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Approach to Nucleation in Astronomical Environments

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TODIAS 東京大学国際高等研究所 TODAI INSTITUTES FOR ADVANCED STUDY

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1-1. Introduction

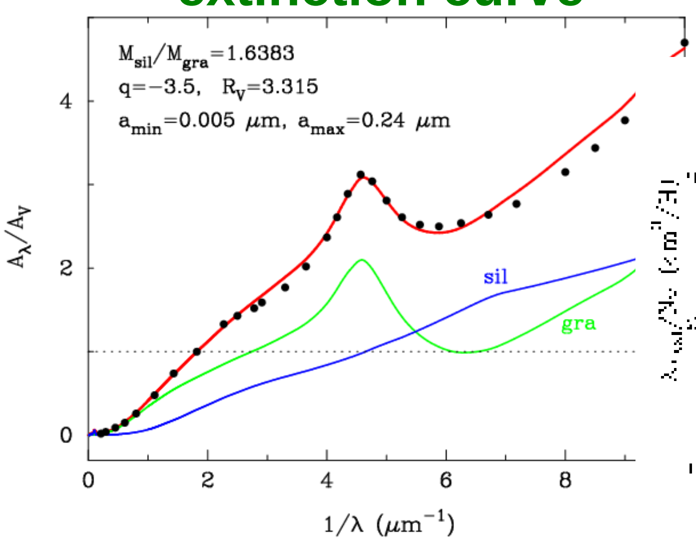
Cosmic dust universally exits in space

when, where, and how is dust formed?

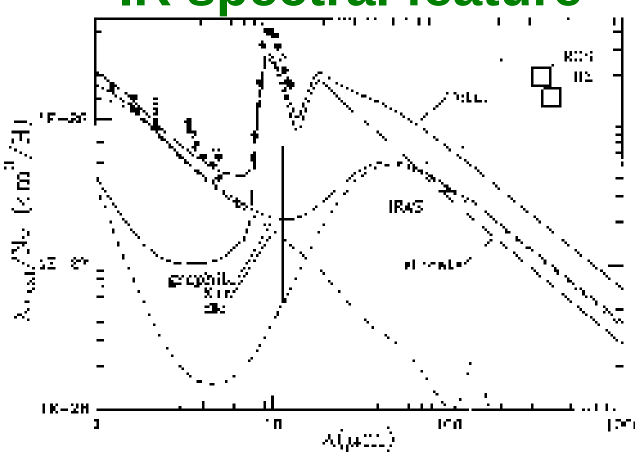
Properties of dust evolves through the processing in the ISM (sputtering, shattering, coagulation, growth ..)

composition, size, and amount of newly formed dust

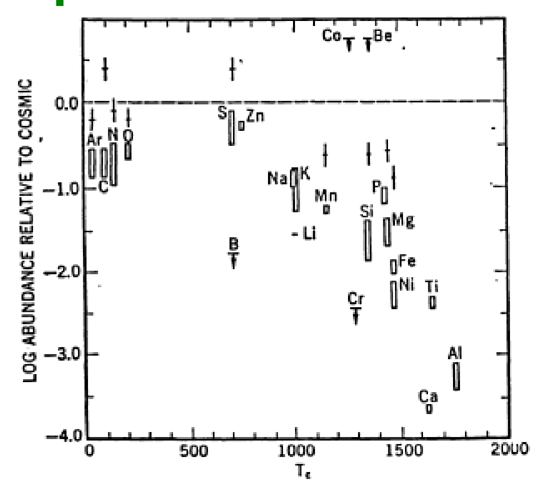
extinction curve



IR spectral feature



depletion of elements



1-2. Formation sites of dust

when, where, and how is dust formed?

in cooling gas outflows

- **abundant metals** (metal: atomic number > 5)
- **low gas temperature (T < ~2000 K)**
- **high gas density (n > ~10^6 cm^{-3})**

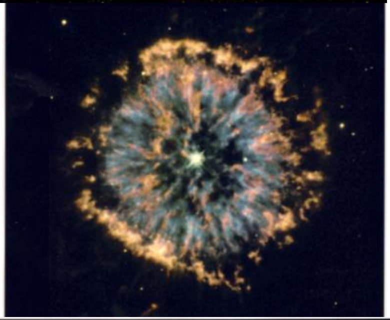
possible formation sites of dust

— expanding ejecta of supernovae

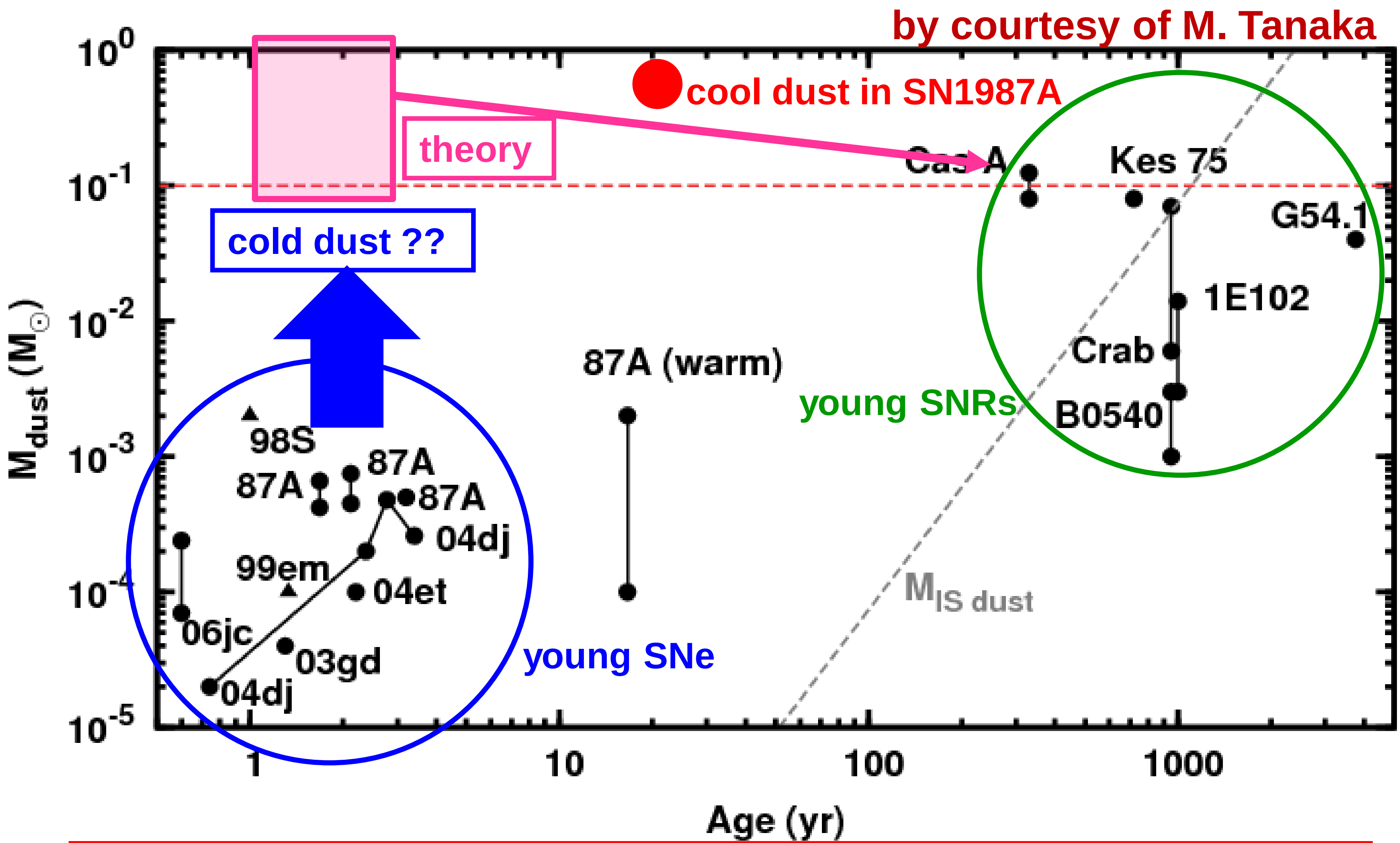
— mass-loss winds of AGB stars

— molecular clouds (grain growth only)

