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Mineral formation in stellar winds

V. Formation of calcium carbonate

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Abstract. An emission band around 92 μm found in a few IR spectra from highly evolved stars was proposed to be due to the presence of carbonate dust grains in the circumstellar material (Kemper et al. 2002a, Nature, 415, 295). This contribution presents the results of a model calculation for the condensation of calcite ($CaCO_3$) in the stellar wind of AGB stars. It is shown that the quantities of carbonate dust formed relative to the quantities of silicate dust are negligibly small. This results from the fact that carbonates form at a much lower temperature than the silicate dust components. Carbonate dust formation then is suppressed by the strong acceleration of the wind material by radiation pressure on the silicate dust and the subsequent rapid dilution of the wind material. This makes it highly improbable that carbonate dust can be formed in stellar outflows.

Key words. stars: circumstellar matter – stars: mass-loss – stars: winds, outflows – stars: AGB and post-AGB

1. Introduction

Since the ISO satellite allowed a detailed far infrared spectroscopy of circumstellar dust shells, a large number of broad solid state emission bands have been detected in that wavelength region. Many of them are now identified by comparing observed emission bands with laboratory measured absorption spectra of materials which, because of their chemical composition, are possible candidates for condensates in stellar outflows with either an oxygen rich or carbon rich element mixture (Molster 2000; Molster et al. 2002a,b,c). Most of the identified features are associated with the most abundant minerals which may condense in an oxygen rich element mixture, the magnesium-iron silicates. Some features have been identified with diopside, corundum, silica and some other solids (for an overview see Molster & Waters 2003). There remain, however, a number of features for which presently no identification is possible.

Kemper et al. (2002a,b) recently claimed that a broad and rather strong not yet identified feature in the wavelength region 88 μm … 98 μm observed in a few objects (NGC 6302, Kemper et al. 2002b; NGC 6537, Molster et al. 2002a) can be identified with calcite with composition $CaCO_3$ or with a mixture of calcite and dolomite ($Ca_{0.5}Mg_{0.5}CO_3$); see also Molster & Waters (2003). This identification is based essentially on this single feature. A second feature at about 65 μm due to dolomite is claimed to contribute to an observed broad group of features extending from about 55 to above 70 μm, but this interpretation is not really convincing. Earlier attempts to identify features of carbonates at much lower wavelength with observed circumstellar dust features were not successful (McCarthy et al. 1977; Knacke & Krätschmer 1980).

In this contribution we will show that it is unlikely that carbonates can be formed in the outflows of evolved stars. The basic reason for this is that the upper stability limit of carbonates against decomposition occurs in a hydrogen rich environment with very low pressure at rather low temperatures. The outflowing gas then has already achieved highly supersonic outflow velocities due to radiative acceleration by radiation pressure on the more stable silicates. These condense at much higher temperatures and the subsequent rapid dilution of the outflowing wind material then suppresses any further growth of other kinds of dust in that zone, which in particular also holds for carbonates.

2. Condensation of carbonates

2.1. Chemical equilibrium condensation

The formation of carbonates requires that three oxygen atoms are available for each C atom in the carbonate. Because of the exceptional high bond energy of the CO molecule this condition cannot be met in a carbon rich element mixture where the oxygen is completely consumed by CO formation. We consider therefore an oxygen rich element mixture where sufficient O is left over to form oxygen bearing minerals like silicates and possibly carbonates. This requirement is clearly met by NGC 6302 (see Table 3 in Marigo et al. 2003), one of the two objects for which the presence of carbonate dust grains has been proposed. For NGC 6537, the second object, the abundances

