CIRCUMSTELLAR DUST CONDENSATION SCENARIOS

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Abstract. Circumstellar dust condensation is a ubiquitously observed phenomenon. Its adequate physical description and quantitative theoretical modelling usually require i) the treatment of the microscopic grain formation processes, and ii) the simultaneous determination of the local physical and chemical conditions by calculating a consistent model structure of the system under consideration. In this sense, the actual dust formation process and the individual nature of the dust forming object are intimately coupled. It is the aim of this contribution to visualize this interplay in a rather schematic and abstract way by focusing on the essential interaction of evolution trajectories and dust formation windows for stationary, pulsational, and episodic situations, as well.

1. Introduction

In any gaseous systems, the formation process of macroscopic particles, usually addressed as dust or grains, can be conceived either from the view of thermodynamics as a phase transition occurring beyond some critical limits or from the view of chemistry as a reaction network by which, starting from suitable molecules, more and more complex structures (e.g. clusters) are formed which finally grow to macroscopic specimens exhibiting bulk phase properties. This is in particular relevant for cosmic dust formation, where in the course of cooling flows occasionally conditions evolve which give rise to avalanche dust formation as it is observed in the stellar outflows of late giants and supergiants, like in pulsating shells of Miras and LPVs, but also in the thermally inhomogeneous winds of late carbon rich Wolf-Rayet-stars, in the outbursts of novae and supernovae, and as an irregular phenomenon in the atmospheres of R Coronae Borealis (RCB) stars, by which the spectacular occultations of theses objects are explained.

Despite the individual properties of the different objects and their varying local conditions, effective dust condensation always seems to take place i) if the temperature is sufficiently low, ii) the density of the dust forming species is sufficiently large and iii) the time scale for the object providing favourable condensation conditions is sufficiently long in order to allow for effective dust formation to proceed. Applying these criteria to dust formation in astronomical objects, one is to conclude that effective dust formation usually can be expected only within a rather limited island of the density-temperature-plane, which has to coincide for a sufficiently long time with the corresponding system trajectory guiding the local density and temperature evolution of the dust forming mass elements. Thus, it is essential for the evolution trajectory of any dust forming object to meet this "window" of dust formation. As the thermal, hydrodynamical, and chemical conditions in a dust forming system are strongly influenced by the presence of dust, astrophysical dust formation generally cannot be considered as an isolated problem, but usually requires the consistent calculation of the detailed model structure, including dust formation and growth.

Thus, in many situations a sensitive interplay between model structure and grain condensation is found, revealing circumstellar dust formation as a rather fine tuned self-stabilizing process triggered by an extreme non-linear coupling between shell dynamics, chemistry, radiative transfer and structure formation.

It is the aim of this contribution to discuss this fundamental interrelation for important astronomical dust formation scenarios in order to shed light onto the special conditions required for the particular models and to demonstrate their individual "solution" of the grain condensation problem.

2. The dust formation window

Any theoretical description of primary dust formation (i.e. formation of macroscopic specimens out of the gaseous phase) shows that for the kind of particles to be expected in astronomical systems (graphitic structures, soot, PAHs, "astronomical silicates", carbides, etc.) a rather low and narrow temperature regime ($1000 \ldots 1200$ K $\lesssim T \lesssim 700 \ldots 600$ K) is necessary in order to allow for the large formation efficiencies being observed.

This is a necessary condition imposed by thermodynamics in order to produce high local supersaturation ratios and consequently large constructive reaction rates outbalancing the destructive evaporation processes. As