what kinds of, what size of, how much dust is formed

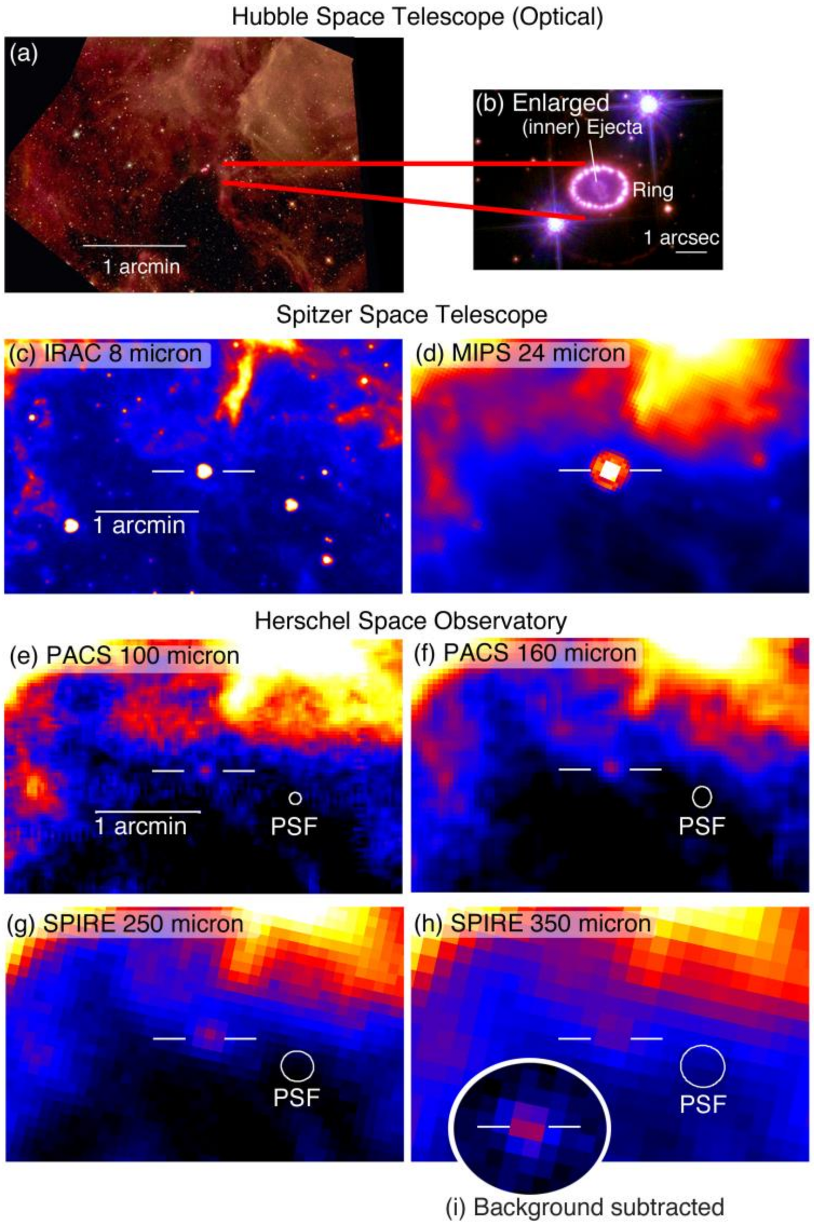

1-3. Missing-dust problem in CCSNe



There is a big difference in the mass of dust between observational estimates and theoretical predictions!!

1-3. Missing-dust problem in CCSNe

Matsuura, ..., TN, et al. 2011, Science



coo

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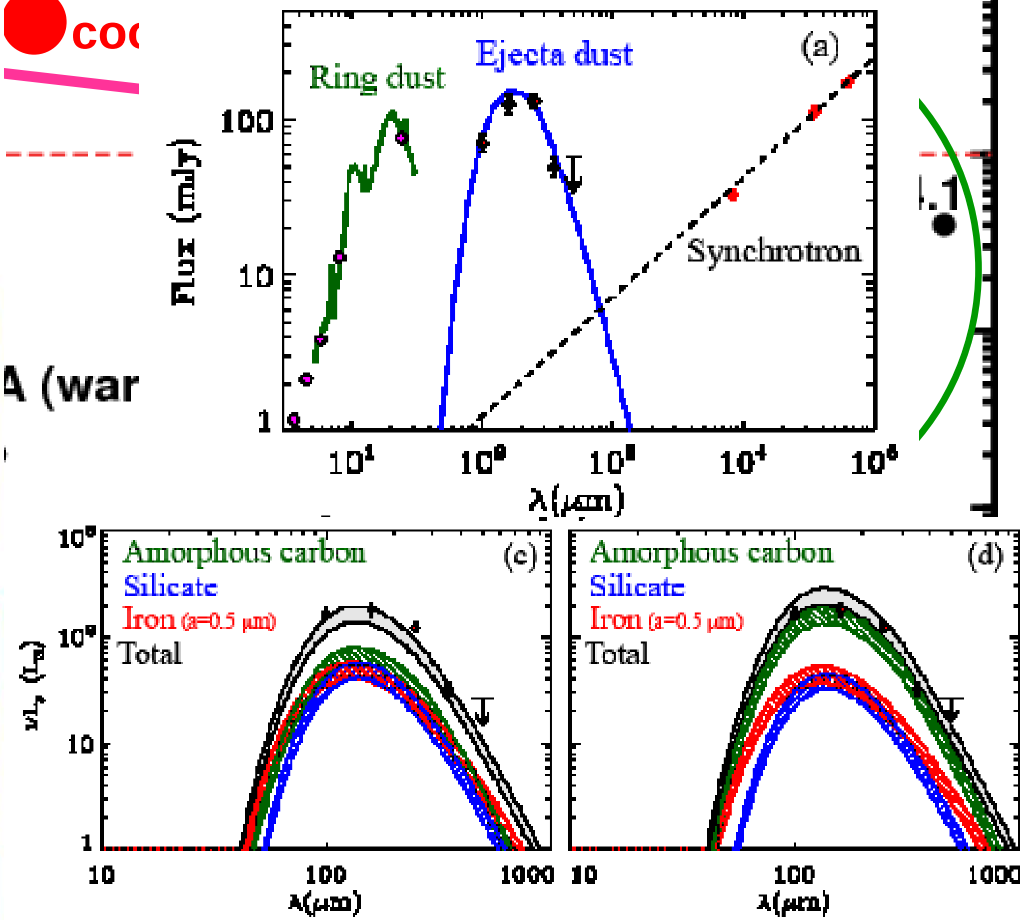
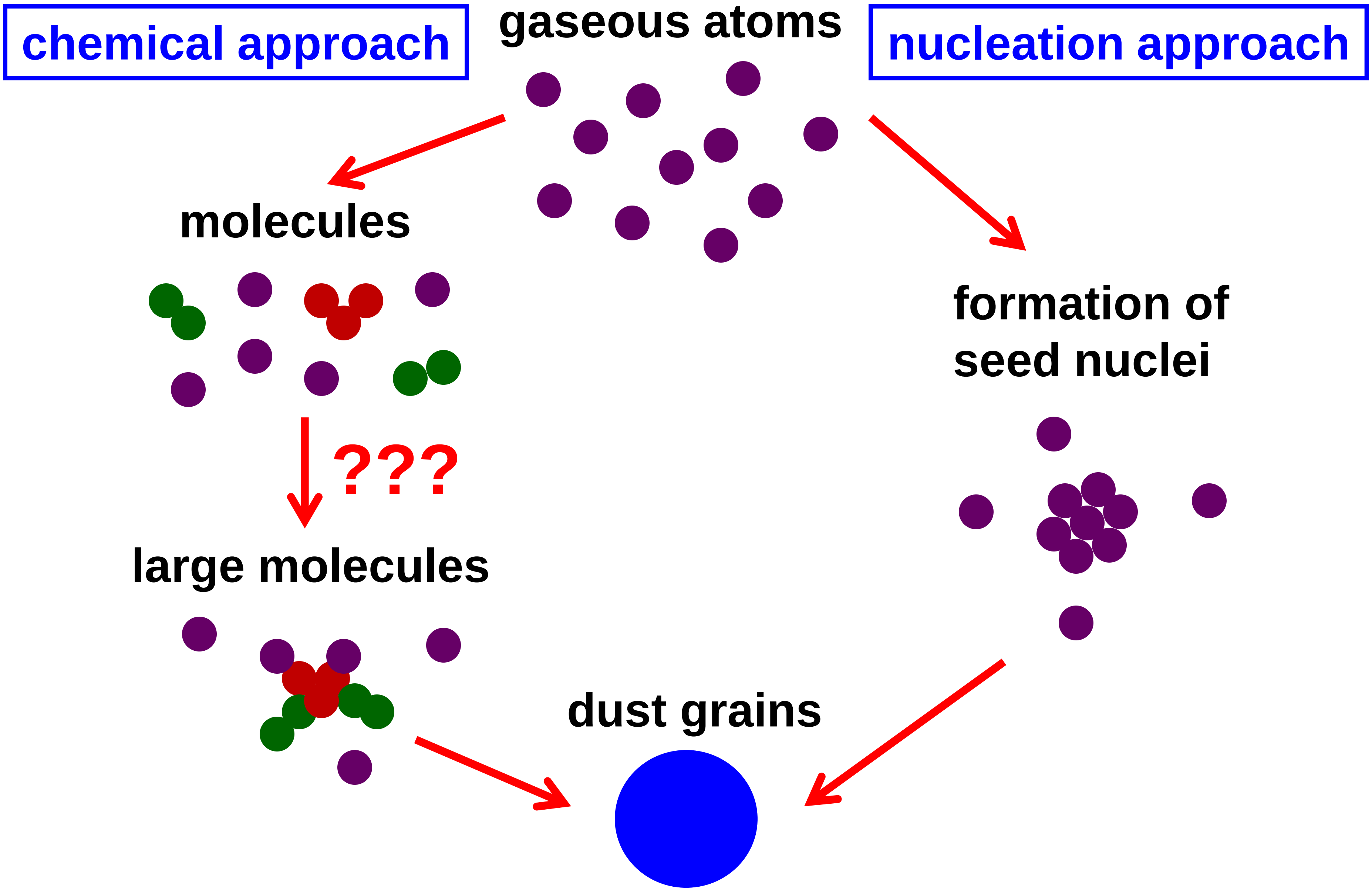