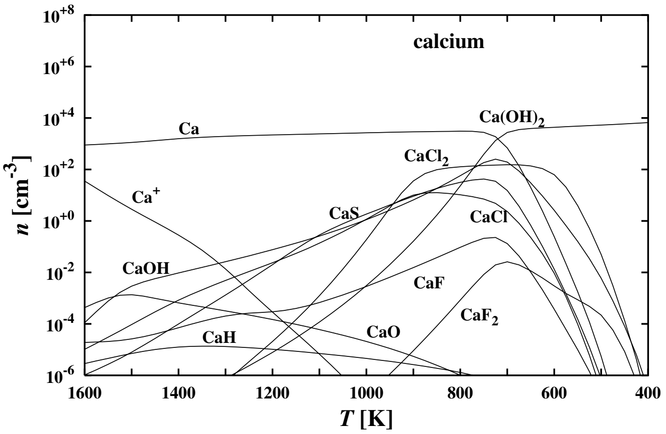

Fig. 1. Particle densities of calcium bearing gas phase species at a pressure of $P = 10^{-10}$ bar for different temperatures.

derived for O and C are equal to each other but the estimated error of the abundance determination of 30% leaves room for a somewhat higher O than C abundance.

2.1.1. Composition of the gas phase

For calculating the condensation of calcium carbonate in a stellar outflow, we need to know the composition of the gas phase since this defines the species from which the carbonate has to be formed. With respect to the abundant elements H, C, N, O, Si, Mg, and Fe which are important for the dust condensation process the composition of the gas phase is quite simple. At temperatures below 1200 K and pressures of the order of 10^{-10} bar or less, which are typical values of T and P in the condensation zone of circumstellar dust shells, the hydrogen is completely associated to H_2, the carbon is completely bound in CO, and the nitrogen is completely bound in N_2. If no solids are condensed, the silicon is nearly completely bound in SiO; only a small fraction is bound in SiS, which can be neglected. If dust is formed the silicon is partially consumed by dust formation, but the remaining fraction in the gas phase stays always in SiO. The oxygen not bound in CO, SiO and in minerals forms H_2O. Mg and Fe in the gas phase are nearly completely present as free atoms. Only at rather low temperatures do they form hydroxides, but then most of these elements are already consumed by dust formation.

The formation of $CaCO_3$ requires reactions with molecules from the gas phase bearing the less abundant element Ca. Figure 1 shows the results of a chemical equilibrium calculation for Ca compounds in a gas with solar element abundances considering the 25 most abundant elements and Rb and Cs as electron donors at low temperature. Element abundances are from Grevesse & Sauval (1998) without the corrections of Allende Prieto et al. (2001, 2002) since these apply only for the sun. The dominating Ca bearing species in the gas phase is the free Ca atom at temperatures above ≈800 K and the molecule $Ca(OH)_2$ at temperatures below ≈700 K, with a gradual transition between the two limit cases between 800 and 700 K. The growth of Ca bearing condensates in circumstellar dust shells requires either the addition of free Ca atoms at temperatures above ≈800 K or of $Ca(OH)_2$ at lower temperatures. Other Ca bearing compounds from the gas phase have an $\approx 10^{-2}$ fold lower abundance and are too rare to be important as growth species. The results shown in Fig. 1 hold for solar-like abundances.

Table 1. Free enthalpy of formation ΔG of carbonates and CaO from free atoms (in units kJ/mol).

Coeff.	Calcite	Dolomite	Lime
a	1.47018e+06	3.03962e+06	–8.97200e+03
b	–2.86005e+06	–5.59899e+06	–1.06340e+06
c	7.25920e+02	1.46089e+03	1.04332e+03
d	–1.08246e–02	8.38699e–03	–1.75619e–02
e	–1.83075e–07	–8.37213e–06	8.35406e–07

The objects for which the detection of carbonates is claimed are highly evolved post-AGB stars with significantly modified abundances of the elements He, C, N, and O (e.g. Marigo et al. 2003), but this obviously would not change the conclusions with respect to the abundance of Ca bearing compounds.