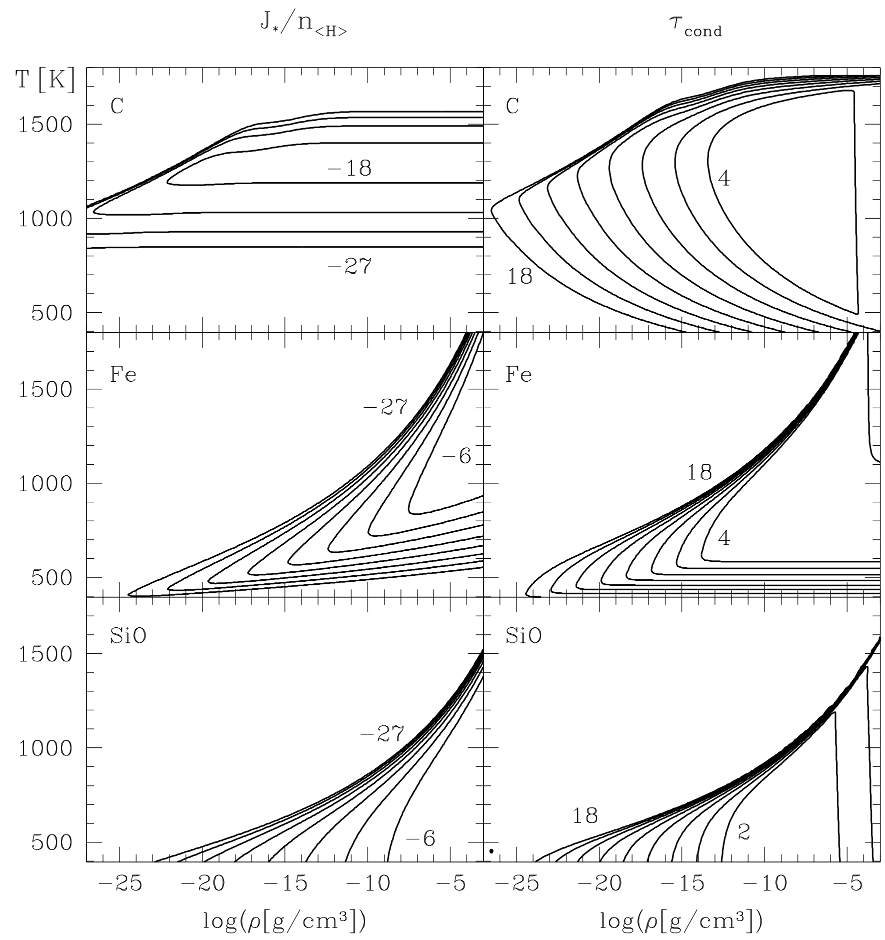

Figure 1. Contour plots showing the critical nucleation rate J_* of amorphous carbon, iron, and SiO-clusters, respectively, normated to the total number density of hydrogen (left panel) and the corresponding condensation time scale $\tau_{\rm cond}$ required for 10% of the condensible material actually to be condensed (right panel). The contour lines are labelled by their logarithmic value in cgs-units, separated by an increment of 3 (nucleation rate) and 2 (condensation time), respectively. In addition to chemical equilibrium and solar abundances, in case of carbon condensation a C/O-ratio of 2 has been adopted.

these addition rates are also proportional to the local molecular number densities of the condensating species, effective dust formation imposes also limitations upon the favourable total density regime i) by the chemical rate network providing the density of the condensating species and ii) by the nucleation and growth timescale measuring the local dynamics of the condensation process. Though for the astrophysical situations of interest this regime of favourable values of the total density is strongly varying, in all cases there exists a minimum density defined by the required minimum condensation efficiency (i.e. time). Thus, for any system of given chemical composition, a region of a potentially high dust nucleation rate can be marked (e.g. Gail and Sedlmayr 1987, Dominik *et al.* 1990, Tielens 1990). For avalanche dust condensation actually to occur, the density-temperature-trajectory of a corresponding mass element has to cross the "dust formation window" during the course of its dynamical evolution. The rates for nucleation (e.g. Fig. 1) and cluster growth, increase with increasing number density of the condensing species. Therefore, the contour lines of these rates, and hence the dust formation window, usually are not closed in the high density limit. This, however, is only an artificial concern because such large densities generally are not realized in the objects under consideration.

In the following, we discuss important situations of astrophysical dust formation and the triggering processes necessary for the system trajectory to meet the target window.

3. Dust forming objects

3.1. STATIONARY CIRCUMSTELLAR OUTFLOWS

Stationary circumstellar outflows approximately seem to be realized for the winds of red giants and supergiants, showing only moderate variability and a long lasting nearly constant mass loss rate, but also by the outflows of novae and supernovae, which after ignition both exhibit a more or less quasi-stationary free expansion.