.1

Herschel detects cool (20K) dust of 0.4-0.7 Msun toward SN 1987A!

es and theoretical predictions!!

2-1. How do dust grains form?



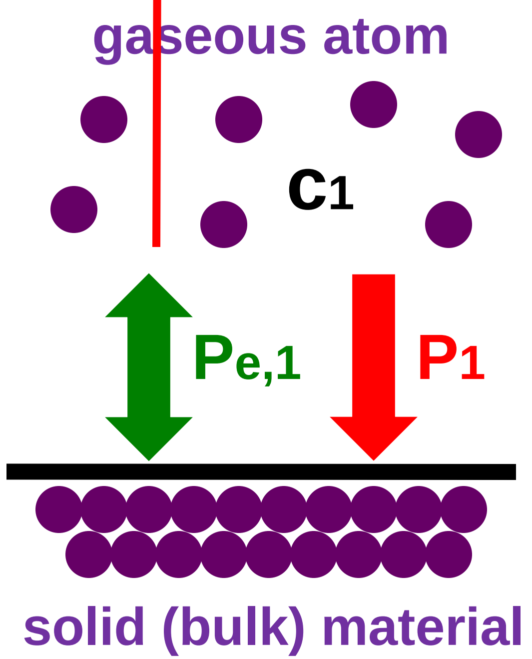
2-2. Supersaturation ratio

① T_{dust} is assumed to equal to $T=T_{gas}$

・ supersaturation ratio, S

➔ ratio of real partial pressure to equilibrium partial pressure

$$\ln S = \ln \frac{P_i}{P_{i,\mathrm{eq}}} = -\frac{\Delta G^0}{kT} + \sum_i \nu_i \ln P_i$$



For condensation of dust,

$S = P_1 / P_{e,1} > 1$

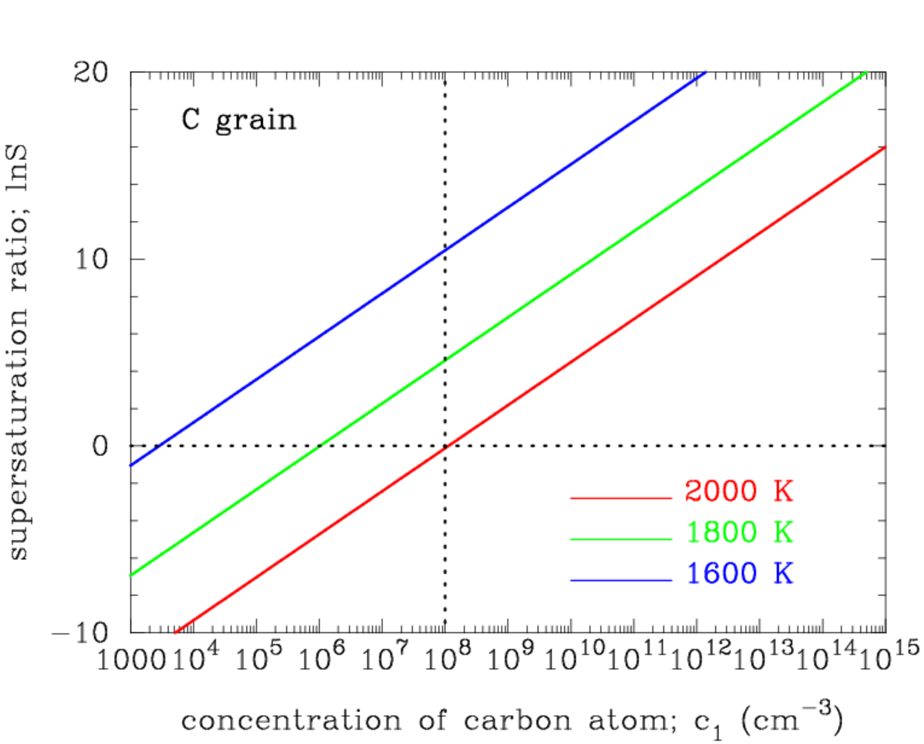
➔ $\ln S = \ln(P_1 / P_{e,1}) > 0$

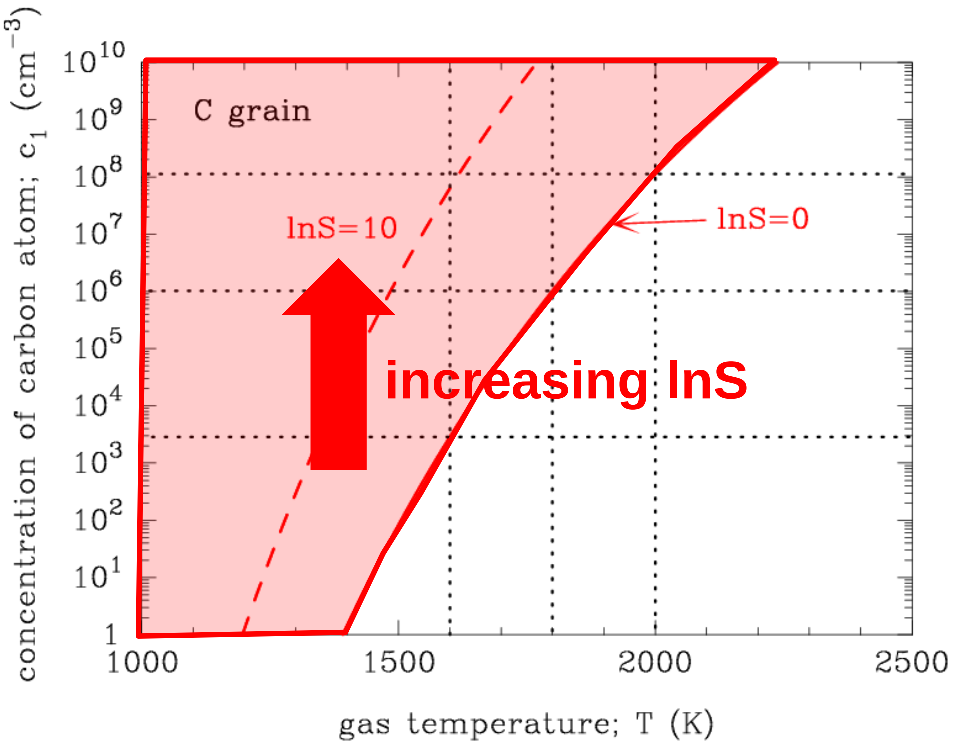
$\ln S = A / T - B + \ln(c_1 kT / P_0)$

where $-\Delta G^0/kT = A/T - B$ ($A=8.64\times10^4$, $B=19$ for C grains)

