GRAIN FORMATION IN THE WINDS OF COOL RED GIANT STARS

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Abstract. The problem of dust formation in the circumstellar envelopes of Asymptotic Giant Branch stars is reviewed. Special emphasis is put on the consistent modelling of the dust forming circumstellar shell, where due to a strong coupling the dust formation process governs the dynamical behavior of the object.

Key words: dust – chemistry – circumstellar shells – long–period variables – RCrB

1. Introduction

Cosmic dust plays an important role in current astrophysics, manifesting itself as an important component of the interstellar medium and dominating the appearance of various objects like red giants and supergiants, and even episodic events, e.g. RCrB stars, novae, and supernovae. For this reason it seems natural that cosmic grain physics, in particular the problem of grain formation, has attracted much interest in the last decades. Especially red giants and supergiants, showing pronounced stellar outflows, have proven to be ideal objects to study in detail the process of grain nucleation and growth.

From a microscopic point of view, grain formation can be conceived as a sequence of chemical reactions, starting with suitable molecules and finally ending with macroscopic dust particles. In this respect, the grain formation process itself seems to be only controlled by proper pressure and temperature conditions and a certain chemical composition of the gas phase providing suitable molecules to condensate. So far the problem appears to be rather simple: Adopting some nucleation theory, first one has to determine regions of high nucleation efficiency in the p–T plane (i.e. regions of sufficiently high particle densities and sufficiently low temperatures), and, second to determine those trajectories along the evolution of a material element which cross the dust forming region for a time sufficiently long to enable effective grain formation in the element. Natural systems for this process are stellar outflows, starting from the initial plasma phase in the stellar photosphere. With decreasing temperature a complex chemistry evolves and finally, at some critical radius, favorable conditions for dust nucleation and growth occur as indicated by the observed steep onset of the optical depth, the high infrared excess and a significant increase of the expansion velocity in the shells of these objects (cf. Fig. 1). With this respect, dust formation in the winds of red giant stars is a physically and mathematically well posed problem, the initial condition of which can be uniquely infered from the atmospheric analysis.

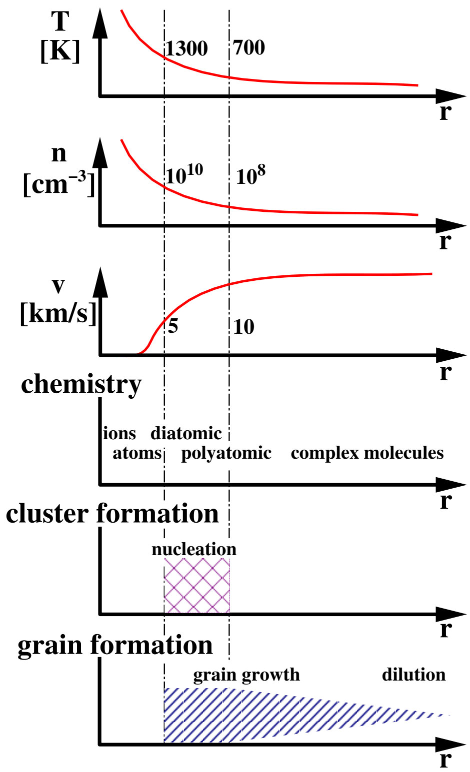

Figure 1. Schematic structure of a dust forming circumstellar shell. Dust nucleation is well confined to a region approximately between 1300 K and 700 K while the region of dust growth extends much farther outwards.

Despite this simple basic picture, astrophysical dust formation appears to be an extremely complicated non–linear process. The reason for this behaviour is that the presence of even a small amount of dust, due to its huge absorption and scattering coefficient, has severe consequences for the local physical and chemical conditions in the dust forming region. In particular the following three effects play an important role:

- *dust is a very effective transmitter of energy* by efficiently absorbing and thermalizing short–wavelength photons and emitting their energy at infrared wavelengths. By this process, dust strongly affects the thermodynamical behaviour of the system.