2.1.2. Pseudo-activities of the solids

For all Ca bearing solids listed in the table of Barin (1992) pseudo-activities

$$a = p_{\rm A}^{i} p_{\rm B}^{j} p_{\rm C}^{k} \dots {\rm e}^{-\Delta G/RT} \tag{1}$$

for the formation of a condensed phase with composition $A_iB_jC_k\dots$ from elements A, B, C, … via the reaction

$$i{\rm A} + j{\rm B} + k{\rm C} + \dots \longrightarrow {\rm A}_i{\rm B}_j{\rm C}_k\dots({\rm s})$$

have been calculated using the partial pressures of free atoms from the chemical equilibrium calculation for the gas phase. ΔG is the change of free enthalpy for this reaction, which is calculated from the thermochemical data given in Barin (1992). An analytical fit of the form

$$\Delta G = \frac{a}{T} + b + cT + dT^2 + eT^3 \tag{2}$$

to the tabular data was derived for all substances. The coefficients for the carbonates and lime (CaO) are given in Table 1.

Chemical equilibrium between the gas phase and a solid would require that the activity a of the solid calculated from Eq. (1) satisfies $a = 1$ (e.g. Atkins 1994). Condensates for which the activity a calculated from Eq. (1) satisfy $a < 1$ would vaporize and can never be formed. Condensates for which the activity a calculated from Eq. (1) satisfies $a > 1$ would condensate and consume as much material from the gas phase as possible until the condition $a = 1$ is met. Usually those materials are formed in chemical equilibrium as condensates, which (i) have the highest pseudo-activities; and (ii) consume as much as possible of the condensible elements.

The pseudo-activities of some of the Ca-compounds of interest are shown in Fig. 2. As is readily seen, the activities a of the carbonates calcite ($CaCO_3$) and dolomite ($CaMg(CO_3)_2$) start to exceed unity at a much lower temperature than most

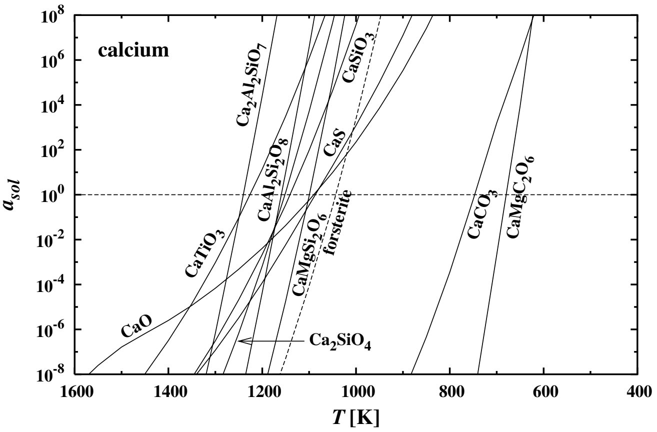

Fig. 2. Pseudo activities of calcium bearing solid compounds at a pressure of $P = 10^{-10}$ bar for different temperatures. The dotted line shows for comparison the pseudo-activity of forsterite.

of the other possible Ca-bearing condensates like gehlenite ($Ca_2Al_2SiO_7$) or diopside ($CaMg(SiO_3)_2$) or lime (CaO), and also at a much lower temperature than the main dust component forsterite (dashed line). Since a solid can exist in chemical equilibrium at most then, if its pseudo-activity equals or exceeds unity, the calcium bearing carbonates would not be formed in chemical equilibrium in an oxygen rich cosmic element mixture.

Under these circumstances, carbonates could be formed in circumstellar outflows only as a result of a strong non-equilibrium condensation process in a rapidly diluting gas, where the condensation of more stable Ca-bearing condensates has not run into completion at the instant when the pseudo-activity of some carbonate first exceeds unity and condensation of carbonates in principle becomes possible from that point on. The carbonates then could be formed as a frozen-in transient state.

Most of the Ca is likely to be condensed in other Ca-bearing compounds in this case. We do not consider the problem of the major Ca-bearing species in this paper, but note that enstatite ($MgSiO_3$) forms a solid solution with diopside ($CaMgSi_2O_6$) (cf. Saxena et al. 1993), i.e. a major part of the Ca is probably incorporated as a solid solution component into pyroxene-like silicate dust material.

In the following we restrict our calculations to the condensation of calcite. Since our final result will be that calcite cannot be formed, this result then also holds for dolomite, since dolomite is less stable than calcite (cf. Fig. 2).