$\ln S$ is higher for lower T and higher c_1

2-3. Behavior of supersaturation ratio



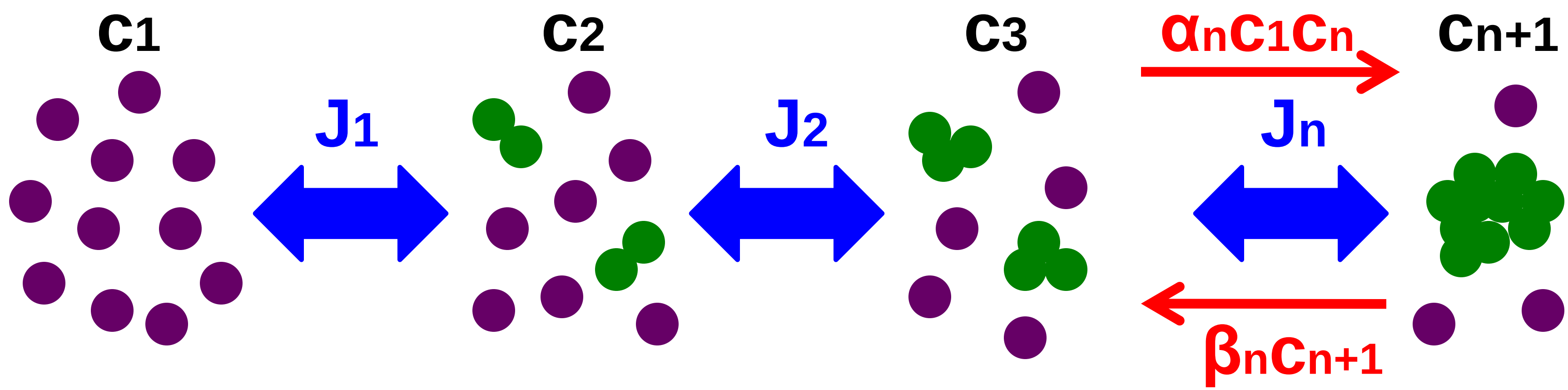


$$\ln S = A / T - B + \ln(c_1 kT / P_0)$$

lnS is higher for lower T and higher c_1

- **number density of carbon atom to be lnS > 0**
  - $c_1 \gtrsim 10^8$ cm^{-3} at 2000 K
  - $c_1 \gtrsim 10^6$ cm^{-3} at 1800 K
  - $c_1 \gtrsim 3\times10^3$ cm^{-3} at 1600 K

3-1. Concept of nucleation



・ Master equations

$$\frac{dc_n}{dt} = J_{n-1} - J_n \quad (n \geq 2)$$

$$J_n = \alpha_n\, c_1\, c_n - \beta_n\, c_{n+1} \quad (\text{unit of } J_n : \text{cm}^{-3}\ \text{s}^{-1})$$

$$\alpha_n = s_n\, S_n \langle v \rangle = s_n\, 4\pi a_0^2\, n^{2/3} \langle v \rangle$$

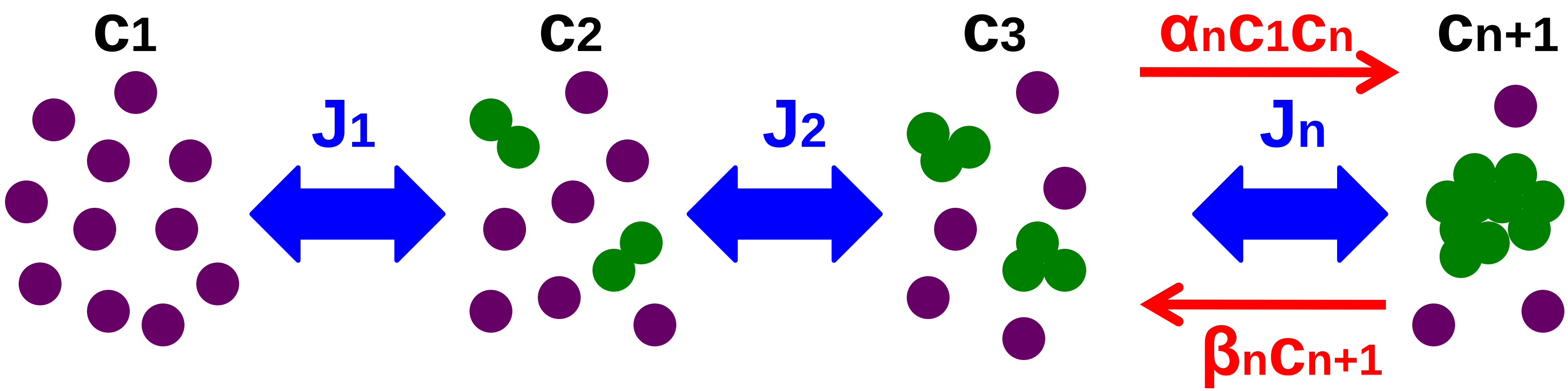
$$\beta_n = \alpha_n\, c_{e,1}\, (c_{e,n} / c_{e,n+1})$$

③ s_n=1 is assumed for every n

② coagulation between clusters is neglected

④ small clusters are assumed to be spheres

3-2. Steady-state nucleation rate



$J_n = \alpha_n c_1 c_n[1 - (c_{e,1}/c_1)(c_{e,n}/c_n)(c_{n+1}/c_{e,n+1})]$

"steady" → $J_s = J_1 = J_2 = \cdots = J_n$ ⑤

$J_s = \{1/(\alpha_1 c_1) + \sum (c_{e,1}/c_1)^n \, 1/(\alpha_n c_1 c_{e,n+1})\}^{-1}$