- *dust is a very effective transmitter of momentum* by transferring the absorbed photon momentum by frictional coupling to the ambient gas. Therefore, dust strongly affects the hydrodynamical structure of the system.
- *dust is a catalyst for chemical reactions:* gas particles absorbed at the grain's surface can react with the grain material or another admolecule to form new species which cannot be formed from the gaseous phase. Therefore, dust strongly determines the chemical behaviour of the system.

As a consequence, any realistic treatment of circumstellar dust formation can only be performed by means of a self–consistent modelling of the dust forming objects, comprising as essential ingredients: thermodynamics, chemistry, cluster physics, radiation matter interaction, and nonlinear dynamics (e.g. Sedlmayr & Winters (1991), Fleischer et al. (1992), Winters et al. (1994a)).

2. Circumstellar dust formation

The consistent treatment of a dust forming shell of a red giant requires the consideration of at least the three closely coupled complexes: circumstellar chemistry, the dust nucleation and grain growth problem, and of the hydrodynamical and thermodynamical wind structure.

2.1. CIRCUMSTELLAR CHEMISTRY

In principle, chemistry plays a three–fold role with regard to circumstellar shells:
i) for the interpretation of the observed molecular lines, i.e. the diagnostics of the objects, the detailed chemical structure and thus the local concentrations of the molecular species have to be known,
ii) the chemical species present determine the transport coefficients in the atmosphere and hence the local physics in the inner parts of the shells (e.g. temperature, density, ...), and
iii) the chemistry determines in particular the local abundance of the dust forming species and, thereby, the primary (high–temperature) condensates to be expected.

To give a general picture of the complex processes to be involved in modelling the chemistry of the circumstellar shell, Fig. 2 depicts a sketch of the various chemical processes which might be important.

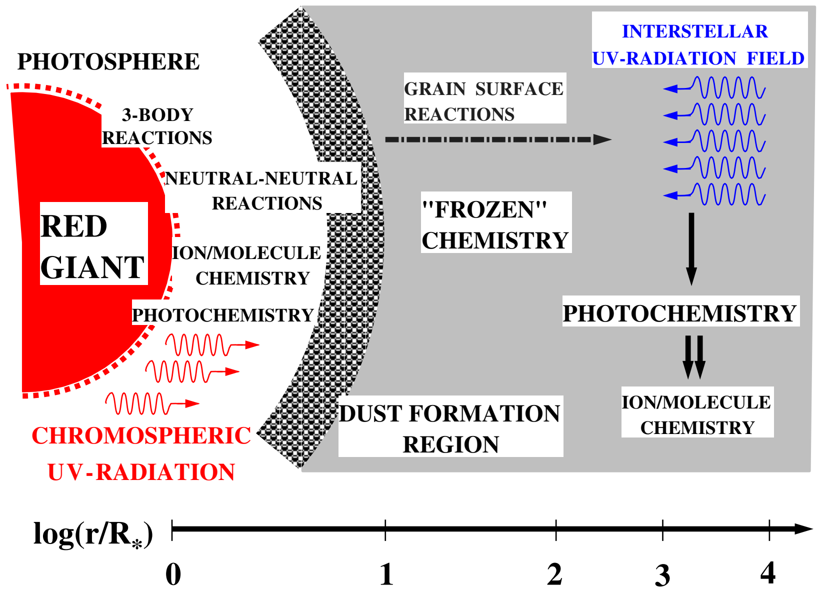

Figure 2. Chemical processes in different regions of the circumstellar shells around red giants (adopted from Patzer (1996))

2.1.1. *Chemical equilibrium (CE)*

This most simple approach requires the chemical reaction timescales to be small compared to all other timescales determining the structure of the outflow (e.g. the hydrodynamical timescale). This condition only holds for sufficiently high particle densities, small velocity fields, and systems where photoreactions can be neglected, i.e. for radiation fields of negligible UV portion. This situation seems to be realized for the cool photospheres and the inner shell regions of cool C-stars and M-stars without chromospheres. This CE condition is very severe and easily violated even by the presence of weak UV contributions and/or by moderate velocity fields (e.g. Goeres et al. 1988, Beck et al. 1992). Their model calculations for α Ori indicate dramatic deviations of particular species from CE caused already by a very moderate photospheric UV field ($T = 3000K$) or by small temporal variations of the radiation field as observed for α Ori (Dupree et al. 1987).

