A Dust Aggregate Model Based on Numerical Simulations of Aggregate Collisions

ダストアグリゲイト同士のDEM(?)衝突シミュレーション

和田 浩二
千葉工業大学 惑星探査研究センター

田中秀和¹, 陶山徹², 木村宏³, 山本哲生¹
¹北大低温研, ²新潟県立自然科学館, ³CPS
A collision of BCCAs
8192+8192 ice particles (r=0.1\textmu m, \xi_c = 8\textAA)
Collision velocity = 22 m/s
Background

Collisional growth of dust ($< \mu m$) → Question mark → Planetesimal formation ($> km$)

Structure evolution of dust aggregates in protoplanetary disks

When and how are aggregates compressed and/or disrupted?

Numerical simulation of dust aggregate collisions!
Ballistic Cluster-Cluster Aggregation (BCCA)

- In the early growth stage, undeformed BCCAs are formed because of their low collision velocity (< \( \text{mm/s} \))
- A series of hit-and-sticks of comparable aggregates
- Fluffy structure (fractal dimension < ~ 2)

How are the BCCA structures compressed?

Dominik & Tielens 1997;
Wada et al. 2007, 2008; Suyama et al. 2008
Background

Collision velocity of dust in protoplanetary disks < several 10 m/s

e.g., < ~50 m/s (Hayashi model, without turbulence)

Is it possible for dust to grow through collisions?
To what extent is dust compressed?

Experimental: Blum & Wurm 2000, Wurm et al. 2005
Ballistic Particle-Cluster Aggregation (BPCA)

- Formed by one-by-one sticking of monomers

- Compact structure (fractal dimension ~ 3)

Dust should be compact in high velocity collisions causing their disruption

Collisions of BPCA clusters implication for growth and disruption of compact dust
Objective

To construct a structural evolution model of dust aggregates by numerical simulations of aggregate collisions

Collisions of BCCA & BPCA clusters

- Compression process  \( (BCCAs) \)
  Gyration radius \( \rightarrow \) Degree of compression

- High-velocity collisions  \( (BPCAs) \)
  Number of particles in the largest remnant \( \rightarrow \) Growth efficiency
  Coordination numbers in the largest remnant \( \rightarrow \) Degree of compression
Simulation Method
Grain interaction model

Elastic spheres having surface energy

Normal

Sliding

rolling

twisting

JKR theory

\[ \delta \]

\[ s \]

\[ \xi \]

Critical sticking velocity: exp.~10 × theo.!?

JKR and rolling resistance have been tested with experiments using ~1µm SiO₂ particles. (Heim et al. 1999; Poppe et al. 2000; Blum & Wurm 2000)

Johnson, Kendall and Roberts (1971)
Johnson (1987), Chokshi et al. (1993)
Dominik and Tielens (1995,96)
Wada et al. (2007)
Grain interaction model

Elastic spheres having surface energy

Normal Sliding Rolling Twisting

\[ \delta, \xi, \phi > \text{critical displacements} \]

- Critical slide: \[ s_{\text{crit}} \sim 1.5 \text{ Å} \] (for 0.2 µm quartz)
- Critical roll: \[ \xi_{\text{crit}} \sim 2 \text{ Å} \] (or \( \sim 30 \text{ Å} \) (Heim et al., 1999))
- Critical twist: \[ \phi_{\text{crit}} \sim 1^\circ \]

\[ E_{\text{break}} \]: Energy to break a contact
\[ E_{\text{roll}} \]: Energy to roll a pair of grains by 90°

Johnson, Kendall and Roberts (1971)
Johnson (1987), Chokshi et al. (1993)
Dominik and Tielens (1995, 96)
Wada et al. (2007)
Dominik and Tielens (1997)

Each grain motion is directly calculated, taking into account particle interactions

- Modeling grain interactions seriously

**D&T “recipe”**

- 2-D, Head-on collision
- Small size (40 + 40 grains)
- Initial structure: only 1 type

**Limitations:**

- Max. compression
- Catastrophic disruption

\[ E_{impact} = \begin{cases} \sim n_k E_{roll} \\ > 10 n_k E_{break} \end{cases} \]

- Energy to roll a grain by 90°
- Energy to break a contact
- Number of contacts in initial aggregates

Confirmed by experiments (Blum & Wurm 2000)
Collisions between BCCA clusters

: Compression process
Collisions of BCCA clusters

- BCCA clusters are composed of 512, 2048, or 8192 particles (10 types randomly produced)
- impacted by head-on collision