$(c_{e,1}/c_1)^n \, (1/c_{e,n+1}) = (1/c_1) \exp[g(n)]$

where $g(n) = \mu(n-1)^{2/3} - (n-1)\ln S$

→ $J_s = \{1/(\alpha_1 c_1) + \sum 1/(\alpha_n c_1^2) \exp[g(n)]\}^{-1}$

3-3. Critical radius

$$J_s = \{1/(\alpha_1 c_1) + \sum 1/(\alpha_n c_1^2) \exp[g(n)]\}^{-1}$$

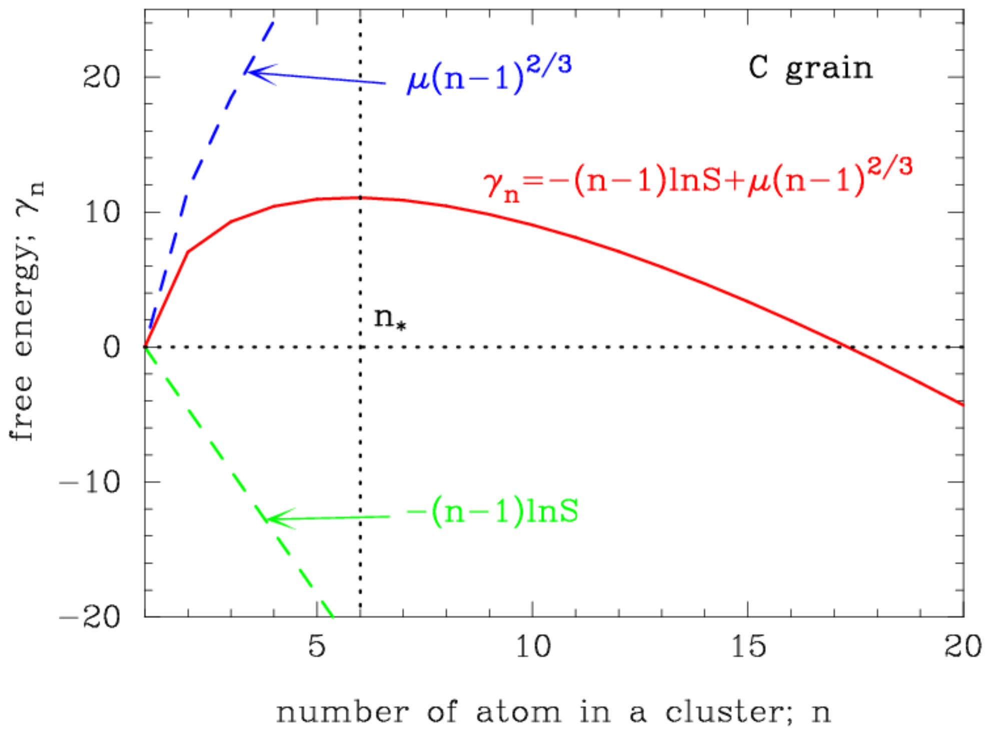
$$g(n) = \mu(n-1)^{2/3} - (n-1)\ln S$$

$$\mu = 4\pi a_0^2 \sigma / kT$$ (σ = 1400 erg cm^{-3} for C grains)

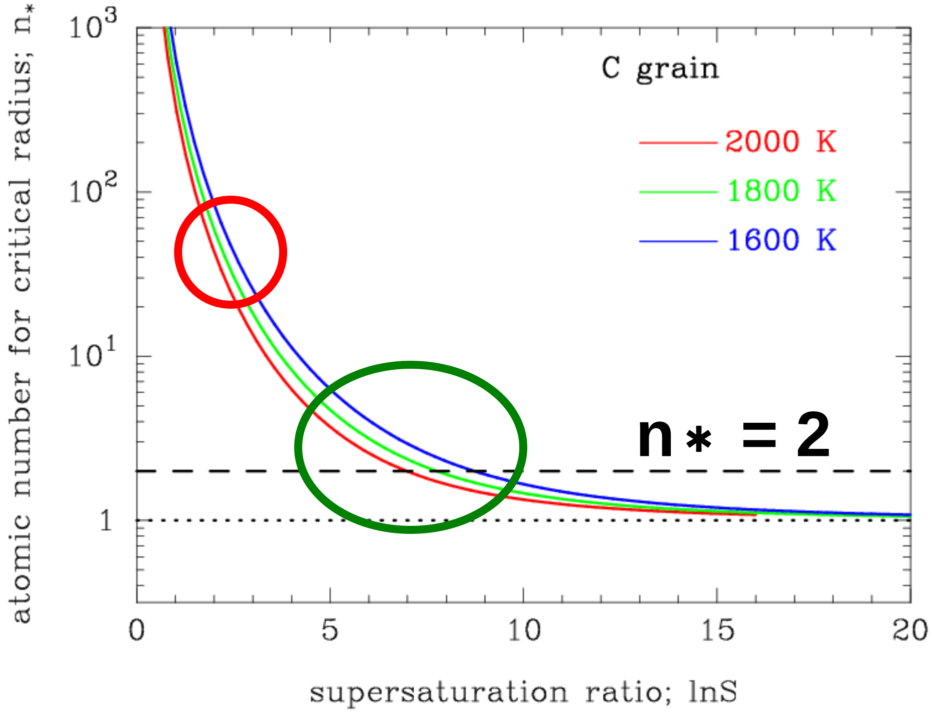
⑥ **The surface energy of small clusters is assumed to be the same as that of bulk**

critical radius

$$(n_* - 1)^{\frac{1}{3}} = \frac{2\mu}{3 \ln S}$$



3-4. Critical radius of nucleation



critical radius

$$(n_* - 1)^{\frac{1}{3}} = \frac{2\mu}{3 \ln S}$$

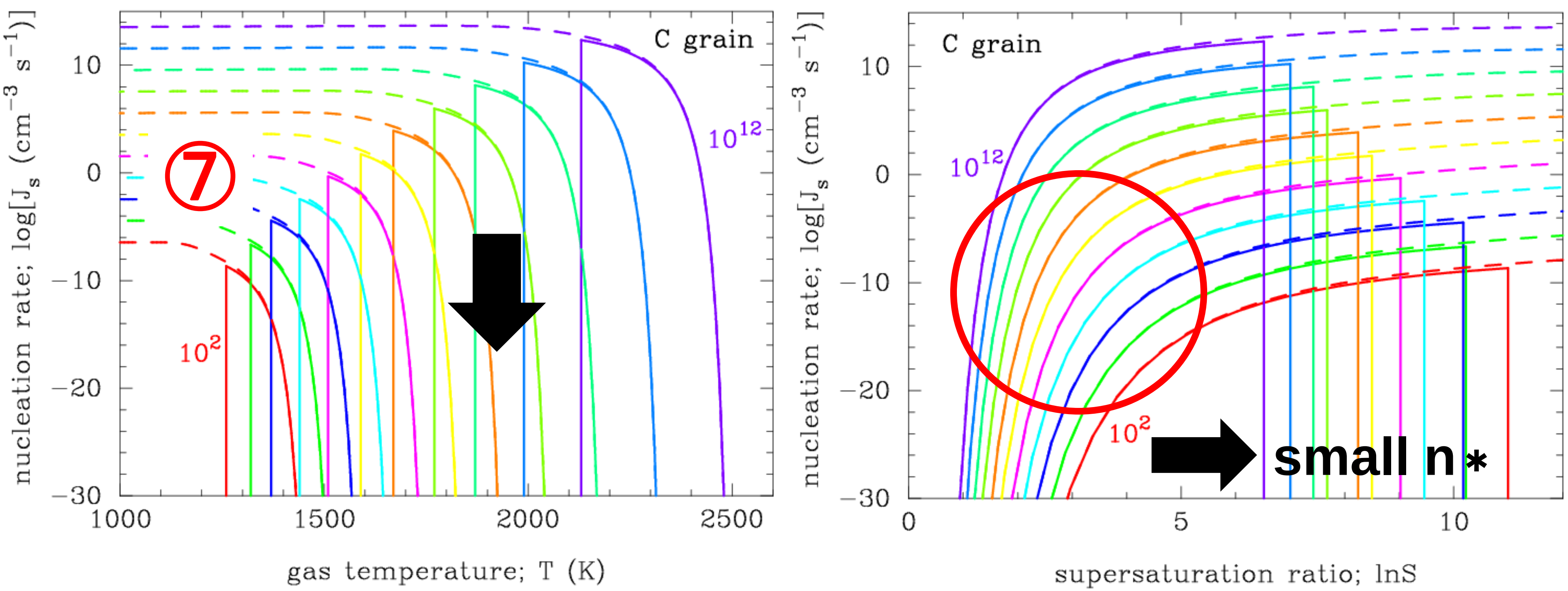
⑦ **$n_* = n_* - 1$**
assuming $n_* \gg 1$

$$J_s = \{1/(\alpha_1 c_1) + \sum 1/(\alpha_n c_1^2) \exp[g(n)]\}^{-1}$$

$$J_s(t) = \alpha_s \Omega \left(\frac{2\sigma}{\pi m_1} \right)^{\frac{1}{2}} \Pi c_1^2(t) \exp\left[-\frac{4}{27} \frac{\mu^3}{(\ln S)^2} \right]$$

