Dust formation around old stars and its feedback on the dust forming system

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Necessary conditions for dust formation

- suitable chemistry $\Rightarrow$ condensing species (high-T condensate)
- "low" temperature $\Rightarrow$ stable clusters
- "high" density $\Rightarrow$ growth to macroscopic grains

$\Rightarrow$ Stellar sources of interstellar dust

Asymptotic Giant Branch stars
Red Giant Branch stars, Red Supergiants
ejecta of Supernovae and Novae
Wolf-Rayet stars, RCrB stars

(also Brown Dwarfs, but the material is not injected to the ISM)
Two different approaches to describe dust formation

nucleation theory

Kinetic nucleation theory
   Critical cluster
Moment equations
   =>
Possibility to construct self-consistent dust shell models

Ex: Gail, Gauger, Patzer, Sedlmayr, Winters, Woitke
   Dorfi, Feuchtinger, Höfner

non-equilibrium chemistry

Chemical pathway
   Critical reaction
Rate network
   =>
Possibility to construct complex non-equilibrium chemical models under prescribed thermodynamical conditions

Ex: Cherchneff, Gobrecht, Plane
Dust formation

is a chemical process

E.g.:

\[(\text{Al}_2\text{O}_3)_{N-1} + \text{Al}_2\text{O}_3 \rightleftharpoons (\text{Al}_2\text{O}_3)_N\]
\[(\text{Al}_2\text{O}_3)_{N-1} + 2 \text{Al} + 3 \text{O} \rightleftharpoons (\text{Al}_2\text{O}_3)_N\]
\[(\text{Al}_2\text{O}_3)_{N-1} + \text{Al}_2\text{O} + 2 \text{H}_2\text{O} \rightleftharpoons (\text{Al}_2\text{O}_3)_N + 2 \text{H}_2\]
\[(\text{TiO}_2)_{N-1} + \text{TiO}_2 \rightleftharpoons (\text{TiO}_2)_N\]

\[(\text{C})_{N-1} + \text{C} \rightleftharpoons (\text{C})_N\]
\[(\text{C})_{N-2} + \text{C}_2 \rightleftharpoons (\text{C})_N\]
\[(\text{C})_{N-2} + \text{C}_2\text{H}_2 \rightleftharpoons (\text{C})_N + \text{H}_2\]
\[(\text{SiC})_{N-1} + \text{SiC} \rightleftharpoons (\text{SiC})_N\]

... 

Most simple case: **monomer addition**, linear chain, \(M_1\) is the monomer, e.g., \(\text{Al}_2\text{O}_3\), \(\text{TiO}_2\), \(\text{C}_1\), \(\text{SiC}\):

\[M_1 \rightleftharpoons M_2 \rightleftharpoons \ldots \rightleftharpoons M_{N-1} \overset{\tau_{gr}^{N-1}}{\underset{\tau_{ev}^{N-1}}{\rightleftharpoons}} M_N \overset{\tau_{gr}^N}{\underset{\tau_{ev}^N}{\rightleftharpoons}} M_{N+1} \rightleftharpoons \ldots \rightleftharpoons M_{N_{max}} \rightleftharpoons \ldots\]

Growth time scale:

\[
\frac{1}{\tau_{gr}^{N-1}} = f_1 v_{N-1,1}^{rel}(T_g) A(N-1) \alpha(M_1, N-1, T_g, T_{\alpha}(N-1))
\]

Evaporation time scale:

\[
\frac{1}{\tau_{ev}^N} = A(N) \beta(T_{\alpha}(N))
\]
Thermodynamic equilibrium (phase equilibrium, thermal equilibrium \((T_g = T_d)\), chemical equilibrium, denoted by \(\circ\)):

**Detailed balance**

\[
\frac{1}{\tau_{ev}} = \frac{1}{\tau_{gr}}
\]

\[
\Rightarrow
\]

\[
\frac{1}{\tau_{ev}} = f_1 \nu_{N-1,1}^\circ (T_d) A(N-1) \alpha (T_d, T_d)
\]

\[
\Rightarrow
\]

