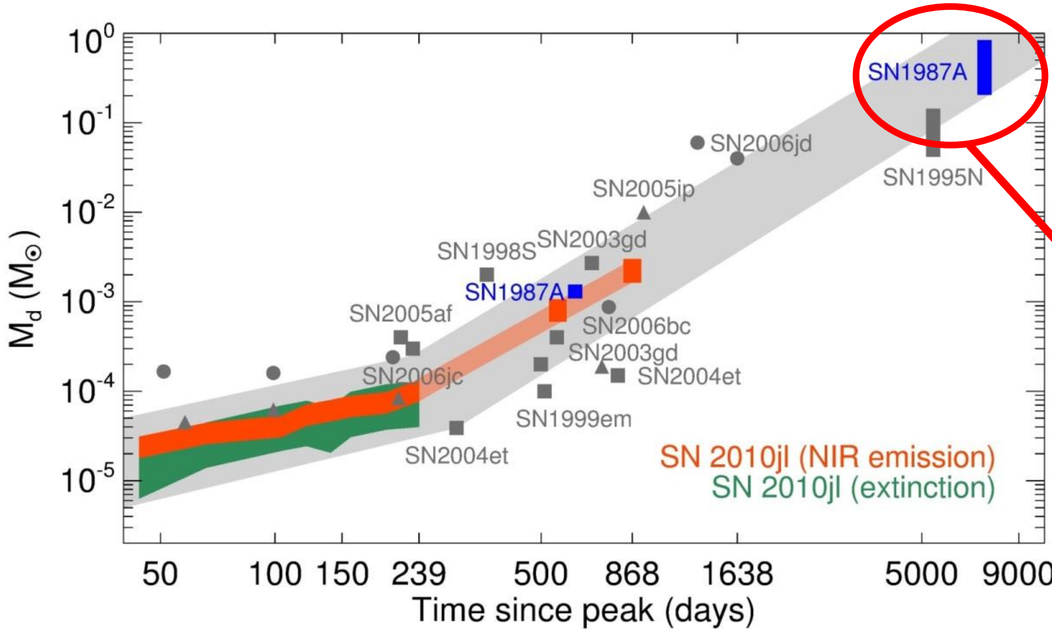
3. When do the majority of grains form?

1-3. Observed dust mass in CC-SNe/SNRs



Dust mass formed in the ejecta is dominated by cold dust

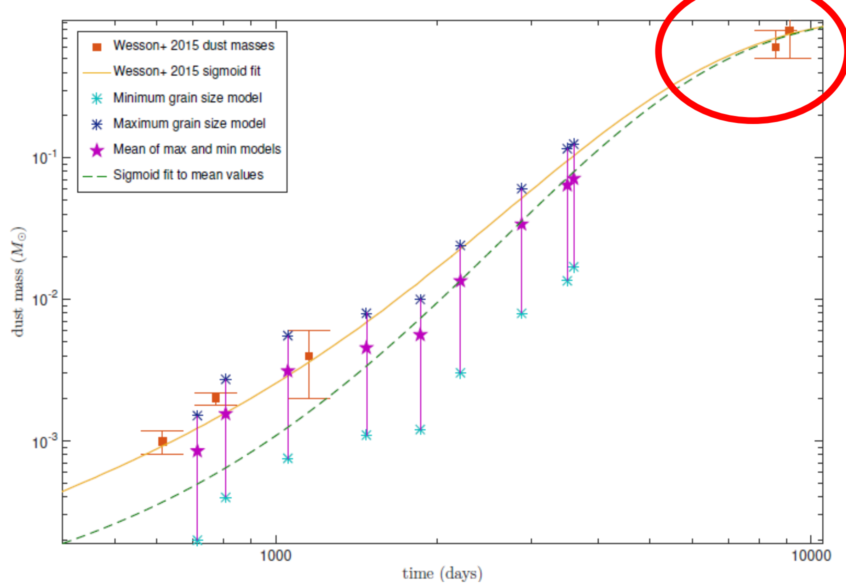
1-4. Dust mass increases with time?



Dust mass estimated from IR emission

Gall et al. (2014, Nature)

Most of dust grains (> 0.1 Msun) form at ~20 yr post-explosion



Evolution of dust mass in SN 1987A derived from extinction of optical emission lines

Bevan & Barlow (2016)

1-5. Key questions for dust formation

1. How much dust grains form?

- FIR/submm obs. ➜ 0.1-1 M_{sun}
- theoretical works ➜ 0.1-1 M_{sun}

2. What is the size distribution of dust?

➜ what fraction of dust is destroyed by RS?
➜ smaller grains are destroyed more efficiently

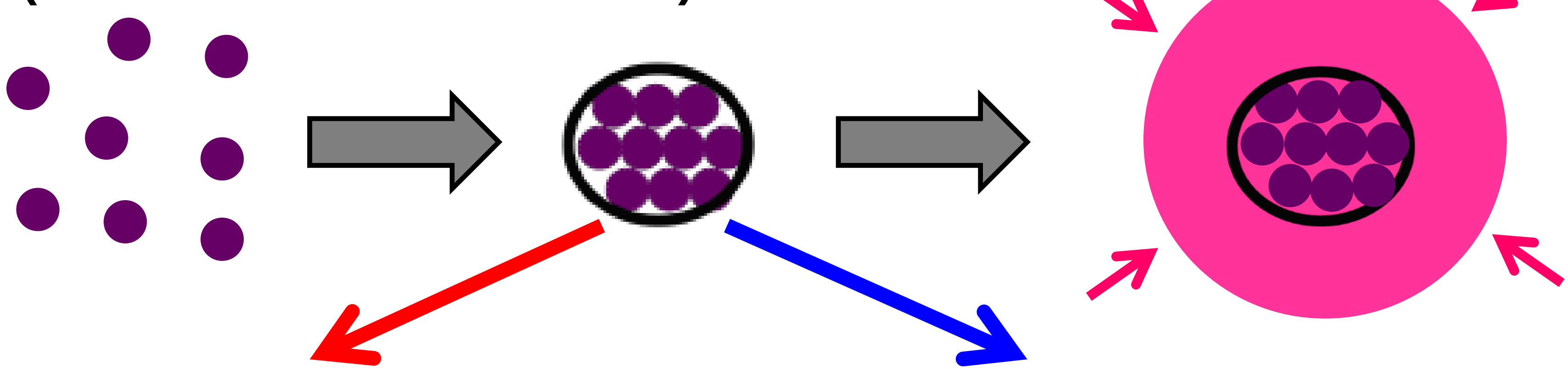
3. When do the majority of grains form?

