Dust Grain Processing: A New Computational Method Applied to a Protostellar Accretion Shock

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Abstract. By applying a new computational multi–component method for the modelling of dust grain processing to a protostellar accretion shock we gain insight on the exact evolution of the grain size distribution function in the postshock region, where various processes act size–dependently on the grains.

1 Introduction

The supersonic infall of gas and *dust* during the collapse of a molecular cloud core to form a protostar is associated with a high–density accretion shock, which stands at the protostellar disk. The accreting dust particles are processed within such shocks by various physical and chemical processes, which generally act differently on grains of different composition, size, and velocity. Consequently, the grain size spectrum is dramatically changed as the dust grains pass through the shock front in entering the protostellar nebula. This development of the grain size distribution function *can generally not* be investigated simply by following separately the motion and size evolution of a few selected grain sizes.

Adopting the dissociative accretion shock model of Neufeld and Hollenbach (1994) we present an application of a *new computational multi–component method* for the modelling of dust grain processing (Krüger et al. 1995), which also accounts for drift velocities of the grains relative to the gas flow. Thereby, we gain insight of how exactly the size distribution function of silicate grains evolves as it is being affected by the evaporation of heated grains and by grain sputtering.

2 Basic Equations of the Multi–component Method

The fundamental differential balance or conservation equation for the grain size distribution function derived by Krüger et al. (1995) accounts for discontinuous processes (e.g. coagulation and shattering; the number and/or the size of the affected grains are abruptly changed due to grain–grain collisions) and continuous processes (e.g. sputtering; smooth grain size changes arising from interaction between gas particles and grains). The essential idea of the computational approach is to discretize the size distribution on a *Lagrange-like grid in grain size space* which moves according to the size evolution of selected sample grains. In this way, the grid is self-adapting according to the evolution of the size distribution, which seems much more appropriate than the use of a static grid.

Some simplifications arise from the application to the adopted shock model. In a first step we do not consider possible nucleation or grain growth behind the shock front. Instead, the processing of a *given* initial size spectrum of spherical grains is investigated (cf. Sect. 3). Thus, dust particles of radius a_* are injected at the base of the flow $N_{\rm H}^0$, where the calculation starts. The sole independent variable of the *plan–parallel shock wave* is the hydrogen column density $N_{\rm H}$ behind the shock front. $v_{\rm d}(a, N_{\rm H})$ is the velocity of a dust particle of radius a at position $N_{\rm H}$; $a_{N_{\rm H}}(a_*)$ denotes the radius of the grain (at position $N_{\rm H}$) whose initial radius was a_*:

$$a_{N_{\rm H}}(a_*) = a_* + \frac{a_0}{3} \int\limits_{N_{\rm H}^0}^{N_{\rm H}} \left[n_{<{\rm H}>} v_{\rm d}(a_{N'_{\rm H}}(a_*), N'_{\rm H}) \tau_{\rm net}(a_{N'_{\rm H}}(a_*), N'_{\rm H}) \right]^{-1} {\rm d}N'_{\rm H} \ .$$

$\tau_{\rm net}$ is the net rate of change in grain size and a_0 is the hypothetical radius of a monomer. Details of the gas density structure $n_{<{\rm H}>}$ are given in Sect. 3. For the considered case the general balance equation simplifies to the following special form:

$$-v_{\rm d}(a_*, N_{\rm H}^0) f(a_*, N_{\rm H}^0) + \frac{{\rm d}a_{N_{\rm H}}(a_*)}{{\rm d}a_*} v_{\rm d}(a_{N_{\rm H}}(a_*), N_{\rm H}) f(a_{N_{\rm H}}(a_*), N_{\rm H}) = 0 \ .$$

In order to evaluate this equation we follow the velocity and size evolution of an initial grid of grain radii $a_{*,i}$. Details of the numerical scheme, grid generation, derivation of macroscopic quantities of the dust component etc. are outlined in Krüger et al. (1995).

3 Model of the Dissociative Accretion Shock

We adopted the protostellar accretion shock model of Neufeld and Hollenbach (1994) behind a dense, dissociative J–shock of shock velocity $v_{\rm s} = 50$ km/s, and preshock density $n^0_{<{\rm H}>} = 10^9$ cm^{-3}. The shocked molecular gas is treated as a single fluid, in which the gas (neutrals, ions, electrons, but **not** the dust grains) has one common temperature and velocity. In single fluid J–shocks the gas is heated to high temperatures immediately behind the shock front, and then cools radiatively. The gas temperature profile $T_{\rm g}(N_{\rm H})$ can be characterized by two temperature plateaus and by two drops of the temperature at column densities $\sim 10^{16}$cm^{-2} and $\sim 10^{21}$cm^{-2} behind the shock front (see Neufeld and Hollenbach 1994 for details). Since the thermal pressure in the postshock region is approximately constant, the gas compresses as it cools, and the gas density structure can be approximately calculated from the temperature profile with $n_{<{\rm H}>}(N_{\rm H}) = n^0_{<{\rm H}>}\, v_{\rm s}^2\, \mu\, m_{\rm H} \,/\, (k\, T_{\rm g}(N_{\rm H}))$. As has been argued by Neufeld and Hollenbach (1994), betatron acceleration of the grains is unimportant at the high gas densities occuring in this model.