**Net growth rate:**

\[
\frac{1}{\tau} = \frac{1}{\tau_{gr}^{N-1}} - \frac{1}{\tau_{ev}^{N-1}} = \frac{1}{\tau_{gr}^{N-1}} \left[ 1 - \frac{p_{vap}(T_d) \nu_{N-1,1}^\circ (T_d)}{f_1 k T_d \nu_{N-1,1}^\rel (T_d) \alpha (T_d, T_d)} \right]
\]

\[
= \frac{1}{\tau_{gr}^{N-1}} \left[ 1 - \frac{1}{S b_{therm}} \frac{1}{b_{chem}} \right]
\]

\[
S = \frac{f_1^{CE} k T_g}{p_{vap}(T_g)}, \quad b_{therm} = \frac{p_{vap}(T_g)}{p_{vap}(T_d)} T_g \nu_{N-1,1}^\circ (T_d) \alpha (T_d, T_d), \quad b_{chem} = \frac{f_1}{f_1^{CE}}
\]

\[
S b_{therm} b_{chem}
\left\{
\begin{array}{l}
> 1 : \text{net growth} \\
= 1 : \text{stable} \\
< 1 : \text{net evaporation}
\end{array}
\right.
\]
Critical cluster

Credit: A. Goeres
Nucleation barrier at the critical cluster of size $N_c(T) \sim (10)$ separating the nucleation regime from the growth regime

high supersaturation ratios are required

⇒ Dust formation can be conceived as a two-step process:

1. **Formation of the critical cluster (“nucleation”)**
   - Stationary process in circumstellar dust shells
   - Properties of the clusters have to be known

2. **Growth of these clusters to macroscopic grains**
   - Time dependent treatment necessary
   - Thermodynamic description appropriate
Nucleation rates in the p-T plane
(=> chemical equilibrium)

C/O = 0.5

C/O = 1.3

SiO

Fe

C

TiO₂

Al₂O₃
Equilibrium geometries of (TiO$_2$)$_N$ compounds


Lee et al. 2015, A&A 575, A11
(TiO$_2$)$_N$ cluster distribution

Lee et al. 2015, A&A 575, A11
TiO$_2$ in VY CMa

Equilibrium structures of Ti$_x$O$_y$ systems

(Jeong et al. 2000, J.Phys.B 33, 3417)

\[
\begin{align*}
N=1 & \quad \text{TiO}_2 (C_{2v}) \\
\quad & \quad \text{TiO}_3 (C_3v) \\
\end{align*}
\]

\[
\begin{align*}
N=2 & \quad \text{Ti}_2\text{O}_4 (C_{2v}) \\
         & \quad \text{Ti}_2\text{O}_3 (C_{2v}) \\
         & \quad \text{Ti}_2\text{O}_2 (C_{2v}) \\
\end{align*}
\]

\[
\begin{align*}
N=3 & \quad \text{Ti}_3\text{O}_6 (C_2) \\
         & \quad \text{Ti}_3\text{O}_a (C_{2v}) \\
         & \quad \text{Ti}_3\text{O}_3 (C_{2v}) \\
\end{align*}
\]

\[
\begin{align*}
N=4 & \quad \text{Ti}_4\text{O}_8 (C_{2v}) \\
\quad & \quad \text{Ti}_4\text{O}_a (C_{2v}) \\
\end{align*}
\]

\[
\begin{align*}
N=5 & \quad \text{Ti}_5\text{O}_10 (C_2) \\
\quad & \quad \text{Ti}_5\text{O}_a (C_{2v}) \\
\end{align*}
\]

\[
\begin{align*}
N=6 & \quad \text{Ti}_6\text{O}_{12} (C_{2v}) \\
\end{align*}
\]

“...it is shown that titanium oxides, especially TiO$_2$ molecules, are the most probable candidates to form the primary condensates in circumstellar shells of M stars”