2.1.2. *Chemical non–equilibrium*

This situation requires the solution of the time dependent network of chemical rate equations (non–kinetic equilibrium) in case that velocity fields and/or short time variations of the radiation field have to be considered. This is the usual case for the modelling of long–period variable stars (LPVs), where the dynamical timescales determine the local physics. Such a treat-

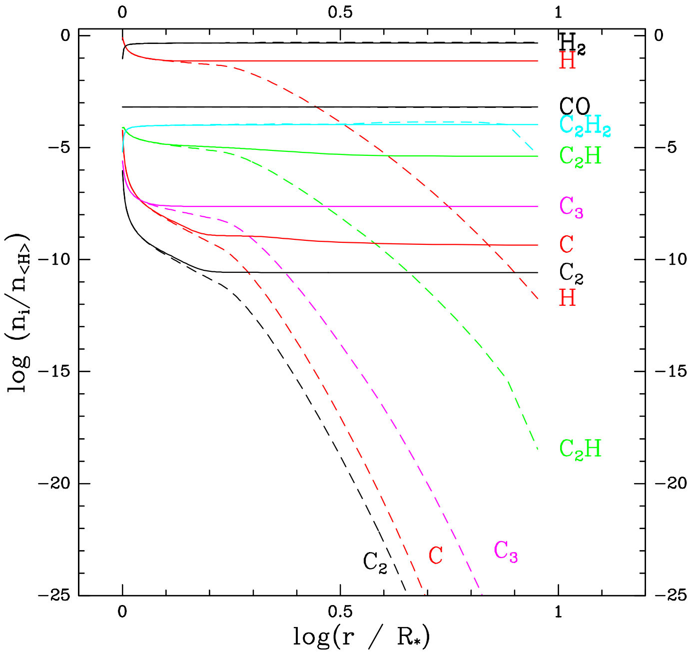

Figure 3. Equilibrium concentrations (dashed lines) and non–equilibrium concentrations (solid lines) for different molecules in a stationary model for a dust driven wind. Due to fast dilution in the wind, a frozen chemistry develops in the non–CE calculation. The figure is adopted from Patzer (1996).

ment is also necessary in the outer regions of stationary outflows, where the hydrodynamical expansion– and acceleration timescale becomes comparable or even shorter than the chemical timescales involved. For these systems often a frozen chemistry evolves due to the rapid decrease of the chemical reaction rates caused by dilution in the wind. As an example, Fig. 3 shows a comparison between a pure CE and a non–CE calculation of the chemical structure for a stationary dust driven wind model describing the dust shell of around a C–star.

2.2. DUST NUCLEATION AND GROWTH

Basically, dust formation can be conceived as a chain of chemical reactions starting with small molecules and ending with macroscopic specimens called dust grains. To follow this idea by a theoretical description, requires in principle to construct and to solve a suitable chemical network, containing in the small regime molecules of increasing size, in the intermediate regime clusters (containing $\approx$ 10 constituents) and in the large particle regime

grains having $\sim 10^{10}$ constituents. This approach however is much to elaborate not only due to the huge number of reaction equations (corresponding to the number of constituents), but also due to the lack of input data necessary to describe the reaction rates, the structure, and the thermodynamical properties of the particles involved.
Applied to PAH formation in C–star outflows, this method turned out to be practically limited to sizes of the polyaromatic molecules having less than six aromatic rings (e.g. Cherchneff et al. 1992).

