

Fractal dimensions of simulated interstellar dust grains

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Abstract

It is known that interstellar dust grains play an important role in the evolution of interstellar clouds. In this work we discuss the results of microscopic modeling of interstellar dust grains for the conditions typical for the regions of star formation using the Monte Carlo method. Impact of the model parameters on the fractal dimension of a dust particle was investigated.

Keywords: astrochemistry – dust, ISM, Monte Carlo method, fractal dimension

1 Introduction

Interstellar dust grains along with atomic and molecular gas are the main components of star-forming regions in our Galaxy. Interstellar dust play a crucial role in physics and chemistry of star formation, as they serve as coolants of collapsing protostars and provide their surface for chemical processes that proceed inefficiently in the gas phase. Polarimetric observations of magnetized star-forming regions suggest that grains have non-spherical shape. This result is confirmed by the captures of interplanetary dust particles with artificial satellites and laboratory experiments on dust growth under conditions similar to that in the interstellar medium. Here, we present the results of microscopic Monte Carlo simulations of the formation of fractal grain particles under interstellar conditions. We explore the impact of model parameters on the resulting fractal dimension of simulated particles and compare it to the experimentally measured fractal dimension of dust grain particles.

2 Methods and calculation

Fractal dimension is studied using a microscopic Monte Carlo model that generates amorphous dust cores of interstellar dust particles. Amorphous core (Fig. 1) is formed by random accretion of carbon atoms on a single initial “seed” carbon atom. The core is constructed using the accretion mechanisms and the numerical functions for the locations of the potential wells which described below.

Preliminary coordinates of the accretion site are randomly selected and projected onto a random point on the surface of the unit sphere according to the algorithm described in [1].

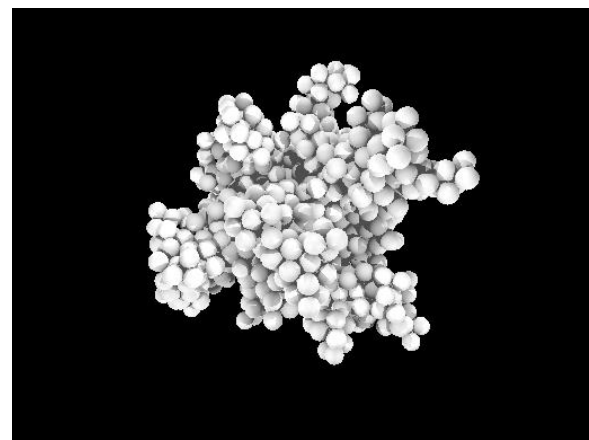


FIGURE 1 A sample of amorphous core containing 1000 carbon atoms

Each atom of the grain has its own potential approximated by the Lennard-Jones potential:

$$U(r) = 4 * \varepsilon * \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], \quad (1)$$

where r – distance between arbitrary point and selected atom;
 ε – the depth of the potential well; σ – the distance at which the interaction energy becomes zero.

The potential of two interacting atoms can be calculated as described in [2]:

$$U(r) = 4 * \sqrt{\varepsilon_1 \varepsilon_2} * \left[\left(\frac{(\sigma_1 + \sigma_2)}{2r} \right)^{12} - \left(\frac{(\sigma_1 + \sigma_2)}{2r} \right)^6 \right]. \quad (2)$$

We take into account atoms of only one chemical element (carbon, in our case), so this formula will match with formula (1).

TABLE 1 Simulation results for various values of the Lennard-Jones potential constants

| № of simulation | Particle | $\varepsilon/k, K$ | $\sigma, \text{\AA}$ | Reference | ρ in the center (half of the radius) | ρ total |
|-----------------|-------------------|--------------------|----------------------|-----------|---|--------------|
| 1 | C | 52 | 3.098 | [4] | 2.63 | 2.44 |
| 2 | C | 80.516 | 3.67 | [5] | 2.44 | 2.28 |
| 3 | C | 47.85 | 3.89 | [6] | 2.38 | 2.25 |
| 4 | | 21 | 3.098 | | 2.62 | 2.43 |
| 5 | | 104 | 3.098 | | 2.63 | 2.43 |
| 6 | | 52 | 2.098 | | 3.03 | 2.72 |
| 7 | | 52 | 4.098 | | 2.4 | 2.26 |
| 8 | Without potential | – | – | | 2.62 | 2.44 |
| 9 | C (100000 atoms) | 52 | 3.098 | [4] | 2.65 | 2.52 |

The potential of the grain surface at arbitrary point is a linear superposition of potentials of all individual atoms. Magnitude of the potential at arbitrary point of the surface is calculated as a superposition of the interaction potentials of atoms located within a radius of $2.5 \sigma_{\max}$ around the location of interest. We considered σ_{\max} to be the maximum possible σ in the system.

Total three-dimensional potential U at specific point is calculated as

$$U = \sum_{i=0}^n U_i(r_i), \quad (3)$$

where U_i is the pairwise interacting potential; r_i – the distance between the interacting atoms.

To determine mutual position of atoms in the system we calculate the coordinates of the minima of the three-dimensional potential field in which atoms are located. For each accreting atom we calculate the value of a local minimum of the potential. The atom is then placed there. The calculations of the minima are carried out using the gradient descent algorithm.

Fractal dimension (ρ) is calculated as

$$\rho = \log_R N, \quad (4)$$

where R – the radius of the smallest sphere that contains the constructed grain core in units of particle radius, N – the number of atoms inside the sphere.