- obs. ➜ ~20 yr (dust mass gradually increases with time)
- theory ➜ ~1-2 yr (within 5 yr)

2-0. Two approaches for nucleation

1. Nucleation
(formation of stable clusters)

2. Grain growth



○ Classical nucleation
(kinetic nucleation)

(Kozasa+1989, 1991, Yamamoto+2001, Todini & Ferrara 2001, Nozawa+2003, 2008, 2010, Schneider & Bianchi 2007, Fallest+2011, Keith & Lazzati 2011, Schneider+2012, Nozawa & Kozasa 2013, Lazzati & Heger 2016, Marassi+2015, Bocchio+2016)

○ Chemical nucleation
(molecluar nucleation)

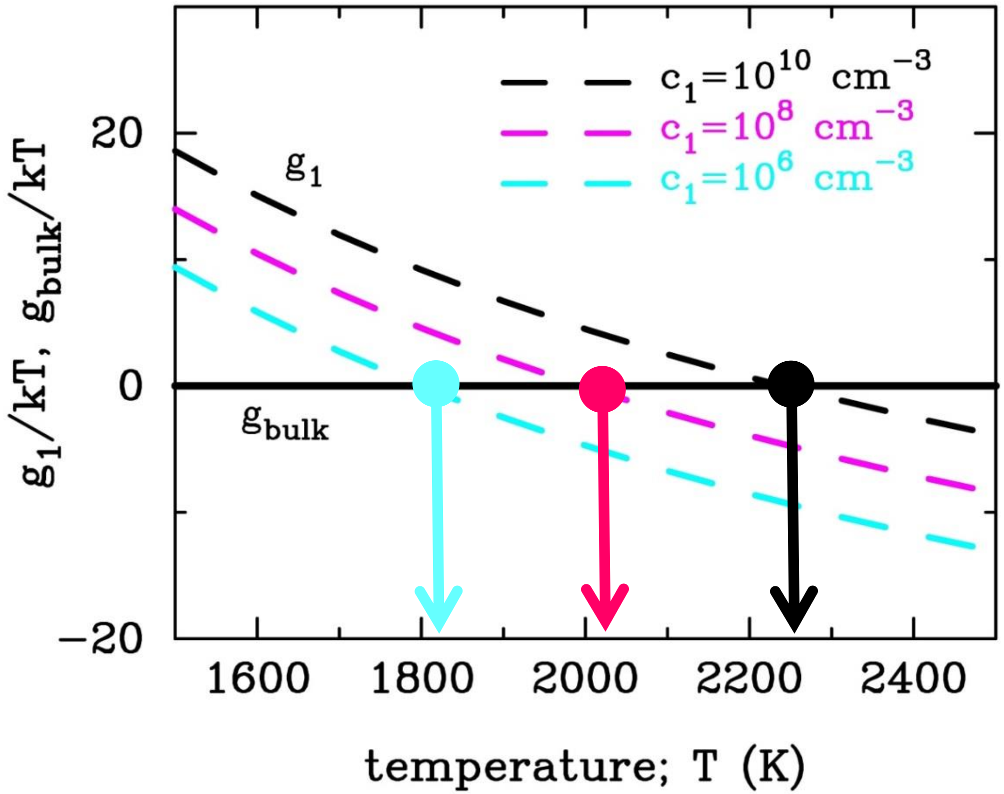
(Clayton+1999, 2001, Deneault+2003, Cherchneff & Dwek 2009, 2010, Sarangi & Cherchneff 2013, 2015 Biscaro & Cherchneff 2014, 2016) Sluder+2016)

2-1. Phase transition

○ Gibbs free energy

gas $$G_1 = n\ g_1(T) = n\ g_1^0(T) + nkT \ln\left(\frac{P_1}{P^0}\right)$$

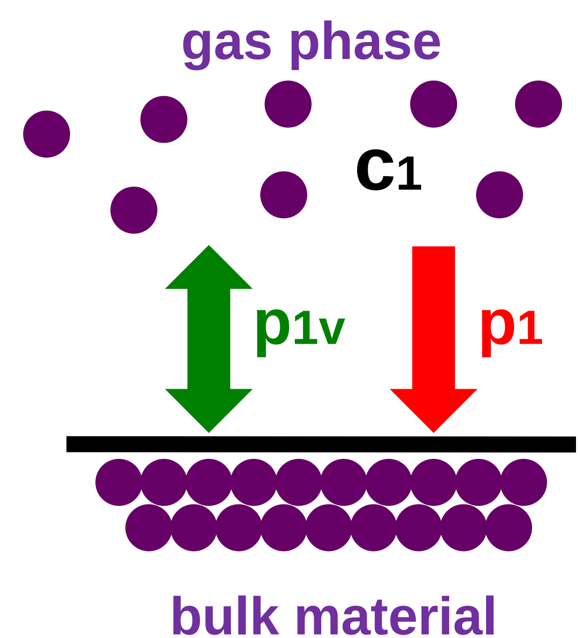
solid $$G_{\mathrm{bulk}} = n\ g_{\mathrm{bulk}}(T) = n\ g_{\mathrm{bulk}}^0(T)$$



○ Supersaturation ratio, S

$$\begin{aligned}
\ln S &= \left(g_1 - g_{\mathrm{bulk}}\right)/kT \\
&= -\frac{1}{kT}\left(g_{\mathrm{bulk}}^0 - g_1^0\right) + \ln\left(\frac{P_1}{P^0}\right) \\
&= \ln\left(\frac{P_1}{P_{1,\mathrm{v}}}\right)
\end{aligned}$$