A detailed inspection of the dust formation process shows however, that the problem can be split into two different phases which can be treated seperately: i) the nucleation process, i.e. the formation of so called critical clusters out of the gas phase, and ii) the growth of these critical clusters to macroscopic specimens. As all clusters smaller than the critical cluster have the tendency to evaporate and all clusters larger than the critical cluster have the trend to grow, the critical cluster plays the role of a 'bottleneck', which any effective dust formation process has to surmount in order to arrive at macroscopic grains. The properties of the critical cluster, defined by an extremum of its Gibbs free enthalpy, are therefore decisive for the whole dust formation problem and its efficiency.

2.2.1. *Nucleation regime*

For the treatment of the first phase – the formation of the critical cluster – usually two different methods are adopted:

1. Classical nucleation theory

In this concept, the molecule–cluster transition is conceived as a thermodynamic phase transition governed by the thermodynamic functions of the emerging products and by the supersaturation ratio of the condensating gaseous species. Classical nucleation theory results in a critical cluster having maximum free enthalpy and in a critical nucleation rate, solely given by the thermodynamic properties of the critical cluster and the local supersaturation ratio of the condensating species which has to be larger than unity to allow the formation of the seed particle. This method for example yields excellent results if applied to the formation of water droplets in cloud chamber experiments or in the earth's atmosphere but is highly questionable in application to astrophysical problems. This is due to the fact, that classical nucleation theory conceptually refers to critical clusters having already well defined surfaces (which is true for water droplets consisting of at least 10^9 monomers) but not for astrophysical critical clusters usually having about 5–20 basic constituents. In this case, the surface tension concept cannot be applied and the thermodynamic functions of all individual small clusters involved either have to be provided by suitable laboratory experiments or calculated by molecular dynamics methods (e.g.

Patzer et al. 1995, Köhler et al. 1996). Hitherto however, such an approach is limited to chemically homogeneous clusters, whose composition and the corresponding molecular interaction potentials are known. A similar description of heterogeneous structures is still lacking. For this reason, all nucleation theories applied so far in astrophysics consider the formation of homogeneous critical clusters (Gail & Sedlmayr 1986, Kozasa & Hasegawa 1987, Kozasa et al. 1996, Köhler et al. 1996).

2. Chemical pathway

Until now this approach has been applied to the formation of polyaromatic molecules in C–stars (e.g. Keller 1987, Cherchneff et al. 1992, Goeres 1993, Goeres et al. 1996), polyaromatic carbons in RCrB stars (Goeres & Sedlmayr 1992) and fullerenes in the Krätschmer–Huffman experiment (Krätschmer et al. 1990; Goeres & Sedlmayr 1991). The basic idea of this method is that in the corresponding reaction networks always few dominant reaction pathways can be isolated along which the grain formation process essentially proceeds. By a detailed discussion of the individual reactions a most efficient pathway can be constructed leading from the basic molecule (the monomer) into the regime beyond the critical cluster. On this path the critical cluster is defined as that step having the minimum net growth rate. Application of this method to PAH formation in C–star winds shows that the critical cluster is rather small at low temperatures (less than 20 C-atoms for $T < 1000\,\mathrm{K}$, see Goeres et al. 1996) and therefore only few reaction steps have to be considered.

2.2.2. *Growth regime*

This particle size regime, which is essentially defined by the addition of growth species to the already existing clusters for both, classical nucleation theory and for the pathway description, can be treated with sufficient accuracy by assuming thermal growth (Gail & Sedlmayr 1988, Gauger et al. 1990). This requires the knowledge of the corresponding reaction rates (i.e. the sticking coefficients) which in particular for inorganic grains are only poorly known or even lacking (e.g. Patzer et al. 1995).

3. Models of dust forming circumstellar shells

In the context of circumstellar dust formation, especially three situations have been modelled: i) stationary dust driven winds, ii) shells of pulsating variables like LPVs, and iii) episodic phenomena like RCrB stars, novae and supernovae.