3 Results

Various parameters of the Lennard-Jones potential for the carbon atoms were found in the literature and then utilized to generate the core. Fractal dimension of the core is then calculated. Using the data from Table 1, we performed simulations to assess the influence of model parameters on the fractal dimension of the core. The fractal dimension was measured for the amorphous dust core consisting of 10^3 carbon atoms, except simulation 9, where we modeled the core that consist of 10^5 atoms. Radius of the carbon atom is 1.7 \AA [3]. The fractal dimension was calculated in two ways: for the sphere with radius R and $R/2$. Results are shown in Table 1.

One can see from Table 1 that the structure of the dust particle is inhomogeneous: the core (central part of the grain) always has a denser structure. Results show that the parameters of the potential significantly affect the structure of the core.

Results of simulations show that σ impacts the structure of the core greatly, while the depth of the

potential well ϵ has almost no influence. Moreover, the results of the simulation where the potential does not effect on atom position and where at which atoms are placed at the first intersection of the ray directed from infinity to the first particle of the core and already existing carbon atom (simulation 8) are almost identical to the one with the

potential parameters taken from one of the literature sources (simulation 1). However, as we can see from the figures (Fig. 2 and Fig. 3), the number of atoms in calculations with the potential (Figure 2) changes uniformly, but in calculations without the potential (Figure 3) its number changes non-smoothly, forming “steps” on the figure (e.g., the blue line). This shows differences in the internal structure of the core in different models. Core structures for simulations 1 and 8 are shown in Figure 4. Calculations of fractal dimension with increased number of atoms were made in Simulation 9. In the center of the grain core one can see the condensation of atoms in comparison to simulations with smaller number of atoms in the core, but total fractal dimension remains approximately the same and the structure type remains unchanged.

Note that our model reproduces the structure of the dust cores similar to those observed experimentally under conditions of high-speed collision, corresponding to late stages of evolution of dust particles [7], with $\rho > 2$.

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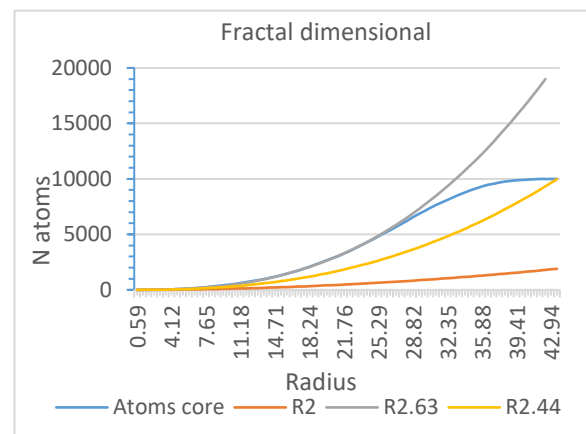


FIGURE 2 – Fractal dimension in the simulation 1.

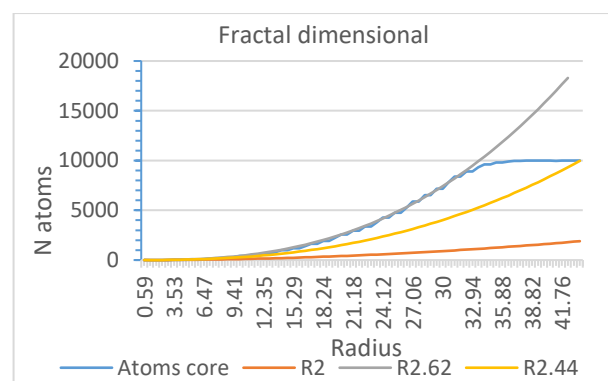


FIGURE 3 – Fractal dimension in the simulation 8.

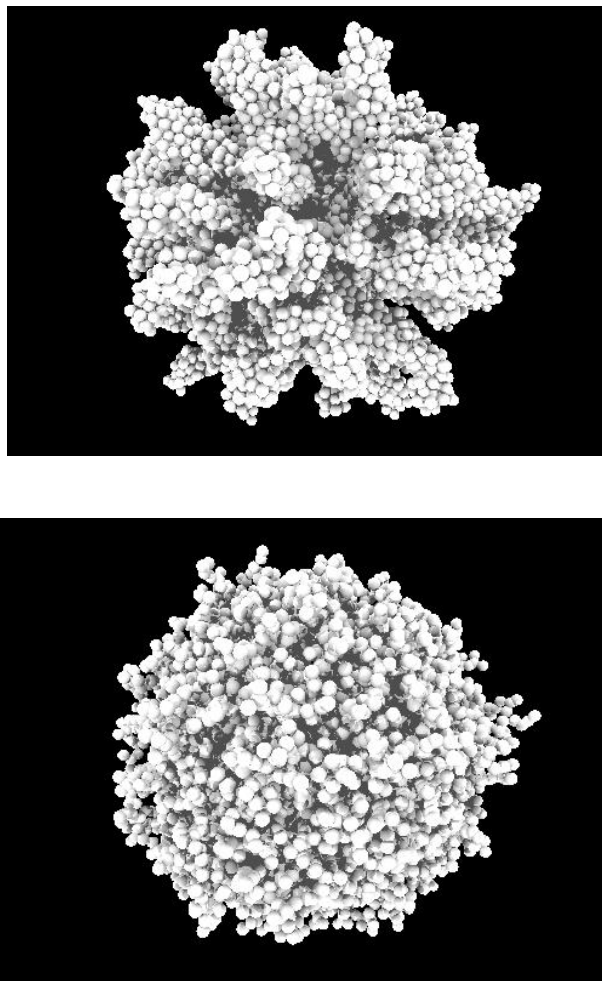


FIGURE 4 – Dust cores in simulation 1 (up) and simulation 8 (down)

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