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FORMATION OF DUST GRAINS WITH IMPURITIES IN RED GIANT WINDS

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1. Introduction and Summary

Among the several proposed carriers of diffuse interstellar bands (DIBs) are impurities in small dust grains, especially in iron oxide grains (Huffman 1977) and silicate grains (Huffman 1970). Most promising are single ion impurities since they can reproduce the observed band widths (Whittet 1992). These oxygen-rich grains are believed to originate mostly in the mass flows from red giants and in supernovae ejecta (e.g. Gehrz 1989). A question of considerable impact for the origin of DIBs is therefore, whether these grains are produced as mainly clean crystals or as some dirty materials.

We have developed a formalism that allows to keep track of the heterogeneous growth of a dust grain and its internal structure during the dust formation process. We have applied this formalism to the dust formation in the outflow from a red giant star.

Since the condensation of dust grains usually becomes effective only at temperatures considerably lower than the evaporation temperature of the condensing refractory materials, we find that at the time of onset of dust formation, a variety of different refractory materials is stable against evaporation. It is therefore highly unlikely that the condensation process produces a pure crystal of a certain stoichiometric composition. Instead, a grain consisting of an amorphous mixture of different materials has to be expected. In the frame of our model we find that about one half of the grain material will be oxygen and the other half will be shared by silicon, iron, and magnesium in a temperature-dependent mixture.

Since the grain materials have to be built up by chemical reactions with different molecules in the gas, it is also to be expected that impurities in the form of single atoms are incorporated frequently into the crystal structures. Since both Fe and Mg are mostly present in atomic form, they are the best candidates for this process. Together with the fact that the produced grains small (about 10^{-6}cm in diameter) makes them a possible sources of the DIB absorption.

We conclude that dust grains formed in stellar winds are heterogeneous amorphous structures, combining different refractory materials in the same grain. The mechanism of formation of the grains is likely to allow for frequent inclusions of impurities.

2. Method of calculation

The growth of the dust grains is calculated with the *moment method for heterogeneous growth* (Dominik *et al.* 1993) which reduces the calculation of the time evolution of the grains size distribution to a set of ordinary differential equations for the moments of the size distribution. The moments are defined by

$$K_j = \int_{a_\ell}^{\infty} f(a,t) a^j da \quad , j = 1, 2, \dots$$

where a is the radius of the (spherical) dust grains, $f(a,t)$ is the size distribution function and a_ℓ is the lower limiting size of a dust grain. The moment equations are given by

$$\frac{d}{dt} K = J_\ell a_\ell^j + j \xi K_{j-1} \quad , j = 1, 2, \dots$$

where J_ℓ is the nucleation rate and ξ is the growth velocity of the grain radii. The equations above are simple to solve. The moments contain the most important information about the dust directly and can also be used to construct the size distribution at any instant. The moment method is discussed in detail in (Gail and Sedlmayr 1988, Dominik *et al.* 1993).

To calculate the growth velocity we consider different refractory materials. We assume that certain molecules containing the relevant atoms can contribute to the growth the material, and they do so in each collision with a sticking probability α. Due to the lack of better data, we assume these probabilities to be 1.
Evaporation rates are calculated from chemical equilibrium. To calculate these rates we construct an equilibrium state of the refractory material with its own vapor and derive evaporation rates for all molecules consisting of atoms which are contained in the solid. If the growth rates are larger than the evaporation rates, the solid is stable in the actual environment and may grow.
If several different materials are stable at the same time, we maximize the condensation rate of each chemical element under the stoichiometric boundary conditions of all stable solids. The method is discussed in detail in (Dominik *et al.* 1993).

3. Model calculation

We have applied the method described above to dust formation in the wind of an oxygen-rich red giant star. The model was calculated with the following assumptions.

- Central star: $L_\star = 10^4 L_\odot, T_\star = 2500K, \dot{M} = 10^{-6} M_\odot/yr$, solar chemical abundances.
- Gas temperature: calculated from radiation dilution: $T(r) = \frac{T_\star}{\sqrt{2}}\{1 - \sqrt{1 - R_\star^2/r^2}\}$.
- Molecular composition of the gas phase: chemical equilibrium.
- Solid phases considered: Si, Fe, Mg, FeO, MgO, SiO_2, Fe_2O_3, Mg_2Si, $MgSiO_3$, Mg_2SiO_3.
- Nucleation rates for Fe and SiO calculated form classical nucleation theory as described in (Draine and Salpeter 1977) and (Gail *et al.* 1984).