(Gail & Sedlmayr 1998, Faraday discussions 109, 303)

Mass-losing red supergiant VY CMa

First detection of TiO$_2$ in space (NOEMA/SMA)

(Kaminski et al. 2013, A&A 551, A113)
Binding energies of $\text{Al}_x\text{O}_y$ compounds

Equilibrium geometries of \((\text{Al}_2\text{O}_3)_n\) clusters and vibrational transitions

Non-equilibrium chemistry of AlO bearing species

at $r = 1R_*$

$\text{Al} + \text{OH} \rightarrow \text{AlO}$
$\text{AlO} + \text{AlO} + \text{M} \rightarrow \text{Al}_2\text{O}_2 + \text{M}$
$\text{Al}_2\text{O}_2 + \text{H}_2\text{O} \rightarrow \text{Al}_2\text{O}_3 + \text{H}_2$
$2\text{Al}_2\text{O}_3 + \text{M} \rightarrow (\text{Al}_2\text{O}_3)_2 + \text{M}$

critical reaction

Condensates in an oxygen-rich model calculation

(Jeong et al. 2003, A&A 407, 191)

TiO₂ seeds,
Mantle growth by
TiₓOᵧ, AlₓOᵧ,
MgSiO₃, Mg₂SiO₄
SiO₂, FeₓOᵧ...

Presolar O-rich grain from Krymka LL3.2 chondrite


Core: O, Al, Ti,
Mantle: O, Si, Fe

Core:
44% Al₂O₃, 44% TiO₂
In mantle only: Si, Fe
Observational study of dust formation in \( \odot \) Ceti


\[ \text{AlO}(6-5): \text{Kaminski et al. 2016, A&A 592, A42} \]

\[ \Rightarrow \text{AlO depletion} \]

\[ \begin{align*}
S\text{-cont. (Jy/beam km/s)} & \quad 0 & \quad 0.08 \\
\text{r (R}_\odot\text{)} & \quad 0 & \quad 10 & \quad 12
\end{align*} \]

\[ \Rightarrow \text{SiO depletion at } r > 4 R_\odot (T \leq 600K) \]


\[ \text{TiO}_2 \text{ more extended than TiO } \Rightarrow \text{ unlikely to be the first condensate!} \]

Quy Nhon - Vietnam

The Cosmic Cycle of Gas and Dust in the Galaxy

July 10, 2018
Carbon dust formation in a gas box with oscillating thermodynamic conditions.
Carbon dust formation in a gas box
Supercooling => hysteresis
Scenario of a dust forming circumstellar shell
Radial structure of a high mass-loss rate model

\[ \alpha = \text{grad}/g\text{grav} \]

- \( M_* = 0.8 \, M_\odot \)
- \( L_* = 1.5 \times 10^4 \, L_\odot \)
- \( T_* = 3000 \, \text{K} \)
- \( \varepsilon_C/\varepsilon_O = 1.30 \)
- \( P = 650 \, \text{d} \)
- \( \Delta v_p = 8 \, \text{km/s} \)
- \( \dot{M} = 4.5 \times 10^{-5} \, M_\odot/\text{yr} \)
- \( v_{\text{exp}} = 17.3 \, \text{km/s} \)
- \( \frac{\rho^d}{\rho^g} = 1.1 \times 10^{-3} \)

Summary and conclusions

Two different physical descriptions of the astrophysical dust formation problem are at hand
The required input data start to become available

Dust formation has to be treated in a consistent way, i.e. taking into account the coupling of the dust component to its surroundings

Time-dependent hydrodynamic models of pulsating, dust forming circumstellar shells reveal nonlinear phenomena induced by the self-regulating dust formation process:

- spatial structuring of the dust shell
- dust induced shocks
- back-warming
- temporal structuring of the shell, eigen-timescale

Chemical non-equilibrium calculations start to reproduce observed molecular abundances
Both approaches seem ready to be combined!