solid stable for lnS > 0（S>1）



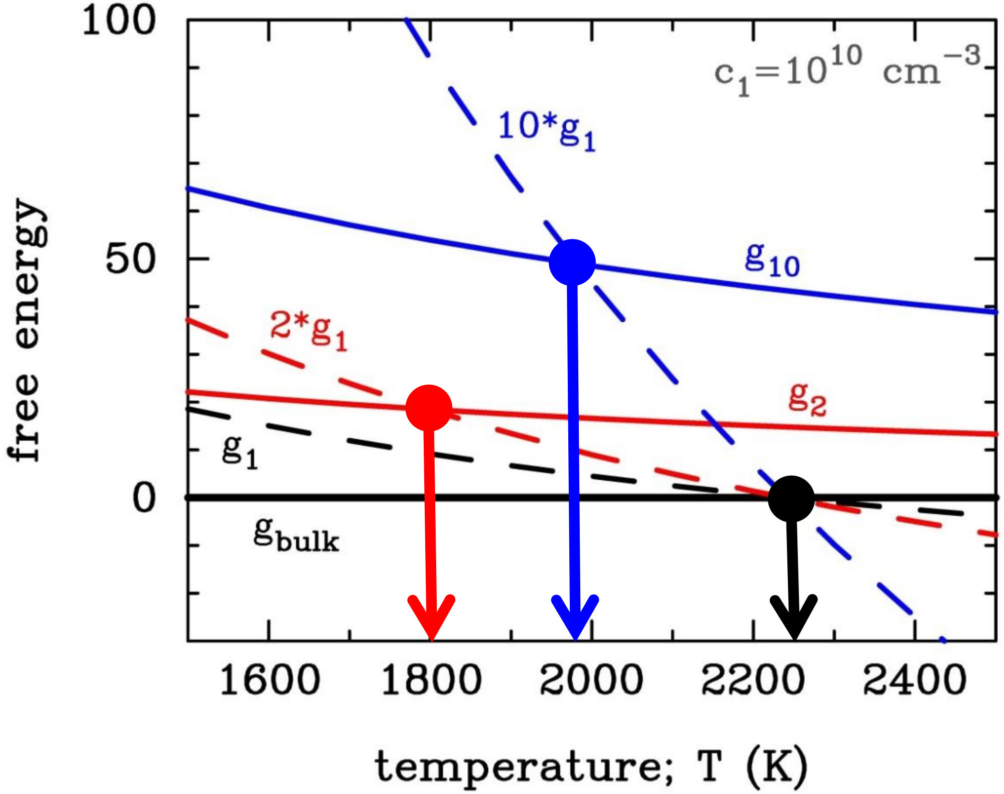
2-2. Formation of clusters

○ Free energy for clusters

$$\boxed{G_n = n\ g_n(T) = n\ g^0_{\rm bulk}(T) + E_{\rm bar}}$$

capillary approximation

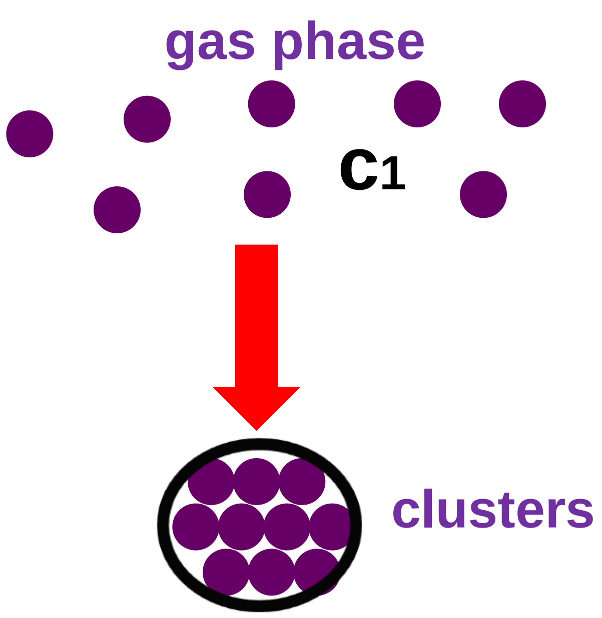
$$\boxed{G_n = n\ g^0_{\rm bulk}(T) + 4\pi a_0^2 n^{\frac{2}{3}} \sigma}$$



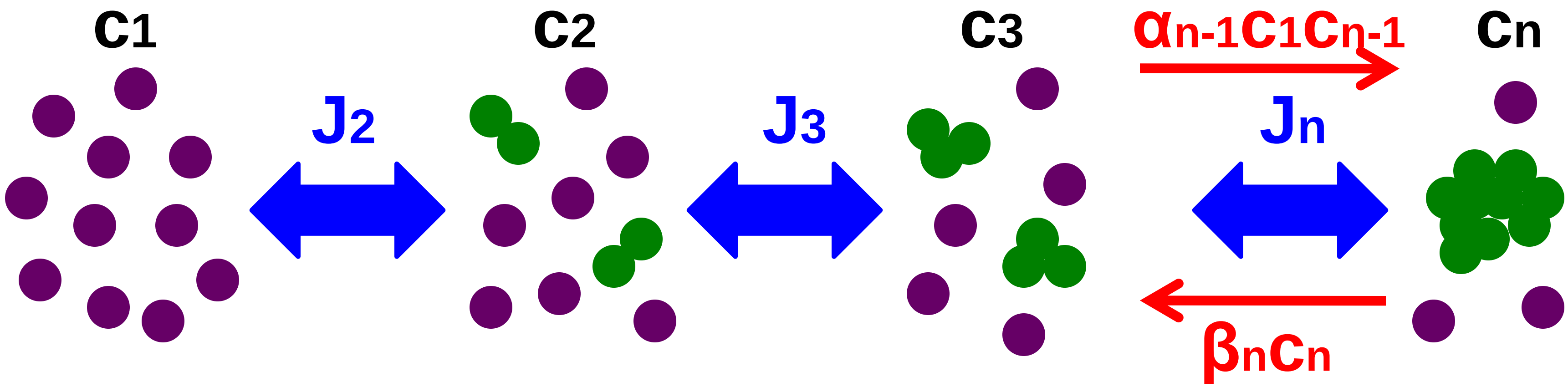
○ Energy involved in cluster formation

$$\boxed{\begin{aligned} W_n &= (G_1 - G_n)/kT \\ &= n \ln S - E_{{\rm surf},n}/kT \end{aligned}}$$

where $E_{{\rm surf},n} = 4\pi a_0^2 n^{\frac{2}{3}} \sigma$



2-3. Kinetic nucleation



○ Master equations

$$\frac{dc_n}{dt} = J_n(t) - J_{n+1}(t) \quad \text{for} \quad 2 \le n \le n_*,$$

$$J_n(t) = \alpha_{n-1} c_1 \left[c_{n-1} - c_n \exp(\gamma_n) \right]$$

$$\alpha_n = \eta_s 4\pi a_0^2 n^{\frac{2}{3}} \left(\frac{kT}{2\pi m_n} \right)^{\frac{1}{2}}$$

sticking coefficient, η_s = 1

$$\gamma_n = \frac{1}{kT} \left(E_{\mathrm{surf},n} - E_{\mathrm{surf},n-1} \right) - \ln S$$

energy barrier : ~ 10

2-4. Classical nucleation

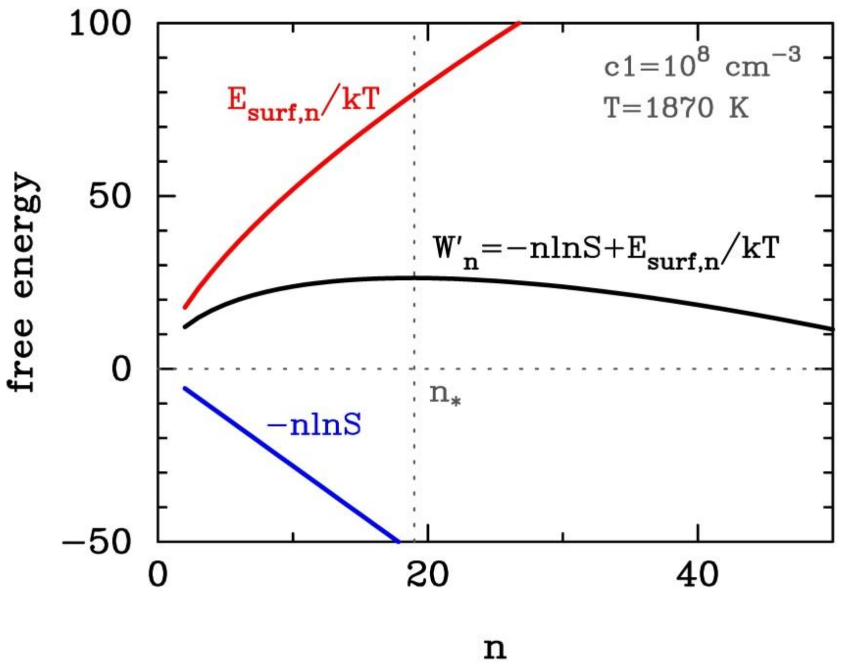
○ Steady-state nucleation rate

(assuming $J_s = J_2 = J_3 = \ldots = J_n$)