The following figures show chemistry and dust formation in the model as a function of the gas temperature.

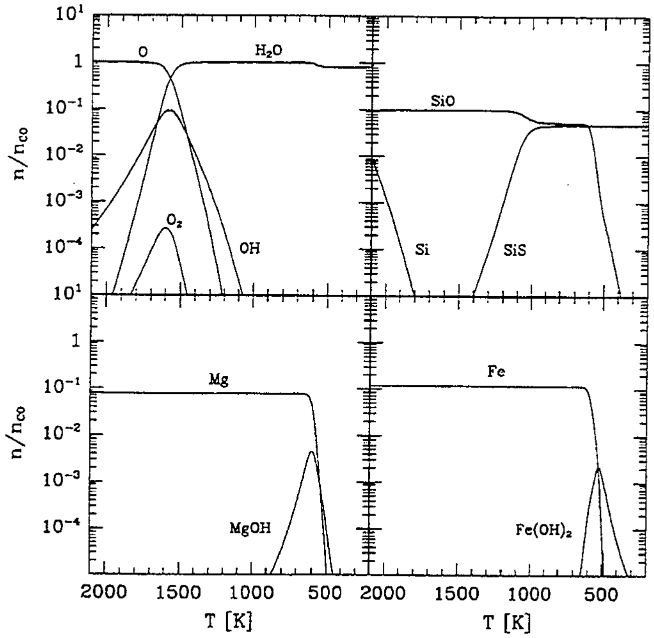
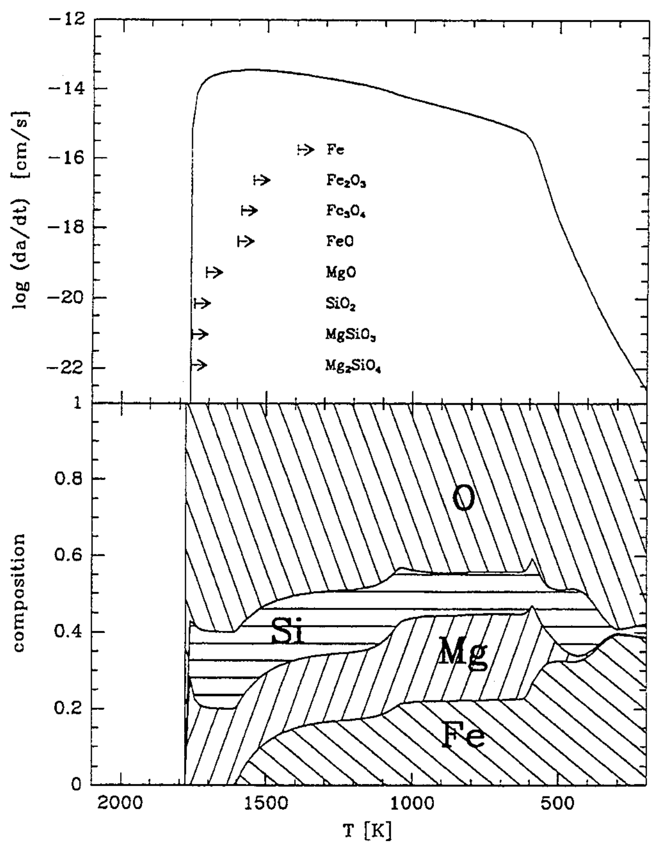


Figure 1: Chemical composition of the gas phase
The figure to the left shows the concentrations of the molecules most important for dust formation. Oxygen is mainly present as H_2O, except for temperatures above 1500K, where atomic O is more important. Silicon is at higher temperatures mostly in SiO, at lower temperatures also in SiS. Both Iron and Magnesium are present in atomic form. The sharp drop-off of the densities of SiO, Mg, and Fe around 600K is due to consumption of these molecules by dust formation.