3.1. STATIONARY DUST DRIVEN WINDS

This phenomenon, which only occurs for objects showing negligible variability and extremely high mass loss rates, is confined to the upper right region of the HR diagram (cf. Dominik et al. 1990). The physical condition for a stationary dust driven wind to exist is that the dust formation region is situated inside the sonic point of the wind in order for the radiation pressure on dust being able to levitate the atmosphere beyond the escape point and to determine the mass loss rate of the star (Gail & Sedlmayr 1987, Sedlmayr & Dominik 1995). A good example for such an object is IRC +10216, the selfconsistent model of which (assuming spherical symmetry, radiative equilibrium, chemical equilibrium, and applying classical nucleation theory to describe the formation of amorphous carbon grains) not only provides the observed velocity field, the temperature structure, and the optical depths, but also the observed spectral appearance and the detailed shell structure leading to the observed visibilities (Winters et al. 1994a).

3.2. PULSATING VARIABLES

Most red giants surrounded by a circumstellar dust shell are long–period variables (e.g. Jura 1986) with pulsation periods on the order of $P \approx 1\,\mathrm{yr}$. Modelling their circumstellar dust shells therefore requires a fully time–dependent treatment of the problem. The results of such calculations reveal a very complex structure of the circumstellar shell (e.g. a layered distribution of the dust component, dust induced or dust accelerated shocks) and the existence of an eigenperiod of the circumstellar shell leading to the effect of *multiperiodicity* which is caused by the very strong and highly non–linear coupling among hydrodynamics, thermodynamics, chemistry, and dust formation and –growth (see Fleischer et al. 1991,1992,1995 and Fleischer et al., this volume). These phenomena provide a physical explanation for the internal structures and the *multiperiodic* long–term behaviour of the observed infrared lightcurves (e.g. Feast et al. 1984, Le Bertre et al. 1992) and of the observed brightness profiles and visibilities (e.g. Ridgway & Keady 1988, Danchi et al. 1994) of these objects as discussed in Winters et al. (1994b,1995).

3.3. DUST FORMATION IN RCRB STARS

A third important astrophysical application of dust formation theories concerns the study of episodic phenomena like nova– and supernova outflows or the RCrB occultation events. Whereas the first two cases can simply be treated by adopting a stationary flow, dust formation in RCrB environments turns out to be triggered by a critical phenomenon causing an instantaneous phase transition from molecules to carbon dust (cf. Goeres & Sedlmayr 1992). As RCrB even in the quiet state shows more or less periodic variations, the trigger mechanism might be some critical shock wave causing an extreme local increase of the temperature (up to $\approx 50000\,\mathrm{K}$) and thereby providing an exellent initial condition for a subsequent cooling flow down to well below the radiative equilibrium temperature within only a few days (Woitke et al. 1996). This idea appears to be very appealing because it explains not only the observed large optical depths causing the obscuration but even seems to solve the long standing debate between observers and theoreticians concerning the expected site of dust formation. Previous theories always claimed dust formation to take place at a distance of about 10 stellar radii, where the temperature is low enough for grains being able to form. This contradicts the observations which can only be explained if dust formation takes places very close to the star. This discrepancy could be resolved by the above suggested mechanism as it yields extreme supercooling and therefore high nucleation rates even at about 2 stellar radii (Woitke et al. 1996). However, a consistent modelling of this mechanism would require a 3–dimensional treatment of cloud formation which seems to be out of scope of present–days capabilities. Moreover, atmospheres of RCrB stars seem to be close to their Eddington limit (Asplund et al., this volume), suggesting sporadic "blop" outflows of matter which also could provide favourable conditions for dust formation along their cooling tracks.

4. Conclusions

The consistent modelling of red giants and supergiants, novae, and supernovae including chemistry and dust formation, and the investigation of the obscuration phenomenon of RCrB stars all yield results being in excellent agreement with the observed spectral appearance and the derived timescales characterizing these objects. Nevertheless, all theories applied so far, still suffer from rather restrictive assumptions either with regard to the microscopic physics (e.g. chemical equilibrium, classical nucleation theory, ...) or in order to reduce the numerical effort (e.g. spherical symmetry, ...). These limitations should be surmounted in future work in order to arrive at a realistic consistent description and understanding of these interesting objects. This is a particular need in view of already existing and of future high precision instruments, which collect a wealth of very detailed observations, waiting to be interpreted on an equivalently high level.