$$\boxed{J_s \propto \exp\left(-W_n\right)}$$

$$\boxed{W'_n = -W_n = -n \ln S + \frac{4\pi a_0^2 \sigma}{kT} n^{\frac{2}{3}}}$$

$$\boxed{n_{\rm crit} \simeq \left(\frac{8\pi a_0^2 \sigma}{3kT \ln S}\right)^3}$$



$$\boxed{J_s(t) = \eta_s\ \Omega_0 \left(\frac{2\sigma}{\pi m_1}\right)^{\frac{1}{2}} c_1^2(t) \exp\left[-\frac{4}{27(\ln S)^2}\left(\frac{4\pi a_0^2 \sigma}{kT}\right)^3\right]}$$

formation rate of stable clusters

2-5. Basic equations for dust formation

1. Nucleation

・Kinetic

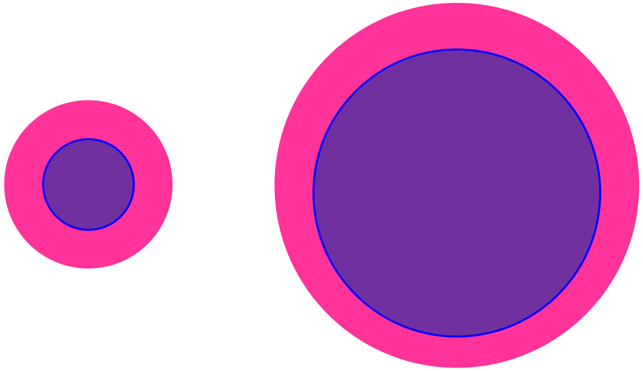
$$\frac{dc_n}{dt} = J_n(t) - J_{n+1}(t) \quad \text{for} \;\; 2 \leq n \leq n_*,$$

・Classical

$$J_s(t) = \eta_s \, \Omega_0 \left(\frac{2\sigma}{\pi m_1} \right)^{\frac{1}{2}} c_1^2(t) \exp \left[-\frac{4}{27(\ln S)^2} \left(\frac{4\pi a_0^2 \sigma}{kT} \right)^3 \right]$$

2. Grain growth

$$\frac{da}{dt} = \eta_{\rm g} \Omega_0 \left(\frac{kT}{2\pi m_1} \right)^{\frac{1}{2}} c_1(t)$$



・free expansion

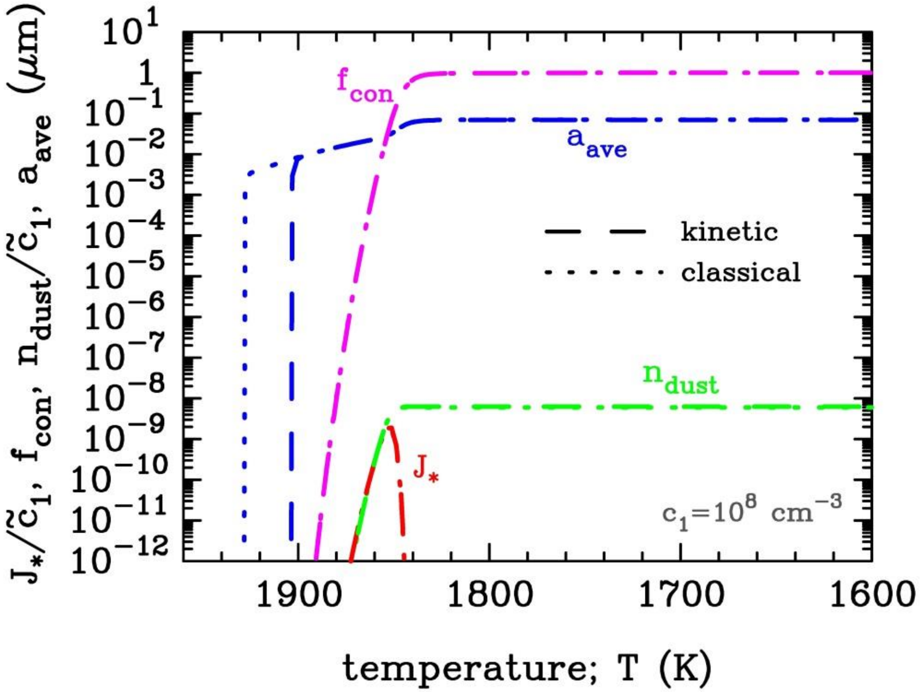
$$\tilde{c}(t) = c_0 \left(\frac{t}{t_0} \right)^{-3},$$

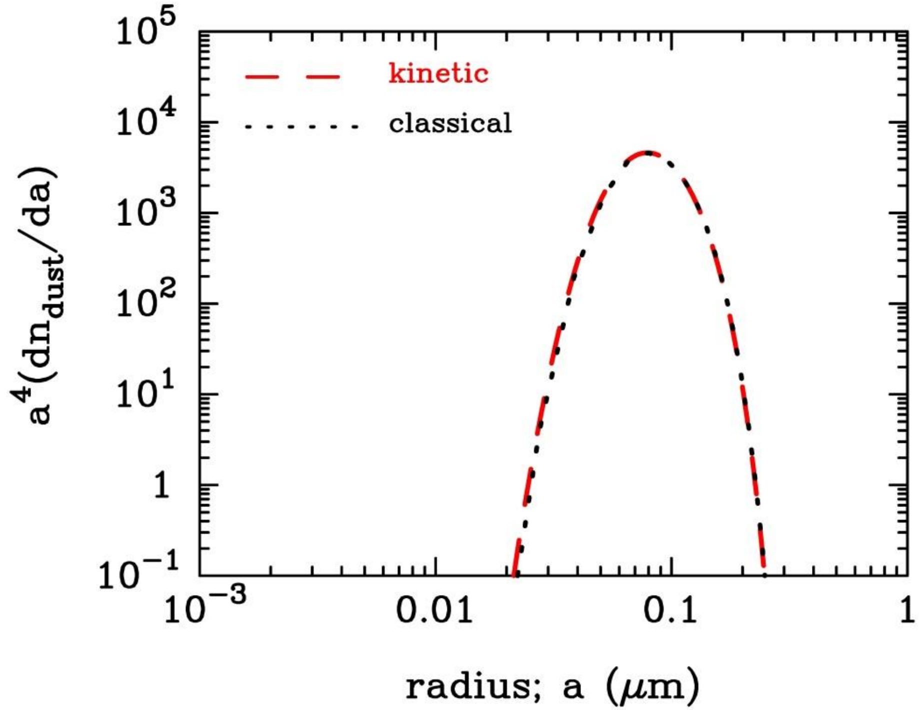
・gas cooling

$$T(t) = T_0 \left(\frac{t}{t_0} \right)^{-3(\gamma-1)},$$

(γ=1.25)