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

3-5. Comparison of steady-state nucleation



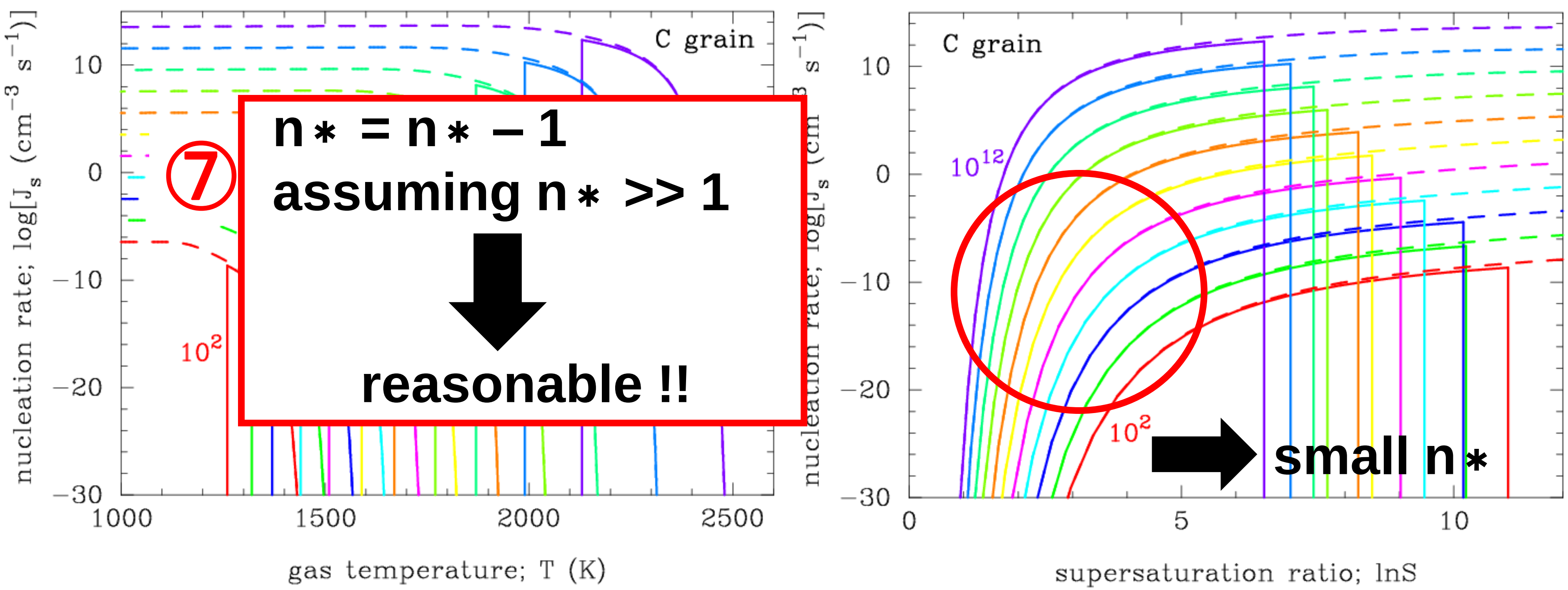
- **solid line : approximation formula for nucleation rate**

$$J_s(t) = \alpha_s \Omega \left(\frac{2\sigma}{\pi m_1} \right)^{\frac{1}{2}} \Pi c_1^2(t) \exp\left[-\frac{4}{27} \frac{\mu^3}{(\ln S)^2} \right]$$

- **dashed line : summation form for nucleation rate**

$$J_s = \{1/(\alpha_1 c_1) + \sum 1/(\alpha_n c_1^2) \exp[g(n)] \}^{-1}$$

3-5. Comparison of steady-state nucleation



- **solid line : approximation formula for nucleation rate**

$$J_s(t) = \alpha_s \Omega \left(\frac{2\sigma}{\pi m_1} \right)^{\frac{1}{2}} \Pi c_1^2(t) \exp\left[-\frac{4}{27} \frac{\mu^3}{(\ln S)^2} \right]$$

- **dashed line： summation form for nucleation rate**

$$J_s = \{ 1/(\alpha_1 c_1) + \sum 1/(\alpha_n c_1^2) \exp[g(n)] \}^{-1}$$

4-1. Non-steady nucleation rate

$$J_s = \{1/(\alpha_1 c_1) + \sum 1/(\alpha_n c_1^2) \exp[g(n)]\}^{-1}$$

"steady" → $J_s = J_1 = J_2 = \cdots = J_n$ ⑤

$$J_n = \alpha_n c_1 c_n [1 - (c_{e,1}/c_1)(c_{e,n}/c_n)(c_{n+1}/c_{e,n+1})]$$

$$\rightarrow J_n = \alpha_n c_1 \{c_n - c_{n+1} \exp[g'(n)]\}$$

$$g'(n) = \mu [(n-1)^{2/3} - (n-2)^{2/3}] - \ln S$$

・ Master equations

$$dc_n/dt = J_{n-1} - J_n \quad (2 \leq n \leq 100)$$

$T = T_0 (t / t_0)^{-3/4}$ (T_0 = 3000 K, t_0 = 150 day)

$c_1 = c_{10} (t / t_0)^{-3}$ ($c_{10} = 10^5 - 10^8$ cm^{-3})

4-2. Basic equations of dust formation

Equation of conservation for atoms

$$1 - \frac{c_1(t)}{\tilde{c}_1(t)} = \int_{t_0}^{t} \frac{J(t')}{\tilde{c}_1(t')} \frac{4\pi}{3\Omega} r^3(t,t') dt'$$

Equation of grain growth

$$\frac{\partial r}{\partial t} = \alpha_s \frac{4\pi a_0^3}{3} \left(\frac{kT}{2\pi m_1} \right)^{\frac{1}{2}} c_1(t) = \frac{1}{3} a_0 \tau_{\rm coll}^{-1}$$

⬇

· number density of dust grain, $n_{\rm gr}$

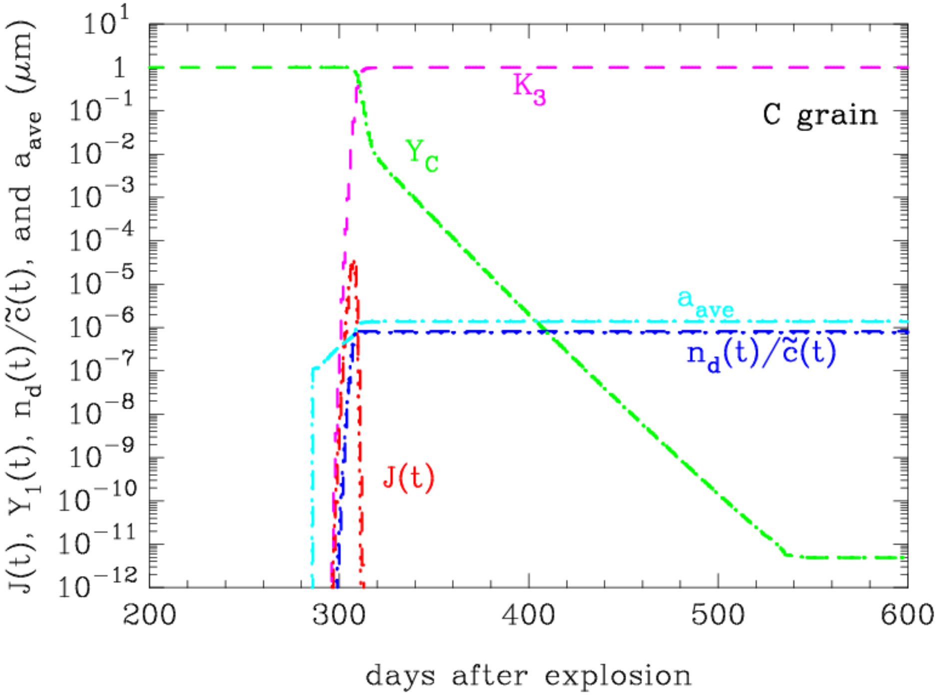
$$\frac{n_{\rm gr}}{\tilde{c}_1(t)} = \int_{t_0}^{t} \frac{J(t')}{\tilde{c}_1(t')} dt'$$