This common situation can best be illustrated by a schematic temperature-radius or a density-radius plot, respectively, which defines the radial (and temporal) evolution of the thermal conditions of a considered expanding element of matter.

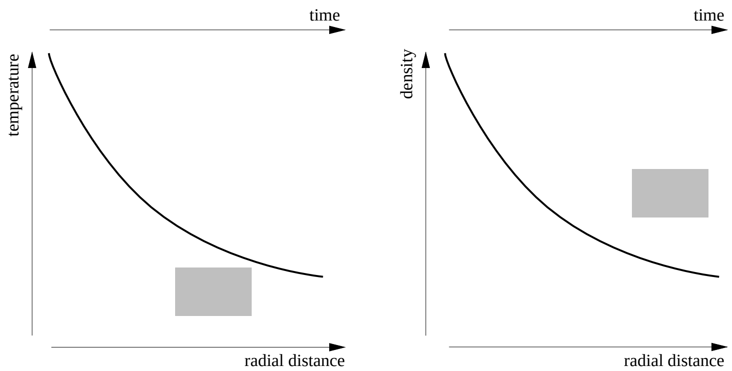

Figure 2. Schematic depiction of dust formation windows (symbolized by dark shaded rectangles) with regard to temperature and density, respectively, relative to a flow trajectory (demonstrating the evolution of a non-dust forming system).

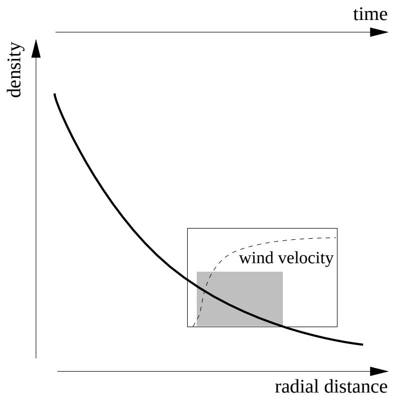

Figure 3. Dust condensation in a stationary stellar wind. When the wind trajectory meets the dust formation window, effective nucleation and grain growth starts.
The insert indicates the steep increase of the wind velocity due to radiative acceleration of the dust component. In case of dust driven winds, the position of the dust formation window, in particular the local onset of dust formation, is closely correlated with the position of the critical point of the wind.

The exact mechanism of dust nucleation and growth depends very much on the local and global structure of the considered object, and most important on the molecular abundances of the condensating species and the kind of grains to be formed.

3.1.1. *Dust driven winds*

The important case of dust driven winds, where the dust formation process basically determines the stellar mass loss rate, is only found for objects at the upper right region of the Hertzsprung-Russell-diagram (HRD) especially for red giants and supergiants on the Asymptotic Giant Branch (AGB), which exhibit a pronounced mass loss ranging up to $\approx 10^{-5...-4}$ $M_\odot$/yr. For dust driven winds, the inner edge of the dust shell, which marks the site of the onset of dust formation, always has to coincide with the position of the sonic point, defining the subsonic-supersonic transition of the wind velocity field.

By assuming amorphous carbon grain formation in C-star shells, self-consistent dusty wind models can be calculated for very luminous, very cool, low mass stars, situated above some limiting border line in the HRD defined by a necessary minimum mass loss rate ($\dot{M}_{min} \simeq 10^{-6} M_\odot$/yr) for producing a sufficient dust opacity. For dust driven winds, the coincidence between the system trajectory and the dust formation window always is guaranteed by a self stabilizing servo mechanism between dust formation and its dynamical and thermodynamical feedback (cf. Sedlmayr and Dominik 1995).

In case of carbon grain formation via PAHs, the situation is not as clear. Both, the chemical network (Cherchneff 1992) and the chemical pathway (Goeres *et al.* 1996) LTE-descriptions yield a much to small nucleation rate for critical PAHs along the trajectory of an expanding mass element in a C-star shell, which simply means that the system trajectory essentially misses the target window if LTE is assumed. This problem could be solved by recognizing that the size dependent internal temperature of the small PAHs is considerable lower than that of the larger PAHs, which approaches the corresponding bulk value (cf. Cherchneff 1992). By a large non-LTE effect the PAH formation efficiency in the small particle domain would be sufficiently enhanced to allow for an efficient cluster and carbon-grain (soot?) formation.