2-6. Kinetic vs. Classical





・Kinetic nucleation

$$\frac{dc_n}{dt} = J_n(t) - J_{n+1}(t) \quad \text{for} \quad 2 \leq n \leq n_*,$$

(n_*=100)

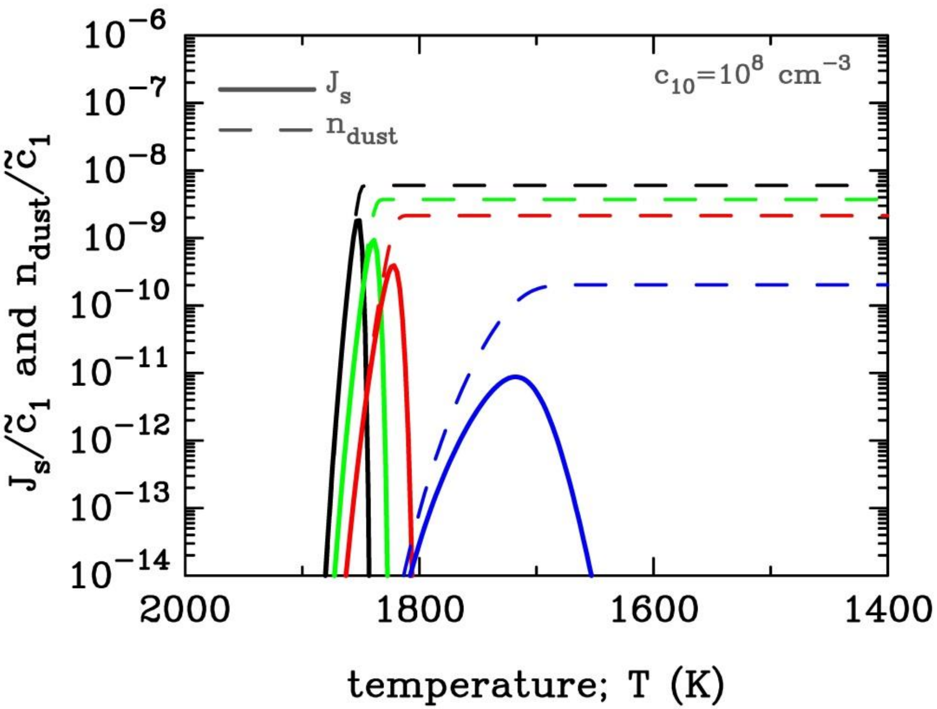
・Classical nucleation

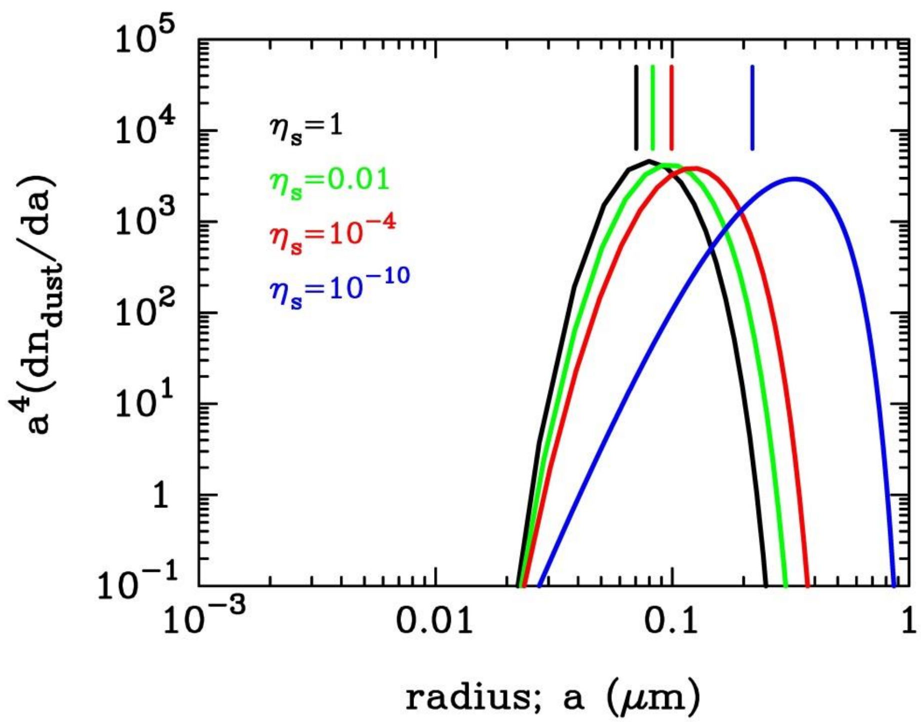
η_s = 1

$$J_s(t) = \eta_s \, \Omega_0 \left(\frac{2\sigma}{\pi m_1} \right)^{\frac{1}{2}} c_1^2(t) \exp\left[-\frac{4}{27(\ln S)^2} \left(\frac{4\pi a_0^2 \sigma}{kT} \right)^3 \right]$$

2-7. Dependence on sticking coefficient

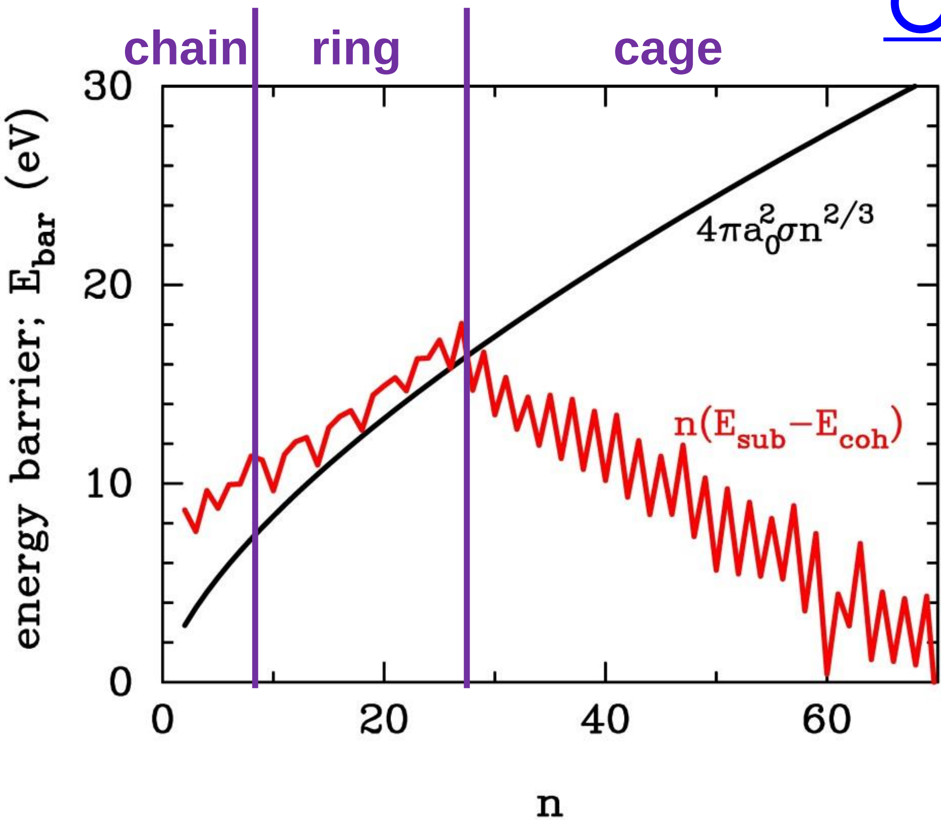
$$J_s(t) = \eta_s\ \Omega_0 \left(\frac{2\sigma}{\pi m_1}\right)^{\frac{1}{2}} c_1^2(t) \exp\left[-\frac{4}{27(\ln S)^2}\left(\frac{4\pi a_0^2 \sigma}{kT}\right)^3\right]$$





$$f_{\rm con} M_C = n_{\rm dust}\ \frac{4\pi}{3}\delta_C a^3 \rightarrow a \propto n_{\rm dust}^{-\frac{1}{3}}$$