We investigate the evolution of an initial MNR power–law size distribution of silicate grains (Mathis et al. 1977) influenced by evaporation of heated grains and by grain sputtering. The evaporation of heated grains is treated according to Neufeld and Hollenbach (1994). The equilibrium grain temperature is determined by balancing the effective cooling via IR emission against the total heating rate, which comprises absorption of UV radiation, heating by impact energy of inelastically scattered gas particles, and energy input due to temporary accomodation of gas particles. These grain heating processes are treated using the methods presented by Hollenbach and McKee (1979) and Draine (1986). Grain sputtering is described by using semianalytical yields derived from experimental data (Tielens et al. 1994).

4 Results and Discussion

Absorption of UV-radiation is the most efficient heating process. Heating due to collisions with gas particles is of less significance, since most gas particles are scattered elastically and simply bounce off the grain surface without transfering much energy. Grain vaporization sets in, if the heating rate per unit grain area exceeds the maximum IR emissivity of the grain at the vaporization temperature, which is approximately proportional to the grain radius, i.e. small grains are heated to their vaporization temperature more easily. Vaporization of heated grains turns out to be the dominant mechanism of grain destruction. There is only little mechanical sputtering of the grains, amounting to a radius change of $\sim 0.5\%$. Due to the moderate gas temperatures thermal sputtering does *not* affect the grains.

The **evolution of the grain size distribution** $f(a, N_{\rm H})$ is presented in Fig. 1 by a sequence of snapshots taken at various column densities $N_{\rm H}$ behind the shock front. Two alterations of f have to be distinguished. The small grains are completely vaporized, which causes a drastic reduction of the value of the size distribution for small radii a. The second effect is the compression of the dust fluid which subsequently follows the compression of the radiatively cooling gas (at $N_{\rm H} \sim 10^{16}$ cm^{-2} and 10^{21} cm^{-2}, cf. Sect. 3) with a specific time lag due to the size dependent distance required to decelerate a grain. This results in a successive upward shift of f, where sections of the size distribution correponding to smaller grain sizes rise first. The shape of the *inbetween* size distribution functions during grain deceleration and vaporization, which **cannot** be described by a power–law (cf. Fig. 1), is a *computational result* of the multi–component method that **cannot** be obtained by simply following separately the motion of test grains through the shock. Macroscopic dust quantities, as for example the absorption coefficient $\kappa_{\rm d}$ of the dust component and the optical depth $\tau_{\rm d}$ corresponding to $\kappa_{\rm d}$, can be easily derived from the obtained size distribution by integration. The optical depth of the dust component is responsible for the weakening of the UV radiation, which in turn determines the grain temperatures and thus the evaporation of grains. In our calculation this interaction between the dust grains and the UV radiation is consistently accounted for.

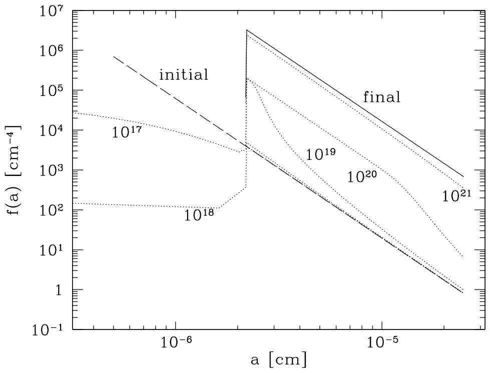

Fig. 1. Evolution of the grain size distribution as function of the particle radius a. $f(a)$ is depicted at various positions $N_{\rm H} = 10^m$ cm^{-2} behind the shock front. The dashed line indicates the initial MNR distribution (Mathis et al. 1977). The solid line designates the final grain distribution.

5 Conclusions

In order to demonstrate the capabilities of the new computational multi–component method for the description of dust grain processing, we have investigated the evolution of the grain size distribution in a protostellar accretion shock. In this way, it has been possible not only to compute the final grain size distribution after processing by the shock but also to determine the shape of inbetween size distributions during grain processing, which cannot be described by a power–law. Essentially, we found that large grains above a certain limit size $a_{\rm vap} = 2.2\,10^{-6}$cm, which depends on the grain material and is roughly proportional the UV-flux $F_{\rm s} \approx 1/2\, n^0_{<{\rm H}>}\, \mu\, m_{\rm H}\, v_{\rm s}^3$ emitted by the shock, are almost unharmed while those below $a_{\rm vap}$ completely vaporize. These results apply to silicate grains and also to other refractory materials such as iron. Ice mantles, on the other hand, will vaporize very quickly regardless of their thickness.

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