Carbonaceous dust from a core-collapse supernova: the need for an improved theory

David Fallest and Davide Lazzati
North Carolina State University, Raleigh, NC

Abstract

Classical nucleation theory assumes that dust grains share the same microphysical properties regardless of their size. These assumptions include the sticking coefficient, shape, and temperature of the grain. Usually, predictions of dust formation consider grains to be completely “sticky" (a sticking coefficient of unity) and to be spherical in shape – conditions which result in maximally efficient nucleation. We discuss the effects of varying these microphysical properties on the nucleation rates, condensation times, and size and mass distributions of carbonaceous grains formed by a type II supernova explosion. Variations of the sticking coefficient and grain shape lead to delayed condensation times and can result in marked differences in the size and mass distributions, which, in turn, can strongly influence the shape of the expected extinction curves. These results, along with the known limitations of the classical nucleation theory, suggest that a more thorough understanding of the physical properties of small grains and a more complete theory of nucleation are necessary.

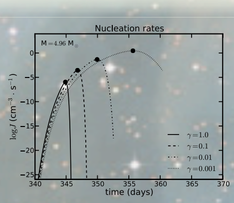
Classical nucleation theory is a thermodynamic theory and may not be applicable in the formation of very small grains. Kinetic nucleation theory may be a better, though more complicated, choice because it is better equipped to deal with grains of all sizes (from grains of fewer than ~100 monomers up to macroscopic sizes) and changes in shape for different sized grains. Moreover, kinetic theory is much better equipped to deal with temperature fluctuations of grains due to interactions with grain monomers and carrier gas atoms. The temperature, or equivalently the energy, of the grain has a large influence on the detachment rate of monomers from the grain.

Motivation

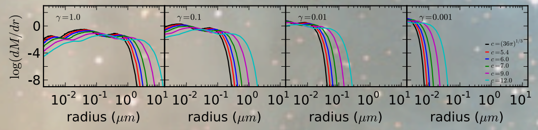
- Possible sources of interstellar dust include outflows from asymptotic giant branch stars, Wolf-Rayet systems, quasars, and supernovae (SNe)
- The amount of dust attributed to each possible source remains unclear
- Theoretical predictions of SNe dust yields are as much as 3 to 4 orders of magnitude larger than observations
- In order to better understand dust formation in the various sources a better theory is required

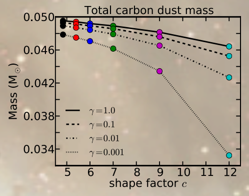
Results and Conclusions

- At early times, reduced sticking coefficient makes grain formation more difficult and suppresses the nucleation rate
- Reducing γ
  - increases the maximum nucleation rate
  - delays time of maximum nucleation to higher supersaturation times
  - makes grain growth difficult resulting in larger numbers of smaller grains
- Increasing c
  - reduces maximum nucleation rate
  - delays time of maximum nucleation
  - allows larger grains to form
- Even though large grains can form, dust dust masses are dominated by smaller grain sizes (between 0.01 and 0.5 μm)
- Total mass of carbon grains formed remains relatively robust (within a factor 1.5)
- Changes in choice of shape factor and sticking coefficient are unlikely to explain discrepancies between theoretical and observational dust yields
- Extinction curves are strongly affected by choice of shape factor and sticking coefficient
- Simulations with large c and γ produce gray extinction curves
- Without knowledge of shape factors and sticking coefficients, predicting extinction curves of SN-condensed dust is impossible

