Abstract

ISO

Formation of Crystalline Silicate in Circumstellar Envelopes of Oxygen–Rich AGB Stars

1. Introduction

- ISO SWS Observations : Waters *et al.*, 1996; A&A **315**, L361
  Emission features between 20 and 45μm around evolved oxygen–rich stars

  - $\diamond$ identification of crystalline silicate features
    - $* \sim 33.5\mu$m $\rightarrow$ olivine $(\mathrm{Mg}_x, \mathrm{Fe}_{1-x})_2 \, \mathrm{SiO}_4$
    - $* \sim 40.4\mu$m $\rightarrow$ pyroxene $(\mathrm{Mg}_x, \mathrm{Fe}_{1-x}) \, \mathrm{SiO}_3$
    - $* \ \underline{x \sim 1}$
  - $\diamond$ the features becomes prominent with decreasing the color temperature
  - $\diamond$ the coexistence of amorphous and crystalline silicate ;
    (amorphous silicate from 10μm feature in NML Cyg)

- steady state dust driven winds

(1) a kinetic theory of crystallization of amorphous silicate based on
   the classical nucleation theory and the laboratory experiment data

(2) the model of dust formation and the temporal evolution of dust
   temperature

(3) Formation of crystalline silicate and the resulting spectral feature, based
   on the result of dust condensation calculations.

2. Crystallization of amorphous silicate

- Formulation of crystallization in amorphous phase based on the classical nucleation theory (crystallization in melt; e.g. Seki and Hasegawa (1981))

    * spontaneous nucleation of crystalline nuclei and the growth

    * diffusion controls the kinetics

2-1 Basic Equations

- nucleation rate of crystalline nuclei $J(t)$

$$J(t) = \frac{2\pi}{\Omega} \left(\frac{\sigma}{kT}\right)^{1/2} \frac{D}{\Omega^{2/3}} \exp\left(-\frac{\Delta G^*}{kT}\right) \quad \text{with} \quad \Delta G^* = \frac{16}{3}\pi \frac{\sigma^3}{\Delta G_{\rm v}}$$

- growth rate of crystal ω

$$\omega = \frac{d\rho(t)}{dt} = \frac{1}{\Omega^{1/3}} D \left[1 - \exp\left(-\frac{\Delta G_{\rm v}}{kT}\right)\right]$$

- volume fraction of crystalline phase $\theta(t)$

$$1 - \theta(t) = \exp\left[-\int_{t=0}^{t} J(t')\frac{4\pi}{3}\rho^3(t,t'))\,dt'\right] \qquad \text{(by Kolmogorov)}$$

Ω ; the molecular volume

σ ; the interfacial energy between crystalline and amorphous phases

$D = D_0 \exp\left(-E_{\rm a}/kT\right)$; the self diffusion coefficient

$\Delta G_{\rm v} = LT_{\rm m}/(T_{\rm m} - T)$; the Gibbs free energy difference between amorphous and crystalline phases

- No reliable basic data available for amorphous and crystalline silicates

- Comparison with the laboratory experiment

    $\Longrightarrow$ evaluation of the basic data

2–2 Evaluation of the basic data

- Laboratory experiment by Hallenbeck and Nuth (1998, Icarus **131**, 198)

  ⋄ annealing of magnesium silicate smoke at given temperatures

  ⋄ IR spectroscopy as a function of annealing time and temperature

  ⋄ Establishment of a dual maxima and then the change of the spectral feature stall at a time written by

$$t_{\text{stall}} = A \exp \left(\frac{E_c}{kT} \right)$$

- Comparison of the measured spectrum with the absorption spectrum calculated by mixing

  a–MgSiO$_3$ by Dorschner et al. (1995) and c–olivine by Koike (1998)
  $\Longrightarrow$

  ⋄ spectrum change during annealing $\rightarrow$ change in degree of crystallization
  ⋄ characteristics of spectrum at stall $\rightarrow$ $\theta = 0.2 \sim 0.25$