- particle: radius = 0.1 \( \mu \text{m} \),
- Ice \((E = 7 \text{ GPa}, \nu = 0.25, \gamma = 100 \text{ mJ/m}^2)\)
- SiO\(_2\) \((E = 54 \text{ GPa}, \nu = 0.17, \gamma = 25 \text{ mJ/m}^2)\)

- Critical rolling displacement: \( \xi_{\text{crit}} = 2, 8, 30 \text{ Å} \)
Example of simulations

Ice, $8192 + 8192$, $\xi_{\text{crit}} = 8 \text{ Å}$

- $E_{\text{impact}} \sim 0.7 E_{\text{roll}}$
  - $V_{\text{impact}} = 0.2 \text{ m/s}$

- $E_{\text{impact}} \sim 0.3 n_k E_{\text{roll}}$
  - $V_{\text{impact}} = 17 \text{ m/s}$

- $E_{\text{impact}} \sim 13 n_k E_{\text{break}}$
  - $V_{\text{impact}} = 39 \text{ m/s}$
Numerical Results on Gyration Radius
Gyration radius $r_g$ : compression process

Ice, $8192 + 8192$, $\xi_{\text{crit}} = 8 \, \text{Å}$

$$ E_{\text{impact}} \sim 0.01 E_{\text{roll}} $$
Impact velocity: $0.024 \, \text{m/s}$

$$ E_{\text{impact}} \sim 0.19 N E_{\text{roll}} $$
Impact velocity: $13 \, \text{m/s}$

$$ r_g = \sqrt{\frac{1}{N} \sum_i |x_i - x_g|^2} $$

$x_g$: center of mass
Gyration radius $r_g$: compression process

$E_{\text{impact}} \sim (0.1 - 1) NE_{\text{roll}}$

Max. compression

Consistent with Dominik & Tielens (1997)
Gyration radius $r_g$: compression process

- Scaled by $E_{\text{impact}} / (N E_{\text{roll}})$
- $r_g$ is normalized by $r_1 N^{1/2.5}$
Gyration radius $r_g$ : compression process

No restructuring

Max. compression & Disruption

slope = $-\left(\frac{1}{d_f} - \frac{1}{d_c}\right)$

Scaled by $\frac{E_{\text{impact}}}{(N E_{\text{roll}})}$

$E_{\text{imp}} \sim N E_{\text{roll}}$

$E_{\text{imp}} \sim E_{\text{roll}}$

$d_f$: fractal dimension of BCCA

$d_c$: fractal dimension of max. compression

$1_{1.25}$

$r_g, \text{comp}$

$r_g, \text{BCCA}$
Gyration radius $r_g$ : compression process

- SiO$_2$, $N = 1024$, $\xi_c = 2$ Å
  - $\xi_c = 8$ Å
  - $\xi_c = 16$ Å
- Ice, $N = 1024$, $\xi_c = 2$ Å
  - $\xi_c = 8$ Å
  - $\xi_c = 16$ Å
- Ice, $N = 4096$, $\xi_c = 8$ Å
- Ice, $N = 16384$, $\xi_c = 8$ Å

- Scaled by $E_{\text{impact}} / (N E_{\text{roll}})$
- $r_g$ is normalized by $\frac{1}{r_1 N^{1/2.5}}$

$E_{\text{impact}} / (N E_{\text{roll}})$
Gyration radius $r_g$: compression process

- Scaled by $E_{\text{impact}} / (N E_{\text{roll}})$
- $r_g$ is normalized by $r_1 N^{1/2.5}$
- Not fully compressed

\[ \frac{r_g}{r_1 N^{1/2.5}} \approx 0.8 \left( \frac{E_{\text{impact}}}{N E_{\text{roll}}} \right)^{-0.1} \]

$(d_f = 2, d_c = 2.5)$

- SiO$_2$, $N = 1024$, $\xi_c = 2$ Å, $\xi_c = 8$ Å, $\xi_c = 16$ Å
- Ice, $N = 1024$, $\xi_c = 2$ Å, $\xi_c = 8$ Å, $\xi_c = 16$ Å
- Ice, $N = 4096$, $\xi_c = 8$ Å
- $N = 16384$, $\xi_c = 8$ Å

$E_{\text{impact}} / (N E_{\text{roll}})$

$df$: fractal dimension of BCCA

$dc$: fractal dimension of max. compression
The number of particles $N(<r)$ within $r$ in an aggregate is shown in the graph. The graph illustrates the dependence of $N(<r)$ on $r$ for different values of $d$, with $d=2.5$ and $d=2$. The critical value of the correlation length is $\xi_{\text{crit}} = 8 \text{ Å}$. The number of particles increases with increasing $V$. The graph includes data for various values of $v$: $0.0055$ (#23), $0.022$ (#22), $0.0884$ (#03), $0.354$ (#06), $1.000$ (#09), and $3.000$ (#12), all labeled as mean values.
Successive collisions in a BCCA mode