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References

Beck H. K. B., Gail H.-P., Henkel R., Sedlmayr E., 1992, *A&A* 265, 626
Cherchneff I., Barker J. R., Tielens A. G. G. M., 1992, *ApJ* 401, 269
Danchi W. C., Bester M., Degiacomi C. G., Greenhill L. J., Townes C. H., 1994, *AJ* 107, 1469
Dominik C., Gail H.-P., Sedlmayr E., Winters J. M., 1990, *A&A* 240, 365
Dupree A. K., Baliunas S. L., Guinan E., Hartmann L., Nassiopoulos G. E., Sonneborn G., 1987, *ApJ* 317, L85
Feast M. W., Whitelock P. A., Catchpole R. M., Roberts G., Overbeek M. D., 1984, *MNRAS* 211, 331
Fleischer A. J., Gauger A., Sedlmayr E., 1991, *A&A* 242, L1
Fleischer A. J., Gauger A., Sedlmayr E., 1992, *A&A* 266, 321
Fleischer A. J., Gauger A., Sedlmayr E., 1995, *A&A* 297, 543
Gail H.-P., Sedlmayr E., 1986, *A&A* 166, 225
Gail H.-P., Sedlmayr E., 1987, *A&A* 177, 186
Gail H.-P., Sedlmayr E., 1988, *A&A* 206, 153
Gauger A., Gail H.-P., Sedlmayr E., 1990, *A&A* 235, 345
Goeres A., 1993, *Rev. Mod. Astron.* 6, 165
Goeres A., Sedlmayr E., 1991, *Chem. Phys. Lett.* 184, 310
Goeres A., Sedlmayr E., 1992, *A&A* 265, 216
Goeres A., Henkel R., Sedlmayr E., Gail H.-P., 1988, *Rev. Mod. Astron.* 1, 231
Goeres A., Keller R., Sedlmayr E., Gail H.-P., 1996, *Polycyclic Aromatic Compounds* (in press)
Jura M., 1986, *ApJ* 309, 732
Keller R., 1987, In Léger A., d'Hendecourt L., Boccara N., (eds), *Polycyclic Aromatic Hydrocarbons and Astrophysics*, p. 387, Reidel Publ. Comp
Köhler T. M., Gail H.-P., Sedlmayr E., 1996, *A&A* (in press)
Kozasa T., Hasegawa H., 1987, *Prog. Theor. Phys.* 77, 1402
Kozasa T., Dorschner J., Henning T., Stognienko R., 1996, *A&A* 307, 551
Krätschmer W., Fostiropoulos K., Huffman D. R., 1990, *Chem. Phys. Lett.* 170, 167
Le Bertre T., 1992, *A&AS* 94, 377
Patzer B., 1996, Dissertation, Technische Universtät Berlin, Berlin, FRG (in preparation)
Patzer A. B. C., Köhler T., Sedlmayr E., 1995, *Planet. & Sp. Sci.* 43, 1233
Ridgway S. T., Keady J. J., 1988, *ApJ* 326, 843
Sedlmayr E., Dominik C., 1995, *Space Sci. Rev.* 73, 211
Sedlmayr E., Winters J. M., 1991, In Crivellari L., Hubeny I., Hummer D. G., (eds), *Stellar Atmospheres: Beyond Classical Models*, p. 397, Kluwer Academic Publishers
Winters J. M., Dominik C., Sedlmayr E., 1994a, *A&A* 288, 255
Winters J. M., Fleischer A. J., Gauger A., Sedlmayr E., 1994b, *A&A* 290, 623
Winters J. M., Fleischer A. J., Gauger A., Sedlmayr E., 1995, *A&A* 302, 483
Woitke P., Goeres A., Sedlmayr E., 1996, *A&A* (in press)