2-8. Energy barrier of clusters



○ Free energy for clusters

$$G_n = n\ g^0_{\mathrm{bulk}}(T) + E_{\mathrm{bar}}$$

・Classical nucleation

$$\boxed{E_{\mathrm{bar}} = E_{\mathrm{surf},n} = 4\pi a_0^2 \sigma n^{\frac{2}{3}}}$$

・Density fluctuation theory

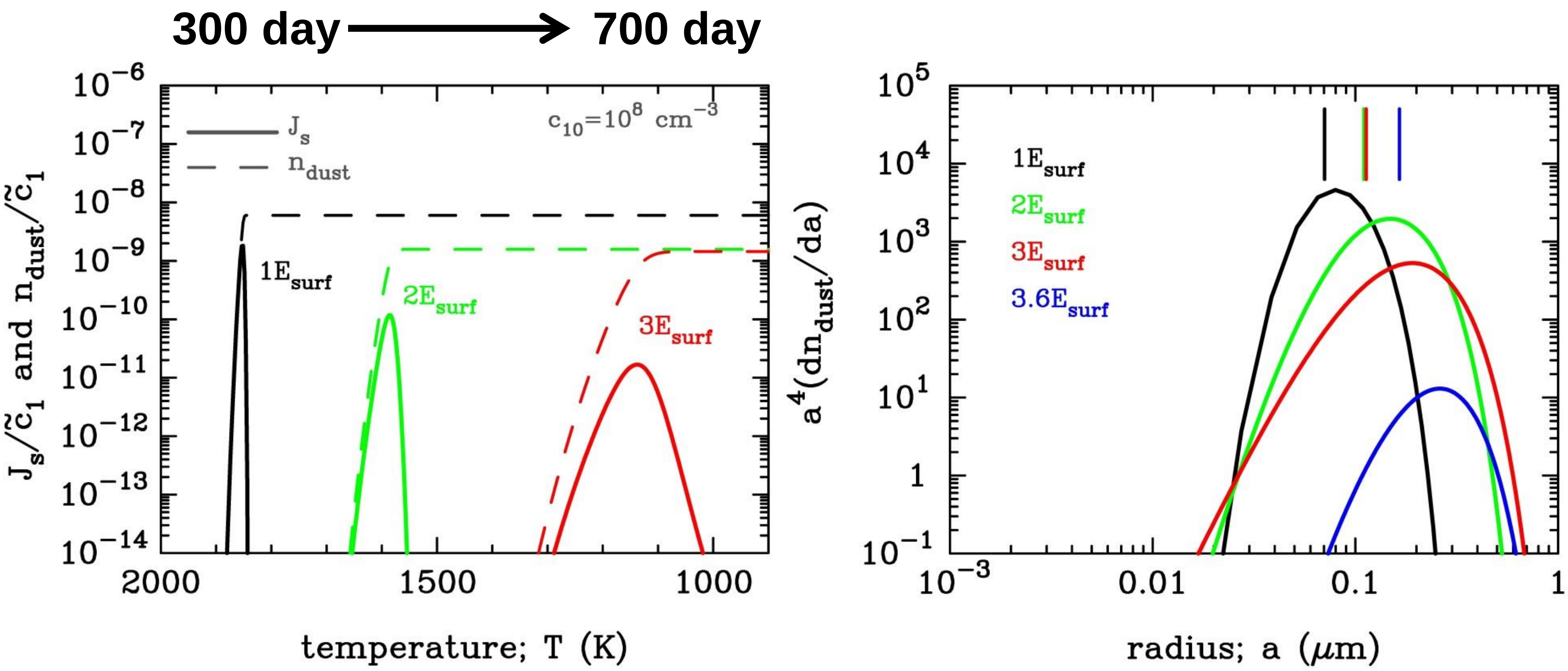
$$\boxed{E_{\mathrm{bar}} = E_{\mathrm{bind},n} = n\left(E_{\mathrm{sub}} - E_{\mathrm{coh}}\right)}$$

Mauney+2015

・Kinetic nucleation

$$\boxed{\frac{dc_n}{dt} = J_n(t) - J_{n+1}(t) \quad \text{for} \;\; 2 \le n \le n_*,}$$

2-9. Dependence on surface energy



- Increasing the surface energy can lead to lower condensation temperature, retarding the formation of dust
- Dependence of sticking coefficient and energy barrier on the resulting size of dust is not strong

3-1. Chemical approach

○ Master equations

$$\boxed{\frac{dc_n}{dt} = \sum^{i}\sum^{j} k_{i,j}\, c_i\, c_j - \sum^{m} k_{m,n}\, c_m\, c_n}$$

○ Arrhenius expression

$$\boxed{k_{i,j} = A_{i,j}\left(\frac{T}{300\ \mathrm{K}}\right)^{\nu}\exp\left(-\frac{E_{\mathrm{act}}}{kT}\right)}$$

Empirical (fitting) formula to account for reaction rates obtained from experiments