The situation is even worse in case of oxygen rich environments (M-type giants and supergiants) where the various nucleating species and the corresponding nucleation sequence along the wind trajectory (cf. Sharp and Huebner 1990) is not yet fully clear. Consequently, the first condensating molecules and their nucleation windows for the primary condensates (aluminium oxides?, titanium oxides?, magnesium oxides? silicon oxides?, iron-magnesium-silicates?, iron?, etc.) and their mutual dependences are still not well known. To develop a reliable quantitative physical description of inorganic cluster and grain formation in oxygen rich objects is of great need for the near future.

In the context of PAH-formation in C-star winds, we already addressed the importance of non-LTE effects for supporting the PAH growth process to yield large production rates. As circumstellar grain condensation turns out to be very sensitively dependent on the local thermal state of the system, generally speaking, non-equilibrium effects should have a great impact on the microscopic dynamics of the formation process, in particular affecting the nucleation rate. Usually three different non-equilibrium situations may contribute:

Supercooling: This effect is a necessary condition for all nucleation situations and simply accounts for the fact that the molecule to solid phase transition only will proceed in a finite time if sufficiently large values of the supersaturation ratio (> 1) of the corresponding nucleating species are realized.

Non-equilibrium chemistry: As the local concentrations of the chemical species strongly depend on the properties of the object under consideration (expansion velocity, radiation fields, shock waves, etc.), in many situations significant departures from the chemical equilibrium concentrations are to be expected. This may also concern the condensating molecules and, thus, cause significant changes of the nucleation and growth rates of the clusters.

Thermal decoupling of the clusters: The internal energetic relaxation of the individual clusters essentially depends on the number of degrees of freedom available for storing the energy. As this quantity is given by the particular structure and the size of a cluster, the resulting "internal temperature" which determines the evaporation rate, i.e. the denominator of the supersaturation ratio, becomes a function of cluster size, geometry, chemical and mineralogical structure, etc. By this effect, the supersaturation ratio (and hence the stability) of particular clusters could be greatly increased, allowing them to survive and to grow even in a potentially hostile environment. Hence, in particular situations, these phenomena may help to modify and to adjust the dust formation window of an object in such a way to coincide with the system trajectory and, thus, to start effective dust production.

3.1.2. *Hot stellar environments*

Unexpectedly, circumstellar dust condensation is not only confined to cool objects, but is also clearly observed in the rapidly expanding dense envelopes of carbon rich late type Wolf-Rayet-stars, i.e. for spectral types WC7. . . 9. As spherical symmetric homogeneous outflows of these stars having stellar temperatures above 20 000 K, in principle do not allow for a gas-solid phase transition, essentially three mechanisms are discussed for breaking this dust preventing symmetry:

- density inhomogeneities (clumps)
- shocks
- temperature fluctuations.

All these effects result basically in different expansion trajectories of individual mass elements, some of them meeting the dust formation window, as is cartooned in Fig. 4. In this way, an intuitive picture of the dust formation scenario is guided, which qualitatively seems to agree with the observations, and at least could be used as a basis for further quantitative descriptions of grain condensation around hot stars.

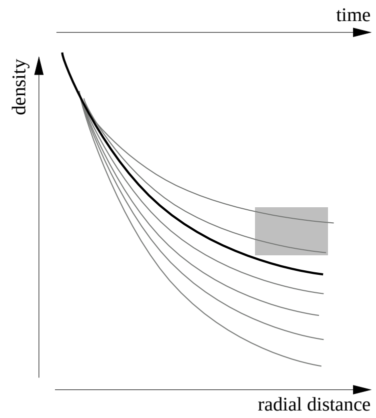

Figure 4. Possible dust condensation scenario in the expanding shell of a Wolf-Rayet star. Because of pronounced density inhomogeneities the evolution of each mass element follows its individual trajectory, some of them crossing the dust formation window. The fat trajectory represents the situation of an homogeneous model, where no dust formation should occur.