· radius of grain nucleated at t_0 and measured at t, $r(t, t_0)$

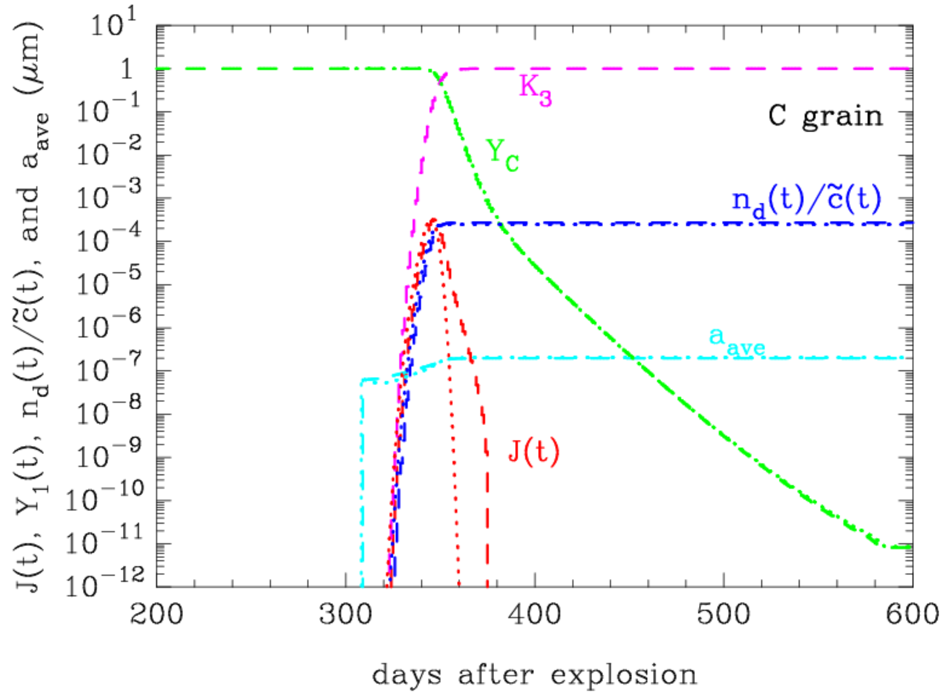
$$r(t,t_0) = r_* + \int_{t_0}^{t} \frac{1}{3} a_0 \tau_{\rm coll}^{-1}(t') dt'$$

4-3. Steady vs. Non-steady (1)

$c_{10} = 10^8$ cm^{-3}



$c_{10} = 10^7$ cm^{-3}

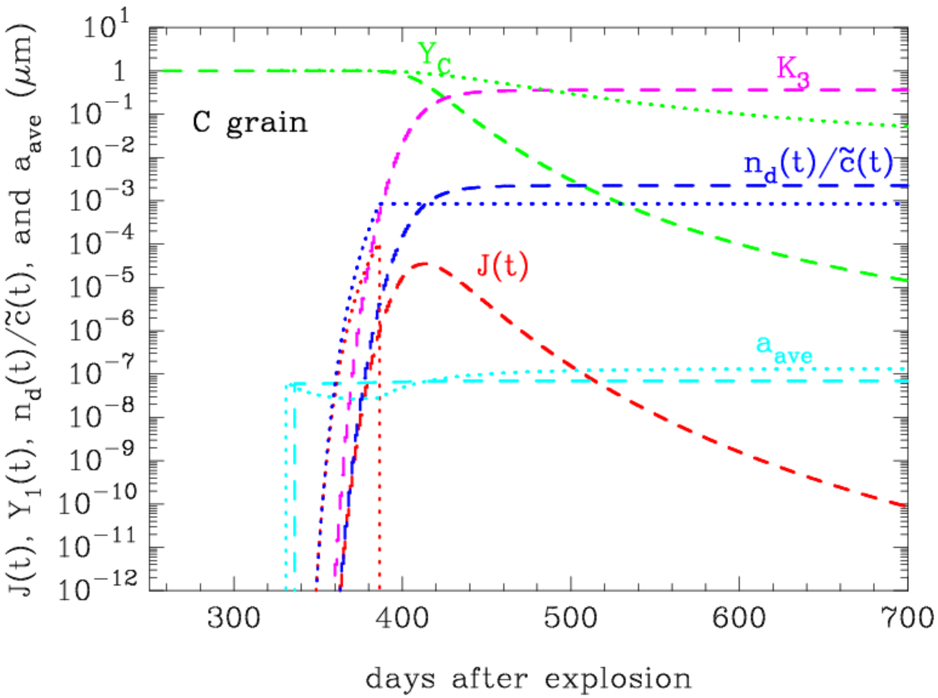


- dashed line : steady-state nucleation rate
- dotted line : non-steady-state nucleation rate

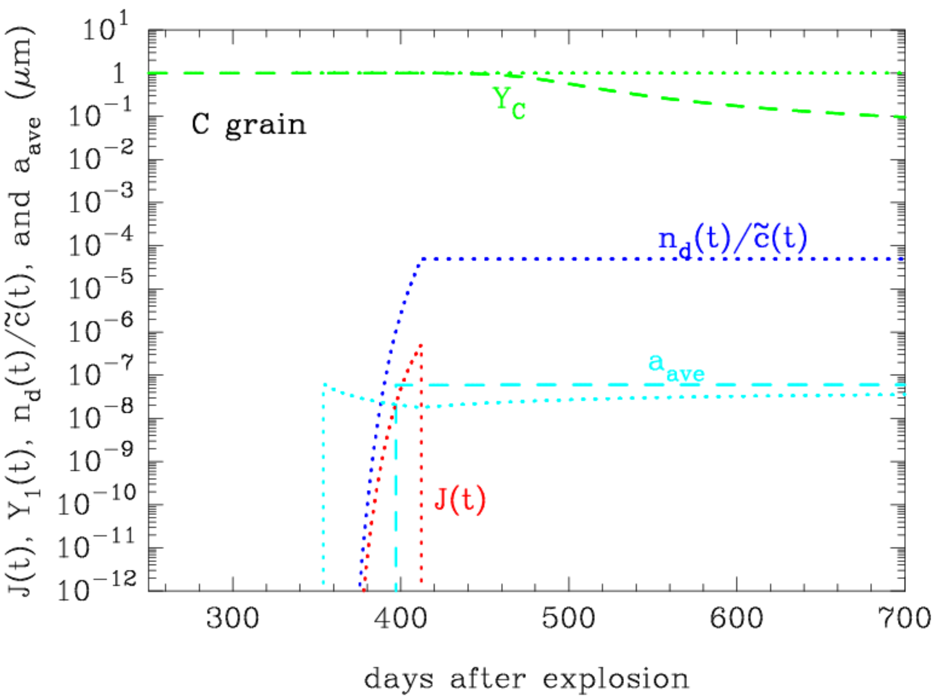
The difference between steady and non-steady nucleation is small for higher initial densities

4-4. Steady vs. Non-steady (2)

$c_{10} = 10^6$ cm^{-3}



$c_{10} = 10^5$ cm^{-3}



- **dotted line : steady-state nucleation rate**
- **dashed line : non-steady-state nucleation rate**

The difference between steady and non-steady nucleation is significant for lower densities