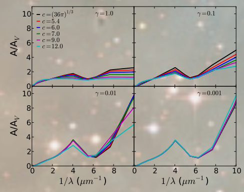

Nucleation rates

Mass distributions




Total carbon dust mass

Extinction curves



Our Model

- Dust grains do not necessarily form as spheres, nor are they completely sticky
- We vary the grain shape using the shape factor c where Σ is the grain surface area and V is the grain volume

$$c = \frac{\Sigma}{V^{(2/3)}}$$

- We chose 6 shape factors: $c = (36\pi)^{(1/3)}$, 5.4, 6.0, 7.0, 9.0, 12.0
- We chose 4 values for the sticking coefficient: γ = 1.0, 0.1, 0.01, 0.001
- We examine the formation of carbon grains from a 20 M$_\odot$ core-collapse SN with Z = 0 (see Umeda & Nomoto (2002))
- We consider the formation of CO molecules to be complete and ignore any dissociation of the molecules, so that carbon grains form only in those regions where the number fraction C/O > 1
- We divide the expanding gases into a series of enclosed mass shells from ~4.93 M$_\odot$ to ~6.21 M$_\odot$ – where the carbon number fraction is highest, ranging from 2×10^{-1} to 8×10^{-9}
- Grains form through nucleation as the expanding SN gas shell cools and becomes supersaturated
- The rate of nucleation can be found through:

$$J_s = \gamma \left(\frac{c^3 v_0^2 \sigma}{18\pi^2 m_0} \right)^{\frac{1}{2}} C_1^2 \exp\left(\frac{-4c^3 v_0^2 \sigma^3}{27(kT)^3(\ln S)^2} \right)$$

- Once grains have nucleated, they grow through the attachment of atoms onto the grains
- The growth of the grains can be found by:

$$\frac{dV}{dt} = \gamma c V^{\frac{2}{3}} C_1 v_0 \left(\frac{kT}{2\pi m_0} \right)^{\frac{1}{2}}$$

- The monomer material available become depleted by the nucleation and growth processes
- We find the amount of depletion by:

$$1 - \frac{C_1(t)}{\tilde{C}_1(t)} = \int_{t_e}^{t} \frac{J_s(t')V(t,t')}{\tilde{C}_1(t')v_0} dt'$$

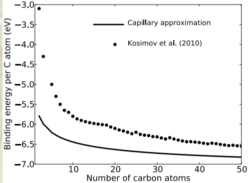
- Each time step we calculate the nucleation rate, grain growth, and depletion of monomers
- We repeat the process until the monomer concentration is substantially depleted
- We vary c and γ to investigate less efficient grain formation and growth

γ = sticking coefficient
c = shape factor
v_0 = molecular volume
σ = surface tension
m_0 = molecular mass
C_1 = monomer concentration
k = Boltzmann constant
T = temperature
$\ln S$ = supersaturation
V = grain volume
$\tilde{C}_1$ = nominal monomer concentration

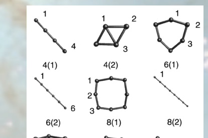
Improving the Theory

- Use kinetic theory which is applicable to large and small clusters (<~100 atoms)
- Use free energies of stable isomers rather than surface tension from capillary approximation
- Use shape factors of stable isomers found by DFT techniques

Grain free energies



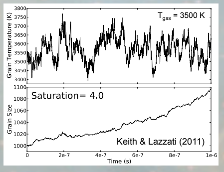
Stable Isomers



Jones (1999)

- DFT can also calculate optical properties of dust grains allowing computation of temperature fluctuations of the grains
- Corrections to the detachment rate of atoms from small grains based on quantum probabilities of phonon accumulation to break a bond
- Include the influence of other dust species
- Include photodissociation of CO molecules and injection of additional carbon atom into available nucleation material
- Account for grain charging and ionization effects on nucleation rates

Grain temperature



Keith & Lazzati (2011)

Acknowledgements

Part of this work is done in collaboration with researchers at the Institute for the Physics and Mathematics of the Universe at the University of Tokyo, Kashiwa Campus, Japan.

This work was funded in part by the NSF East Asia and Pacific Summer Institutes (EAPSI) Japan 2010 fellowship program (award #1015575), and the Japan Society for the Promotion of Science.

IPMU INSTITUTE FOR THE PHYSICS AND MATHEMATICS OF THE UNIVERSE

Rosette Nebula (NGC 2244)
Photo by: Ignacio de la Cueva Torregrosa