2.2. Non-equilibrium condensation of carbonates

If we wish to calculate the formation of calcite by a non-equilibrium condensation process, we need to know the reaction of its formation from the gas phase. Since this reaction seems not to be known[1], we have to make some assumptions concerning this reaction.

In order to form calcite with composition $CaCO_3$ from the gas phase one requires in particular abundant gas phase species which are carriers of the elements Ca, C, and O from which calcite is formed. The gas phase species of highest abundance bearing these elements are free Ca atoms and H_2O and CO molecules. A possible reaction for calcite condensation from the gas phase involving only these species is

$$\mathrm{Ca} + 2\mathrm{H_2O} + \mathrm{CO} \longrightarrow \mathrm{CaCO_3(s)} + 2\mathrm{H_2}. \tag{3}$$

The free enthalpy change ΔG of this reaction is -500.6 kJ/mol, i.e. the reaction is thermodynamically favourable.

Clearly the reaction, as it is written down, is only a net reaction. The true microscopic reactions require a more complex sequence of surface reaction steps involving adsorption and desorption processes, ionization and recombination processes at the surface, and dissociation and association reactions at the surface in order to form the Ca^{2+} cation and the $(CO_3)^{2-}$ anion of the calcite lattice from the gas phase species. The details of the intermediate reaction steps are not known, but we assume that the required reactions are kinetically possible. Further we make the plausible assumption that the rate determining step is the addition of Ca to the lattice since Ca is about two orders of magnitude less abundant in the gas phase than H_2O and CO.

An alternative possibility would be to first form CaO via the reaction

$$\mathrm{Ca} + \mathrm{H_2O} \longrightarrow \mathrm{CaO(s)} + \mathrm{H_2}. \tag{4}$$

Since the activity of CaO exceeds unity at a much higher temperature than the activity of calcite (cf. Fig. 2), this reaction in principle would start first and calcite could subsequently be formed by the reaction

$$\mathrm{CaO(s)} + \mathrm{CO} + \mathrm{H_2O} \longrightarrow \mathrm{CaCO_3(s)} + \mathrm{H_2}. \tag{5}$$

The first reaction has a free enthalpy change of $\Delta G = -437.4$ kJ/mol and the second one a free enthalpy change of $\Delta G = -63.1$ kJ/mole. Both reactions are thermodynamically favourable and therefore this two-step process of calcite formation would also be possible.

Nevertheless we assume that calcite is formed by the reaction (3) since the conversion of CaO into $CaCO_3$ requires the diffusion of O atoms through the calcite layer formed on the lime core. Since formation of $CaCO_3$ is expected to start at temperatures below 800 K solid diffusion becomes a slow process compared to the rapid cooling in the outflow (cf. Gail & Sedlmayr 1999, Sect. 4.4, for a similar case). However, the formation of CaO particles at temperatures above the stability limit of calcite can supply the required seed nuclei for subsequent calcite growth.

CaO is a strongly ionic compound which crystallizes in the NaCl lattice. The bond energy of the basic building block in the solid, the monomer CaO, is 6.93 eV (calculated from thermochemical data taken from Barin 1992). For such a strongly bound ionic compound we can apply the type of estimates for the formation of CaO-clusters as was done in Gail & Sedlmayr (1998) for the case of TiO_2 nucleation, where for the bond energies of clusters scaled results from calculations of bond energies of NaCl-clusters (Martin 1983) and simple approximations

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[1] There is vast literature on carbonate formation from solutions, but seemingly not for precipitation from the gas phase. Some information on carbonate growth can be found in Parker et al. (1993).

Table 2. Data used in the condensation calculation of carbonates.

A	ρ	α
100.773	2.71	0.2

for the rotational and vibrational contributions to the partition functions are used to estimate the thermodynamic functions of ionic clusters. The results show that the onset of CaO nucleation can be expected at a total pressure of 10^{-10} bar at a temperature of about 1000 K. Hence, if calcite condensation becomes possible at a temperature of about 800 K at a total pressure of 10^{-10} bar, seed particles of CaO are available for calcite growth.