- The volume fraction of crystalline phase for a constant temperature is

$$\theta \left(t \right) = 1 - \exp \left[- \left(\frac{t}{\tau_{\text{c}}} \right)^4 \right]$$

  with the characteristic time scale of crystallization

$$\tau_{\text{c}} = \left(\frac{3}{2\pi^2} \right)^{1/4} \left(\frac{kT}{\sigma} \right)^{1/8} \frac{\Omega^{2/3}}{D_0} \exp \left[\frac{1}{kT} \left(E_{\text{a}} + \frac{4\pi}{3} \frac{\sigma^3}{\Delta G_{\text{v}}^2} \right) \right] = \tilde{A} \exp \left(\frac{\tilde{E}_{\text{c}}}{kT} \right)$$

- Fitting the experiment data by the above equation with $t_{\text{stall}} \simeq 0.7\tau_{\text{c}}$,

  $\Longrightarrow$

  $\ln D = 1.47 \times 10^2 - 1.723 \times 10^5/T$ $\qquad$ $\sigma = 731$ dyne/cm

  $\Delta G_{\text{v}} = 1.851 \times 10^4 \, T_{\text{m}}/(T_{\text{m}} - T)$

  for fixed $\Omega = 5.226 \times 10^{-23}$cm^3 and $T_{\text{m}} = 1830$ K

3. Formation of dust grains around O–rich AGB stars

see Kozasa & Sogawa 1997, Ap&SS 251, 165; 1998, Ap&SS 255, 437

⋄ Al_2O_3 grains condense in the inner sonic region
  at $T_{gas} = 1350 \sim 1400$ K, and r_{rg} $(Al_2O_3) = 0.11 \sim 0.2\mu$m

⋄ Accretion of silicate on Al_2O_3 grain starts slightly inside the sonic point
  at $T_{gas} = 1040 \sim 1100$ K and r_{gr}(core–mantle)$= 0.13 \sim 0.3\mu$m

⋄ homogeneous silicate grains condense in the supersonic region
  at $T_{gas} = 920 \sim 990$ K and r_{gr} (silicate) $= 0.0012 \sim 0.006\mu$m

⋄ mass fraction α_m of silicate in the core–mantle grains increases with
  increasing $\dot{M}$; $\alpha_m = 0.03 \sim 0.22$

3–2 Temperatures of dust grains

• Radiation transfer calculations by the Monte–Carlo method

  ⋄ spectral energy distribution

  ⋄ temperature of dust grains after the formation
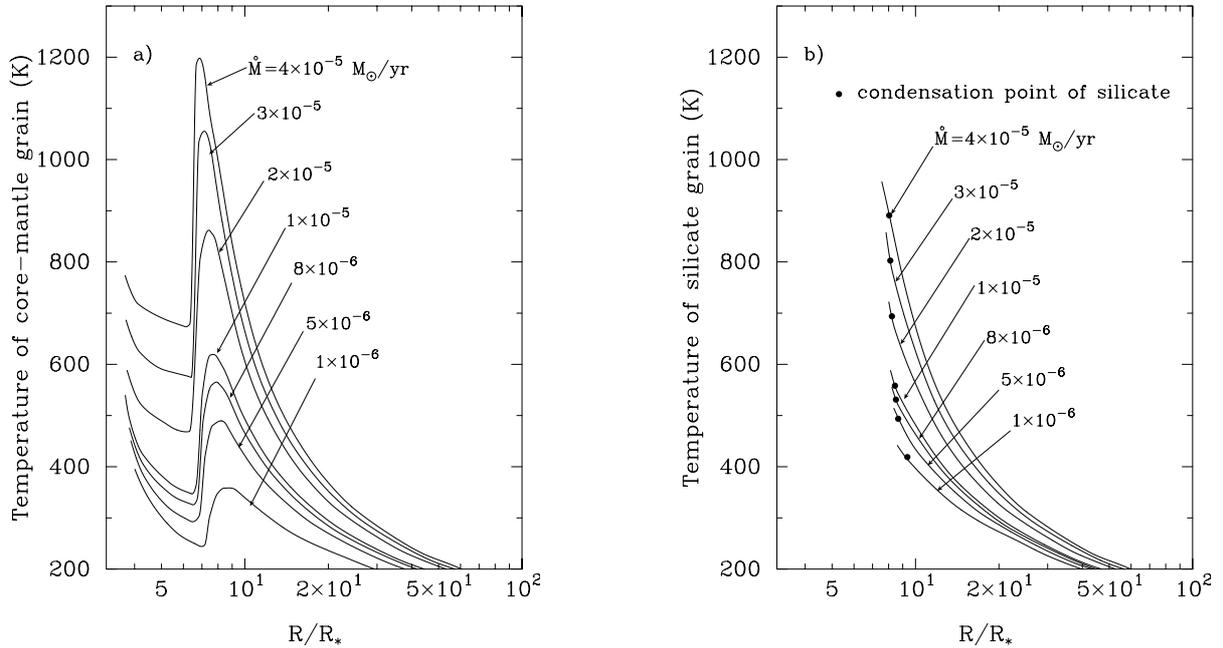
1: Temperatures of dust grains after their formation for the given mass–loss rates; a) for Al_2O_3 and heterogeneous grains, and b) for homogeneous silicate grains