3.2. NOVAE AND SUPERNOVAE

Dust condensation in the high velocity outflows of novae and supernovae resembles in essential features that in stationary stellar winds, where in a cooling flow favourable conditions for cluster formation evolve, determined by the local element abundances, the stellar radiation field, and the appropriate heating and cooling functions. Despite this basic similarity, compared to the elaborate level of treatment of stationary stellar winds, the problem of novae and supernovae dust formation seems to be far from a satisfactory solution. This concerns not only the rare availability of reliable theoretical outflow models, but more specifically the important question of the first condensation species, and hence of the primary condensate, but also the role of non-equilibrium chemistry for the calculation of reliable molecular concentrations.

With regard to dust condensation in supernovae outflows, so far only rather schematic descriptions within the frame of classical nucleation theory exist, based on a given shell thermodynamics, hydrodynamics and chemistry. In order to get an impression of the actual level of approach see Kozasa *et al.* 1989, where dust formation in the outflow of the supernova SN 1987A is investigated.

In the case of novae, a large amount of observational material has been collected which indicates the existence of two distinct classes: dust forming novae (like Nova DQ Herculis 1934) and non dust forming novae (like Nova Muscae 1983). A detailed investigation of the molecular structure of carbon rich nova outflows (Beck 1993) shows that this phenomenon is essentially determined by the interplay of three different time scales: i) the expansion time scale of the neutral flow, ii) the propagation time scale of the ionization fronts affecting the condensating species, and iii) the (global) time scale controlling the spectral (i.e. energetic) evolution of the stellar radiation field. According to this approach, dust formation occurs at some cool neutral part of the flow, which has not yet been overrun by the ionization front. Thus, dust condensation should be restricted to those novae, the trajectory of which meets the formation window *before* the relevant clustering molecules become destroyed and/or (positively) charged.

3.3. MIRAS AND LPVS

In pulsational variables, dust condensation is observed to be a very pronounced phenomenon which not only determines their spectral appearance but more profoundly their shell dynamics and the internal feedback mechanisms regulating the various pulsational modes being realized.

Dynamical modelling of the pulsating shells of Miras and LPVs shows that hydrodynamic waves generated by internal pulsations steepen up to shock waves when traveling outwards through the extended atmosphere and the surrounding circumstellar shell, where they give rise to excellent local conditions enabling layered dust nucleation and growth (Fleischer *et al.* 1992). This is triggered basically by a two-step process, where a shock first

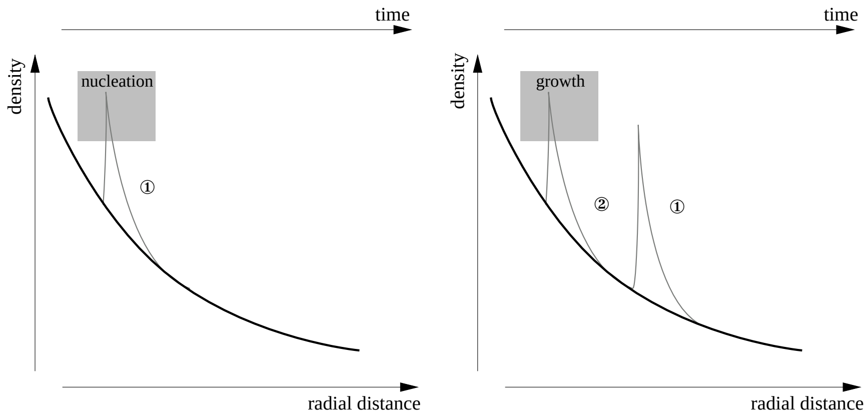

Figure 5. Scheme of dust formation in case of a pulsational variable. Two subsequent shocks are depicted hitting a considered mass element. By the first shock (labelled by (1)), the mass element is compressed and brought up to the dust formation window where avalanche cluster nucleation takes place. This process is stopped by rapid relaxation behind the front. If the mass element is hit by a subsequent shock (labelled by (2)) which is large enough to shift it up into the condensation window again, efficient growth of the already existing nuclei to macroscopic grains proceeds.

overruns a gas element and by the large compression and subsequent strong supercooling favouring efficient cluster nucleation. When this gas element then is hit by the next shock, due to the compression and temperature increase, excellent conditions are realized, allowing for the rapid growth of the seed clusters already present to macroscopic grains. This process demonstrates that pulsations and shock waves provide a natural mechanism for shifting the trajectory of the mass-element into the dust nucleation and the growth window after two subsequent shocks.