5-1. Relaxation time

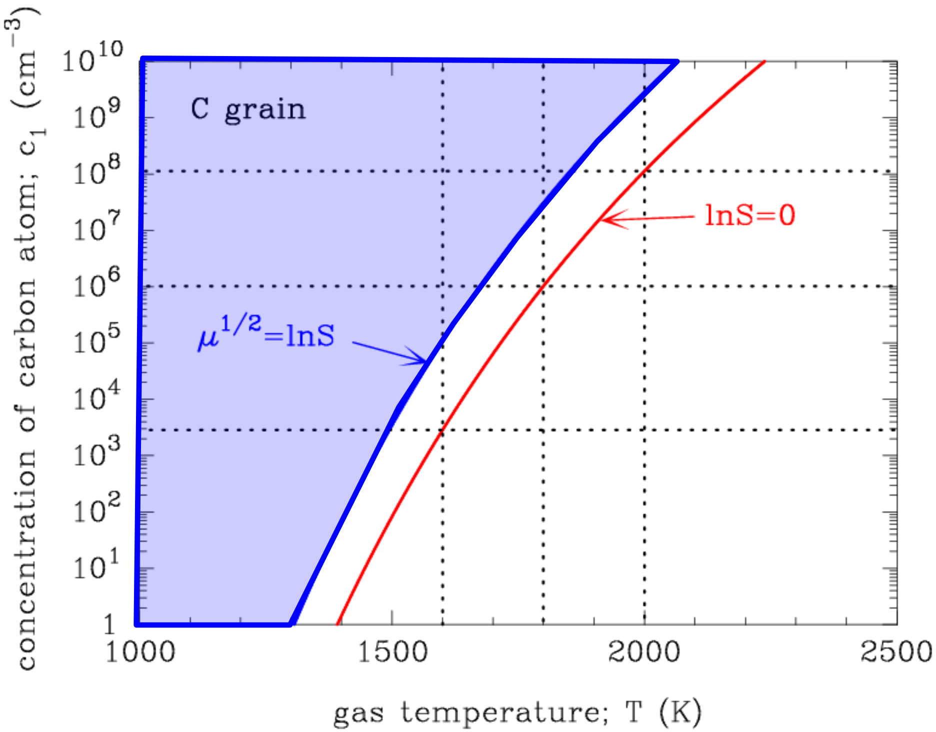
· relaxation time, τ_{relax}

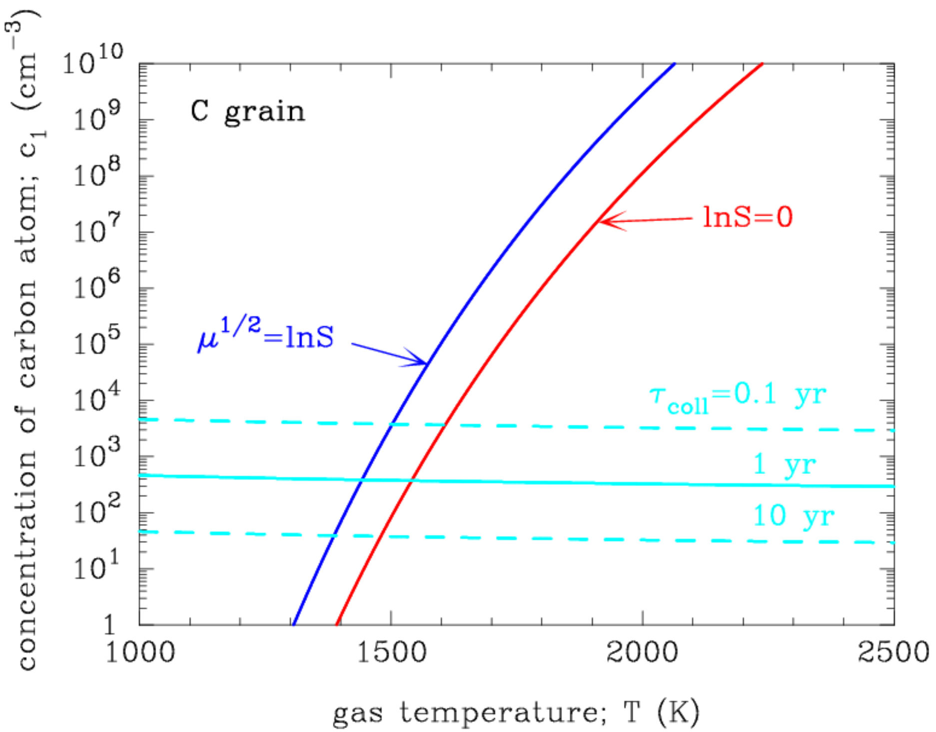
$$\rightarrow \tau_{relax} = \tau_{coll} [(\ln S)^2 / \mu]$$

$$\tau_{coll} = [s_n 4\pi a_0^2 \langle v \rangle c_1]^{-1}$$

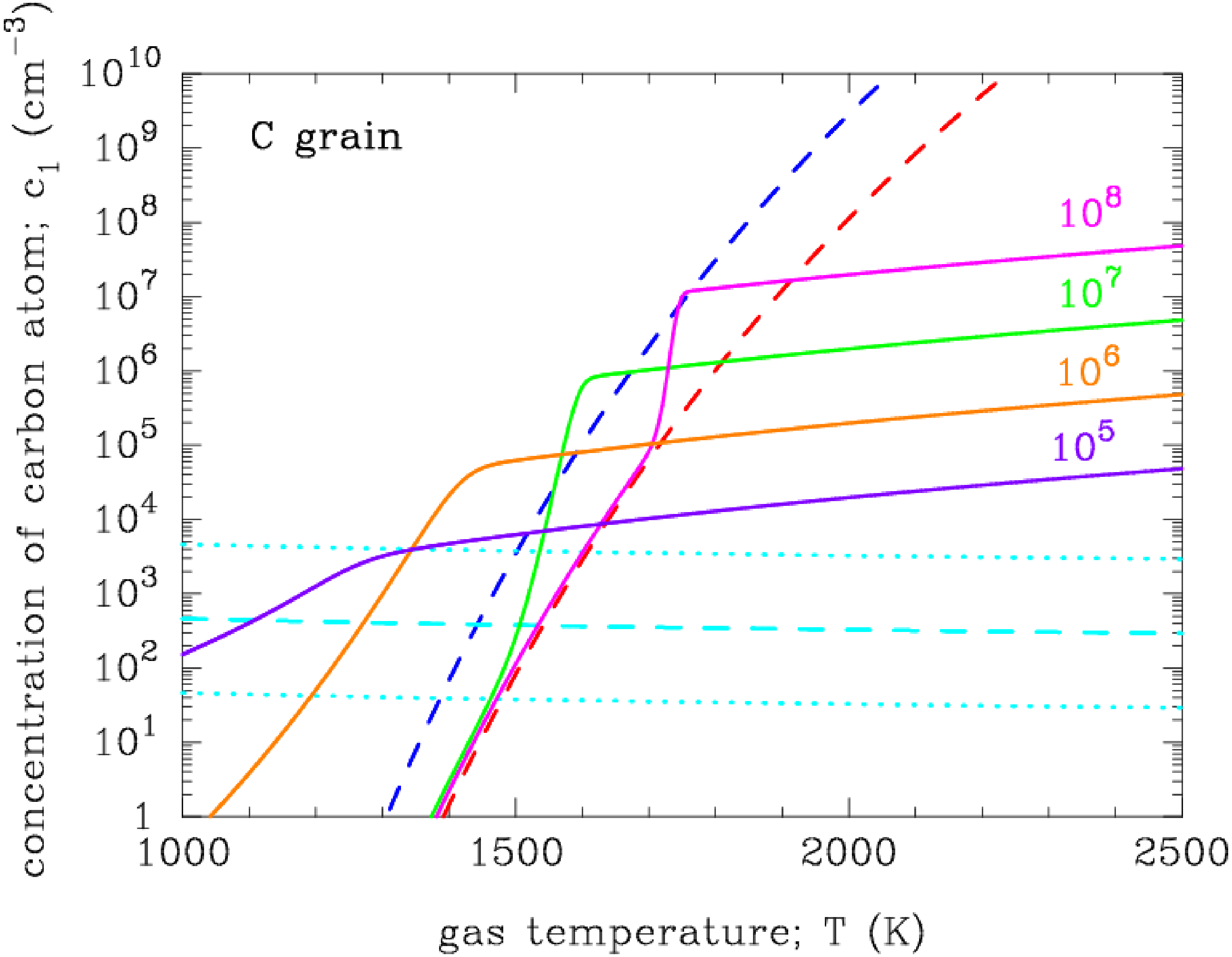
$\tau_{relax} / \tau_{coll} = [(\ln S)^2 / \mu] < 1 \rightarrow$ steady

$\tau_{relax} / \tau_{coll} = [(\ln S)^2 / \mu] > 1 \rightarrow$ non-steady





5-2. Trajectories on T-c_1 plot for dust formation



- higher c_1 ➔ dust condenses at lower lnS ➔ steady
- lower c_1 ➔ dust condenses at higher lnS ➔ non-steady

6. Current problems in dust formation theory

① Dust temperature is assumed to be equivalent to gas temperature

② The coagulation between clusters is neglected

③ The sticking probability is assumed to be one

④ Small clusters are assumed to be spherical

⑤ $J_s = J_1 = J_2 = \cdots = J_{n_*}$ for steady-state nucleation

⑥ The surface energy of bulk material is used as that of small clusters

⑦ $n_* >> 1$ is assumed for classical nucleation rate
➔ this assumption is valid