3-2. Reaction rates for carbon clusters

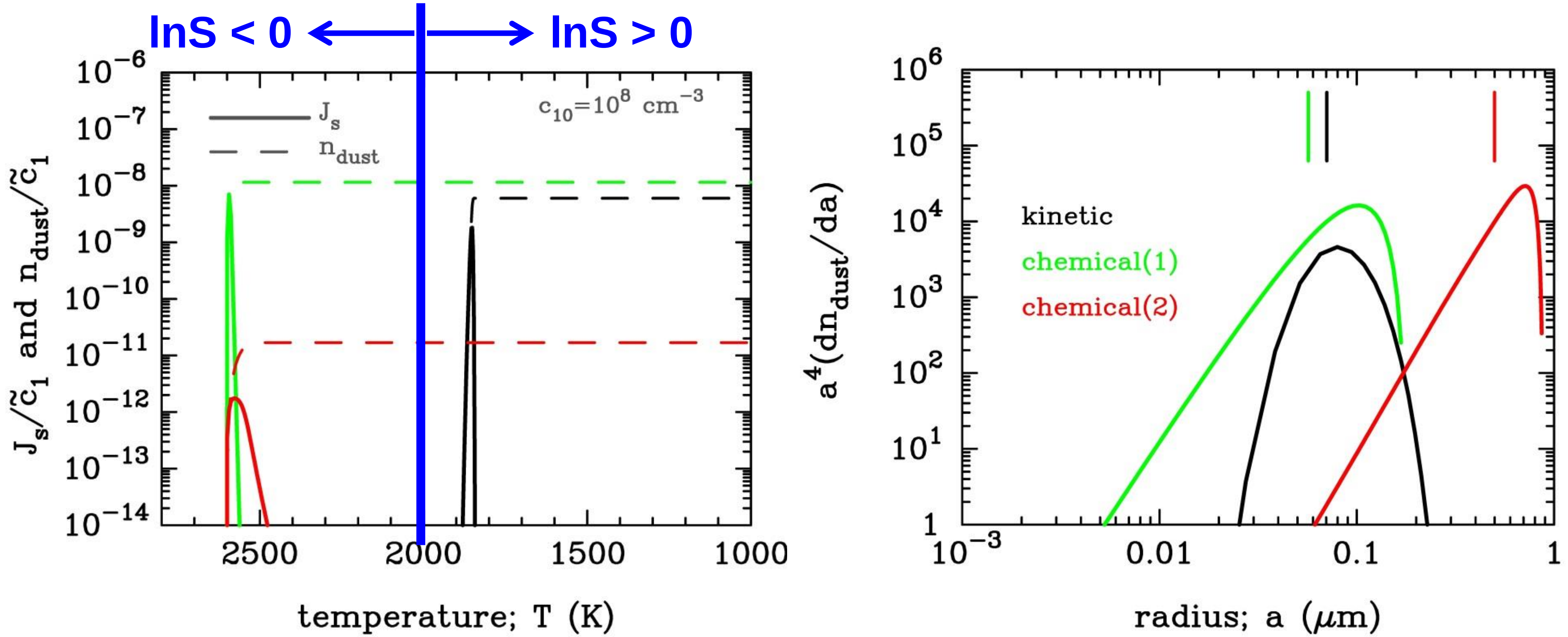
$$k_{i,j} = A_{i,j} \left(\frac{T}{300\ \mathrm{K}} \right)^{\nu} \exp\left(-\frac{E_{\mathrm{act}}}{kT} \right)$$

Carbon – C

C1	C+ C	$\longrightarrow$	C_2+ hν	4.36×10^{-18}	0.35	161.3	Andreazza & Singh 1997
C2	C + C_2	$\longrightarrow$	C_3 + hν	1.00×10^{-17}	0	0	Clayton et al. 1999
C3	C + C_3	$\longrightarrow$	C_4 + hν	1.00×10^{-10}	0	0	Clayton et al. 1999
C4	C + C_4	$\longrightarrow$	C_5 + hν	1.00×10^{-13}	0	0	Clayton et al. 1999
C5	C + C_4	$\longrightarrow$	C_2 + C_3	1.00×10^{-10}	0	0	Clayton et al. 1999
C6	C + C_5	$\longrightarrow$	C_6 + hν	1.00×10^{-10}	0	0	Clayton et al. 1999
C7	C + C_6	$\longrightarrow$	C_7 + hν	1.00×10^{-13}	0	0	Clayton et al. 1999
C8	C + C_6	$\longrightarrow$	C_2 + C_5	1.00×10^{-10}	0	0	Clayton et al. 1999
C9	C + C_6	$\longrightarrow$	C_3 + C_4	1.00×10^{-10}	0	0	Clayton et al. 1999
C10	C + C_7	$\longrightarrow$	C_8 + hν	1.00×10^{-10}	0	0	Clayton et al. 1999
C11	C + C_8	$\longrightarrow$	C_9 + hν	1.00×10^{-13}	0	0	Clayton et al. 1999
C12	C + C_8	$\longrightarrow$	C_2 + C_7	1.00×10^{-10}	0	0	Clayton et al. 1999
C13	C + C_8	$\longrightarrow$	C_3 + C_6	1.00×10^{-10}	0	0	Clayton et al. 1999
C14	C + C_8	$\longrightarrow$	C_4 + C_5	1.00×10^{-10}	0	0	Clayton et al. 1999
C15	C + C_9	$\longrightarrow$	C_{10} + hν	1.00×10^{-10}	0	0	Clayton et al. 1999

Cherchneff & Dwek (2010)

3-3. Chemical vs. Kinetic (Classical)