Consistent model calculations reveal an interesting interplay between the generation of the periodic internal shock waves and the induced global dynamical behaviour of the circumstellar shell essentially driven by radiation pressure of the different dust layers (Winters *et al.* 1994, 1995). Because of this pronounced nonlinear single-periodic, double-periodic, ..., multiperiodic, and even chaotic pulsations of the circumstellar dust, shells can be realized, sensitively depending on the precise values of the fundamental parameters, chosen for characterizing the object considered. Theoretical analysis of this behaviour within the context of dynamical system theory and nonlinear Hamiltonian dynamics allows to construct a Poincaré map, which even in case of very schematic and strongly simplified models reveals their mono-periodic, multiperiodic, or chaotic character (Geyer 1997), as is manifested in the observed infrared light curves of particular objects (e.g. LeBertre 1992). Up to now, consistent dynamical models are available only for C-stars, where the dust formation mechanism is sufficiently understood and effective methods for a reliable theoretical description are available. For the even more important case of inorganic grain formation in the shells of M-Miras, the general situation is still rather unsatisfactory due to the lack of appropriate nucleation theories.

3.4. R CORONAE BOREALIS STARS

Since the discovery of the spectacular occultation phenomena in the light curve of the variable star R Coronae Borealis more than 200 years ago, still no physically consistent description exists, covering all aspects of this most interesting episodic behaviour. However, general agreement exists about the nature of the obscuration, assumed to be caused by efficient soot formation producing an optically thick dust cloud able to occult the central star. As the effective temperatures of RCB stars are rather high with regard to dust condensation, ranging between 4 000 K and 20 000 K, effective dust formation should proceed under the assumption of stationary equilibrium conditions only at considerably large distances of about $10R_*$ from the stellar surface, where the local temperature becomes low enough to allow for carbon grains to condensate. Observations on the other hand favour comparable short distances of only a few stellar radii, in order to explain properties of the stellar atmosphere, characteristic occultation time scales, or specific details of the time variation of individual obscuration features. Thus, in the environments of RCB stars a clear discrepancy exists between theory and observation with regard to the position of the actual condensation window of carbon grains. Nowadays theory aims to remove this gap by postulating

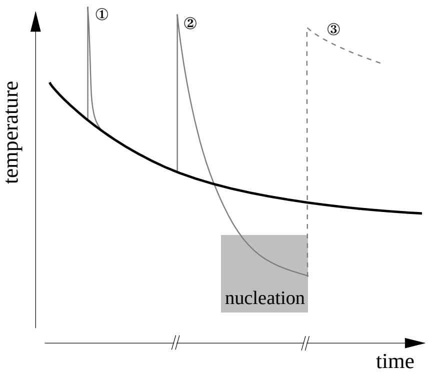

Figure 6. Dust formation by supercooling behind circumstellar shock waves in the envelopes of RCB stars (schematic). The temperature after the passage of a shock wave is depicted for gas elements situated at three different radial positions. Close to the star (1), the density is large, radiative cooling is efficient and raditive equilibrium (black line) is reestablished rapidly after the passage of a shock. At intermediate densities (2), radiative heating and cooling is less effective and, consequently, the re-expansion of the gas behind the shock causes considerable adiabatic cooling, which finally brings the element into the nucleation window. Far from the star (3), the density is too small to allow for any relevant radiative cooling and the gas remains hot after the passage of a shock (cf. Woitke *et al.* 1996).

i) an episodic local density increase over the stellar photosphere due to a blob or clump of matter expelled from the atmosphere due to some kind of a radiative instability in the He ionization zone (Asplund 1997) and ii) a substantial local temperature decrease produced by supercooling after the passage of a shock wave with amplitude above some critical value (Woitke *et al.* 1996).

The central feature of both approaches is a dynamical and thermal instability each of which potentially produces favourable local conditions for dust formation. However, so far no detailed calculations for a quantitative modelling of a RCB light curve based on these suggestions have been performed. Therefore, despite these promising attempts, the consistent final interpretation of the RCB phenomenon is still not at hand, even after more than 200 years of astronomical consideration.

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