4. Formation of crystalline silicate and the spectral features

4–1 Formation of crystalline silicate

- The volume fraction of crystalline silicate in the grains is calculated by

$$\frac{\partial \theta}{\partial t} = \frac{1 - \theta}{\tau_{\mathrm{c}}}$$

  along the thermal history of dust grains undergoing after the formation,

- The characteristic time scale of crystallization τ_{c} is very sensitive to T_{gr}:

$$
\begin{aligned}
T_{\mathrm{gr}} = 1100 \text{ K} \qquad & \tau_{\mathrm{c}} \sim 20 \text{ secs.} \\
1000 \text{ K} \qquad & \sim 30 \text{ days} \\
900 \text{ K} \qquad & \sim 10^{6} \text{ years}
\end{aligned}
$$

  $\Longrightarrow$

  crystallization is impossible for $T_{\mathrm{gr}} \leq 900$ K in the circumstellar envelopes

- The result of calculations:

  $\diamond$ $\dot{M} \leq 2 \times 10^{-5} M_{\odot}/\mathrm{yr}$:   no crystalline silicate $(\theta < 10^{-6})$

  $\diamond$ $\dot{M} \geq 3 \times 10^{-5} M_{\odot}/\mathrm{yr}$:

   $*$ silicate in the core–mantle grains is completely crystallized $(\theta = 1)$.
   $*$ homogeneous silicate grains remain amorphous.

4–2 The spectral feature

- crystalline olivine feature appears at $\sim 33.5 \mu$m
  not so prominent but distinguishable for $\dot{M} \geq 3 \times 10^{-5} M_{\odot}/\mathrm{yr}$

- 10μm feature is dominated by the thermal radiation from homogeneous silicate grains (amorphous) and tend to be in absorption

5 Conclusions

(1) Silicate in the core–mantle grains is crystallized for $\dot{M} \geq 3 \times 10^{-5} M_\odot/\mathrm{yr}$

(2) homogeneous silicate grains remain amorphous

(3) crystalline olivine feature appears around $33.5\mu\mathrm{m}$;
   the feature could tend to be prominent with increasing $\dot{M}$

(4) homogeneous silicate grains dominate the $10\mu\mathrm{m}$ feature;
   the feature tend to be in absorption.

(5) the mass fraction of silicate in the core–mantle grains
   increases with increasing $\dot{M}$

   ⋄ mass fraction of crystalline silicate increases
   ⋄ crystalline silicate emission feature could tend to be more distinctive

⊙ The observed crystalline feature is a diagnostic of the mass loss
   rate.

⊙ Silicate in the core–mantle grains can be crystallized by the
   thermal processing in the massive stellar winds in the latest stage
   of stellar evolution.