Suyama et al. 2008

- Fractal dimension $\sim 2.5$
- Decrease in density

CG by Dr. T. Takeda, 4D2Uproject, NAOJ

![Graph showing density $\rho$ vs. number of particles $N$ with different impact velocities $v_{imp}$: $4.4$ m/s, $1.1$ m/s, $0.27$ m/s. The graph illustrates the decrease in density with increasing number of particles.]
Summary of Compression Process

3D BCCA clusters ($d_f \sim 2$) are not fully compressed

- Fractal dimension for max. compression: $d_c \sim 2.5$

- Gyration radius: $r_g \sim r_1 N^{2.5} \left[ \frac{E_{\text{impact}}}{(n_k E_{\text{roll}})} \right]^{-0.1}$

\[
 r_g \sim r_1 N^{\frac{1}{d_c}} \left[ \frac{E_{\text{impact}}}{(N E_{\text{roll}})} \right]^{-\left(\frac{1}{d_f} - \frac{1}{d_c}\right)}
\]

- Successive collisions also lead to $d_c \sim 2.5$

The results for single collisions are applicable.
Collisions between BPCA clusters

: High-velocity collisions
Initial Conditions and Parameters

Collisions of BPCA clusters

- BPCA clusters are:
  - composed of 500, 2000, or 8000 particles (3 types randomly produced)
  - Impact parameter: $b$ (defined by using characteristic radius $r_c$)

Results are averaged

- Ice ($E = 7.0 \times 10^{10} \text{ Pa}, \nu = 0.25, \gamma = 100 \text{ mJ/m}^2, R = 0.1 \mu\text{m}$), critical rolling displacement: $\xi_{\text{crit}} = 8\text{Å}$
- Impact velocity $v_{\text{imp}} = 6 - 260 \text{ m/s}$

\[ b = \frac{l}{r_c,a + r_c,b} \]

\[ r_c = \sqrt{\frac{5}{3} \frac{1}{N} \sum (x_i - x_G)^2} \]
A collision of BPCAs
8000+8000 ice particles (r=0.1\,\mu m, \xi_c = 8\AA)
Collision velocity = 57 m/s

CG by Dr. T. Takeda,
4D2Uproject, NAOJ
Collisions of BPCA clusters

$N=8000+8000$, ice, $\xi_c = 8\text{Å}$, $v_{\text{imp}} = 70\text{ m/s}$ ($E_{\text{imp}} = 42\text{ NE}_{\text{break}}$)

$b = 0$

$b = 0.39$

$b = 0.69$

$b = 1.00$
Degree of Disruption: Growth Efficiency
Largest fragment mass \( N_{\text{large}} \): growth efficiency

\[ f \equiv \frac{N_{\text{large}}}{N_{\text{total}}} \]

\[ f > 0.5 \rightarrow + \text{ growth} \]
\[ f < 0.5 \rightarrow - \text{ growth} \]

\( f \) dependent on \( N \)
Largest fragment mass $N_{\text{large}}$: growth efficiency

\[ f = \frac{N_{\text{large}}}{N_{\text{total}}} \]

\( f > 0.5 \rightarrow + \) growth
\( f < 0.5 \rightarrow - \) growth

$\nu_{\text{imp}}$ [m/s] (ice)

$E_{\text{impact}} / (N E_{\text{break}})$

$b = 0.19$
Largest fragment mass $N_{\text{large}}$: growth efficiency

$$f = \frac{N_{\text{large}}}{N_{\text{total}}}$$

$b = 0.39$

$$f > 0.5 \rightarrow + \text{ growth}$$

$$f < 0.5 \rightarrow - \text{ growth}$$
Largest fragment mass $N_{\text{large}}$: growth efficiency

$$b = 0.49$$

$$f \equiv \frac{N_{\text{large}}}{N_{\text{total}}}$$

- Growth efficiency:
  - $f > 0.5 \rightarrow + \text{ growth}$
  - $f < 0.5 \rightarrow - \text{ growth}$
Largest fragment mass $N_{\text{large}}$: growth efficiency

\[ b = 0.58 \]

\[ f = N_{\text{large}} / N_{\text{total}} \]