Figure 2: Composition of the condensing material
Upper diagram: The arrows show the stability limits of the different refractory materials under consideration. The first materials to become stable are the magnesium silicates, followed by different oxides. The solid line shows the growth velocity of the grain radii in cm/s.
Lower diagram: Chemical composition of the material condensing on existing nuclei at the temperature given on the x-axis. The fraction of each element (by number, not weight) in the condensing material is proportional to the height of the respective area.



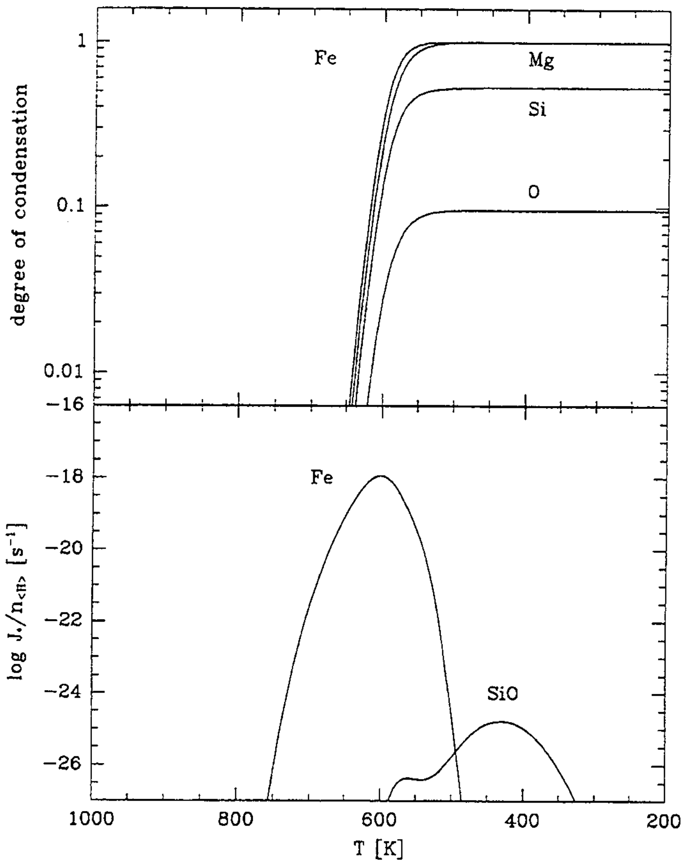


Figure 3: Nucleation rates and degrees of condensation
The *lower diagram*: shows the nucleation rates due to nucleation of pure Fe and SiO.
Upper diagram: Fraction of Fe, Si, Mg, and O that condenses out.
The nucleation rate due to iron shows a strong peak below 800K. At this point dust formation starts. The rapid consumption of condensable material can be seen from the upper diagram. Fe and Mg condense out completely, while some Si remains in the gas phase (as SiS). Only 10% of the available oxygen condense, since the solid cannot bind more oxygen. The nucleation peak of SiO is only very week, since most of the material has already condensed onto the nuclei formed by the iron nucleation.

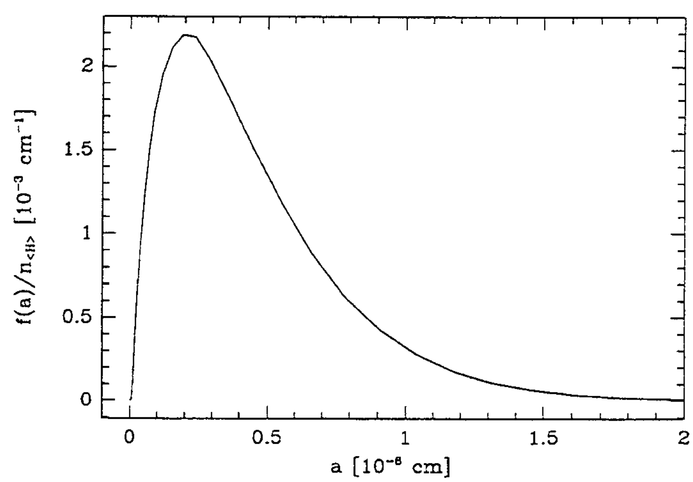


Figure 4: Size distribution of the dust grains entering the interstellar medium
This figure shows the final size distribution of the dust grains as they enter the interstellar medium. The figure clearly shows that the grains are quite small - the mean size is below 10^{-6}cm.

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