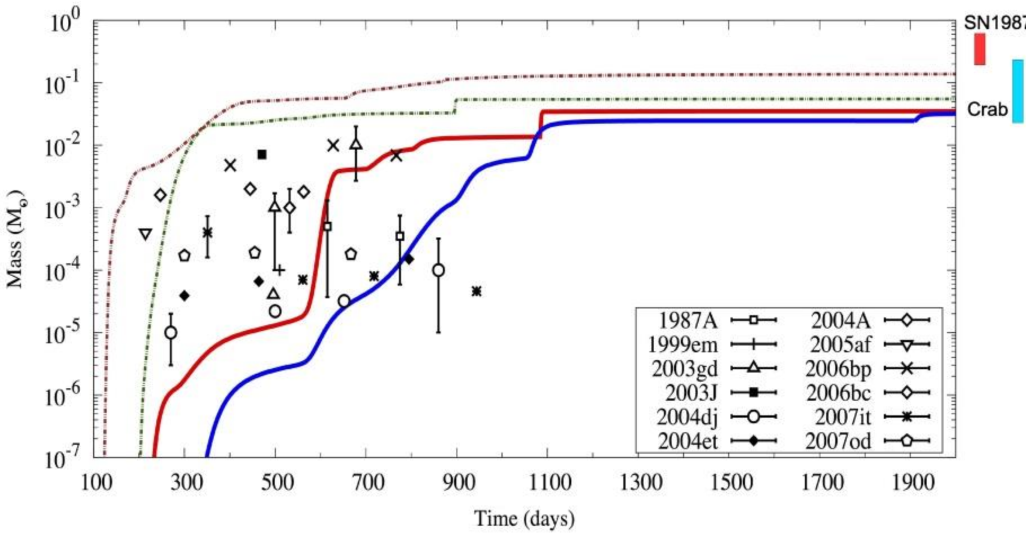
green line: only for forward reactions

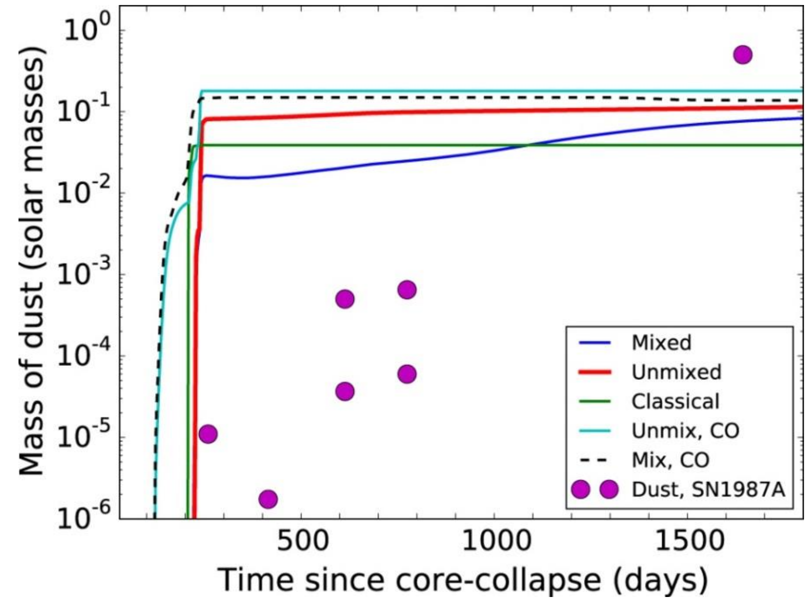
$$\frac{dc_n}{dt} = k_{i,j}\ c_i\ c_j$$

red line: destruction reaction C_2 + O ===> CO + C

If chemical reaction rates and paths are not accurate, the chemical approach may produce erroneous results

4-1. Mass evolution of newly formed dust



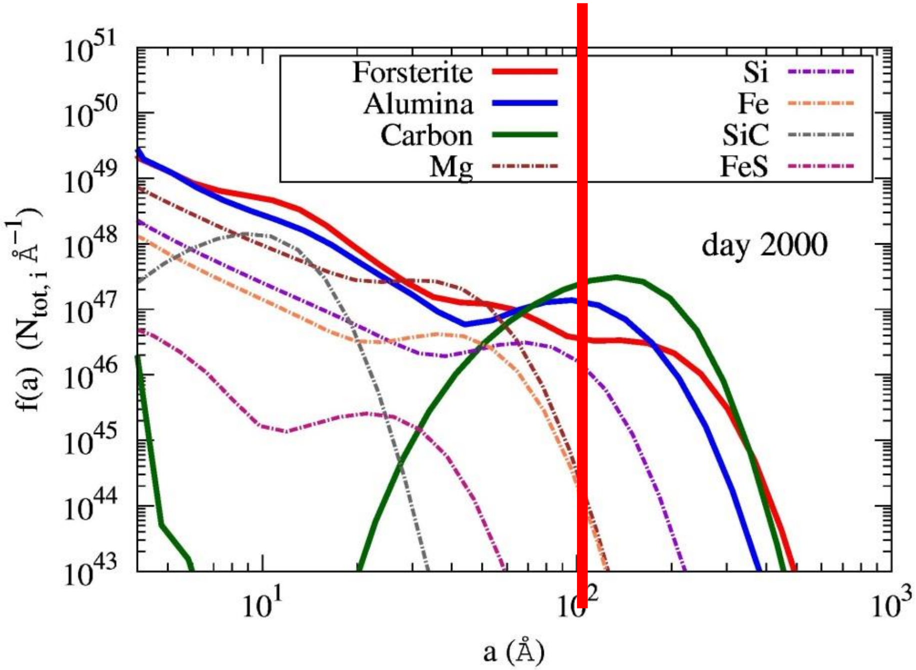


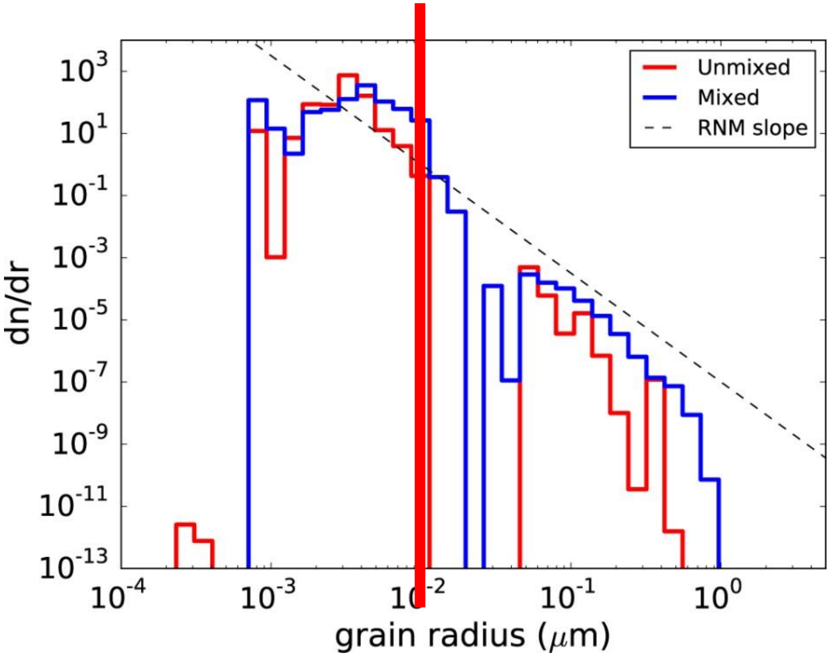
Molecules: chemical
Clusters: chemical
Grains: coagulation
Sarangi & Cherchneff (2015)

Molecules: chemical
Clusters: kinetic
Grains: accretion
Lazzati & Heger (2016)

Both nucleation approaches predict that ~0.1 Msun of dust condenses a few years after the explosion

4-2. Size distribution of newly formed dust





Molecules: chemical
Clusters: chemical
Grains: coagulation
Sarangi & Cherchneff (2015)

Molecules: chemical
Clusters: kinetic
Grains: accretion
Lazzati & Heger (2016)

The radii of newly formed dust ranges from ~0.001 μm to ~1 μm though there are some subtle differences

4-3. Timescale of grain growth

$$\tau_{\rm grow}^{-1} = \frac{1}{a}\left(\frac{da}{dt}\right) = \left(\frac{1}{a}\right)\eta_g \Omega_0 c_1 \left(\frac{kT}{2\pi m_1}\right)^{\frac{1}{2}}$$

$$\tau_{\rm grow} \simeq 50 \left(\frac{\eta_g}{1.0}\right)^{-1} \left(\frac{a}{0.01\ \mu{\rm m}}\right) \left(\frac{T}{50\ {\rm K}}\right)^{-\frac{1}{2}} \left(\frac{M_C}{0.01\ M_\odot}\right)^{-1} \times \left(\frac{V_{\rm core}}{10^3\ {\rm km\ s^{-1}}}\right)^3 \left(\frac{t}{20\ {\rm yr}}\right)^3 \left(\frac{f_{\rm density}}{10}\right)^{-1}\ {\rm yr}$$

At 20 yr, the gas density is too low to form dust grains in the freely expanding ejecta

5. Summary of this talk

1) Classical (kinetic) nucleation

- **well established on the basis of thermodynamics**
- **still one of the good tools to describe dust formation**

2) Chemical (molecular) nucleation

- **consistently follows the formation of a variety of molecules and small clusters, given that reaction paths and rates are well known**

3) Both nucleation approaches predict

- **the formation of dust in the ejecta within 5 yr (seems hard to form massive dust at ~20 yr)**
- **dust size range of 0.001-1 μm**