- $f > 0.5 \rightarrow +$ growth
- $f < 0.5 \rightarrow -$ growth
Largest fragment mass $N_{\text{large}}$: growth efficiency

$$b = 0.69$$

$$f = N_{\text{large}} / N_{\text{total}}$$

$$f > 0.5 \rightarrow + \text{ growth}$$

$$f < 0.5 \rightarrow - \text{ growth}$$

$v_{imp}$ [m/s] (ice)
Largest fragment mass $N_{\text{large}}$ : growth efficiency

$$b = 0.77$$

$$f \equiv \frac{N_{\text{large}}}{N_{\text{total}}}$$

: growth efficiency

\begin{align*}
&f > 0.5 \rightarrow + \text{ growth} \\
&f < 0.5 \rightarrow - \text{ growth}
\end{align*}
Largest fragment mass $N_{\text{large}}$: growth efficiency

$$v_{\text{imp}} \text{ [m/s]} \text{ (ice)}$$

$$b = 0.89$$

$$f = \frac{N_{\text{large}}}{N_{\text{total}}}$$

- Growth efficiency:
  - $f > 0.5 \rightarrow + \text{ growth}$
  - $f < 0.5 \rightarrow - \text{ growth}$

Graph showing $f = \frac{N_{\text{large}}}{N_{\text{total}}}$ vs. $E_{\text{impact}} / (NE_{\text{break}})$. The graph includes data points for different conditions, with colors indicating different cases.
Largest fragment mass $N_{\text{large}}$: growth efficiency

\[ f = \frac{N_{\text{large}}}{N_{\text{total}}} \]

- $f > 0.5 \rightarrow + \text{ growth}$
- $f < 0.5 \rightarrow - \text{ growth}$

Offset collisions independent of $N$

$v_{\text{imp}} \ [\text{m/s}]$ (ice)

$E_{\text{impact}} / (N E_{\text{break}})$
Largest fragment mass $N_{\text{large}}$: growth efficiency

$f \equiv \frac{N_{\text{large}}}{N_{\text{total}}}$

$: growth efficiency$

$f > 0.5 \rightarrow + \text{ growth}$

$f < 0.5 \rightarrow - \text{ growth}$

Average weighted by $b^2$
Growth efficiency averaged

Averaged for $b^2$

$$f = \frac{N_{\text{large}}}{N_{\text{total}}}$$

: growth efficiency

$$f > 0.5 \rightarrow + \text{ growth}$$

$$f < 0.5 \rightarrow - \text{ growth}$$

$\nu_{\text{imp}} [\text{m/s}]$ (ice)

$E_{\text{impact}} / (N E_{\text{break}})$
Growth efficiency averaged

\[ f \equiv \frac{N_{\text{large}}}{N_{\text{total}}} \]

\( f > 0.5 \rightarrow + \text{ growth} \)
\( f < 0.5 \rightarrow - \text{ growth} \)

\( f \approx N_{\text{large}} / N_{\text{total}} \)

\( v_{\text{imp}} \) [m/s] (ice)

\( f > 0.5 \rightarrow + \text{ growth} \)
\( f < 0.5 \rightarrow - \text{ growth} \)

\( f \approx N_{\text{large}} / N_{\text{total}} \)

\( \checkmark \text{small dependence on } N \)
Degree of compression: Coordination number
Coordination number $N_c$

Number of particles in contact with a particle
e.g.,

\[ N_c = 4 \]

\[ N_c = 2 \text{ for BCCA and BPCA} \]

Max. $N_c = 12$ for close-packing

An index of compression:
The more compact are aggregates, the larger $N_c$ is.

What value of $N_c$ is achieved at BPCA collisions?
Coordination number $N_c$ @ BPCA collisions

Mean Coordination Number

$E_{\text{impact}} / (N E_{\text{break}})$

Ice, 8Å, 8000+8000

$u_{\text{col}}$ [m/s]

$b=0.00$ (red)
$b=0.19$ (green)
$b=0.39$ (blue)
$b=0.49$ (pink)
$b=0.58$ (cyan)
$b=0.69$ (yellow)
$b=0.78$ (black)
$b=0.89$ (red)
$b=1.00$ (gray)
average (red)
Why $N_c = 4$?

Particles are stable enough with $N_c = 4$ in 3D:

1D

2D

3D
Summary

Dust aggregates remain *fluffy* only through collisions.

- Fractal dimension $\sim 2.5$
- Coordination number $< 4$

Very fluffy planetesimals could be formed!?

$\sim 10^{-4} \text{ g/cc (Suyama et al. 2008)}$

Other compression processes are required.

Icy aggregates can grow at collision velocity $\sim 50 \text{ m/s}$.

Planetesimals can be formed through collisions of dust.