In the following we do not model the details of the nucleation process, but simply assume that suitable seed particles exist if calcite growth commences.

2.3. Equations for calcite growth

The basic model for dust formation which is used in this paper is that described in Gail & Sedlmayr (1999) and in the papers by Ferrarotti & Gail (2001, 2002, 2003). We do not repeat all details but describe only the specific equations used for calcite condensation as part of the multicomponent dust mixture considered in the model calculation.

We assume for simplicity that the dust grains are spherical particles. The equation for the growth of a grain with radius a is

$$\frac{\mathrm{d}a}{\mathrm{d}t} = V_0 \alpha \, v_{\mathrm{th}} \left(n - \frac{p_{\mathrm{eq}}}{kT} \right) \cdot \tag{6}$$

Here V_0 is the volume of one formula unit ($CaCO_3$ in our case) in the solid which is given by

$$V_0 = \frac{A_{\mathrm{cal}} \, m_{\mathrm{AMU}}}{\rho_{\mathrm{cal}}} \cdot \tag{7}$$

A_{cal} is the atomic weight of calcite and ρ_{cal} the mass-density of calcite. The data used in the calculation are given in Table 2. m_{AMU} is the atomic mass unit.

v_{th} is the thermal velocity of the species responsible for calcite formation

$$v_{\mathrm{th}} = \sqrt{\frac{kT}{2\pi m}} \cdot \tag{8}$$

Since we assume that the addition of Ca is the rate determining reaction step, m is the mass of the Ca atom.

α is the sticking coefficient. No experimentally determined data could be found for this quantity from the literature. For a strongly ionic compound like MgO a sticking coefficient of $\alpha \approx 0.2$ was determined by Hashimoto (1990). We assume that for calcite, which is also a strongly ionic compound (e.g. Parker et al. 1993), the sticking coefficient is similar. This is the value given in Table 2 and represents our best estimate for α. In our model calculations we also did calculations for α-values of $\alpha = 0.1$ and $\alpha = 1$.

p_{eq} is the equilibrium partial pressure of Ca atoms determined from the law of mass-action for the chemical equilibrium between the gas phase and calcite with respect to the reaction (3)

$$p_{\mathrm{H}_2}^2 = p_{\mathrm{Ca}} \, p_{\mathrm{H_2O}}^2 \, p_{\mathrm{CO}} \, \mathrm{e}^{-\Delta G/RT} \, . \tag{9}$$

ΔG is the free enthalpy change in the reaction (3). Thermodynamic data for calcite are give in Table 1, for the molecular species they are taken from Sharp & Huebner (1990).

For the partial pressures of H_2, H_2O, and CO we use the actual partial pressures from the gas phase, which consider the consumption of material from the gas phase due to the condensation process (also by other dust species). The equations for the abundances of the gas phase species are analogous to the equations given in Gail & Sedlmayr (1999). The pressure p_{Ca} calculated from Eq. (9) is used as the equilibrium pressure p_{eq} in the growth Eq. (6).

The actual particle density n of Ca atoms in the outflow in Eq. (6) is determined from the equation

$$n_{\mathrm{Ca}} = \left(\epsilon_{\mathrm{Ca}} - \frac{4\pi}{3} \frac{a^3 - a_0^3}{V_0} \epsilon_{\mathrm{cal}} \right) N_{\mathrm{H}} \, . \tag{10}$$

ϵ_{Ca} is the element abundance of Ca. a_0 is the radius of the seed particles on which the calcite grains grow and ϵ_{cal} is the abundance of seed particles per hydrogen nucleus. N_{H} is the fictitious particle density of free H nuclei, if these all were present as free atoms. This equation supposes that no Ca is bound in other dust species which is most likely not correct since part of the Ca is consumed by the formation of Ca-bearing solid solution components with pyroxene-type silicate dust. Thus, the usage of Eq. (10) somewhat over-estimates the growth rate of calcite dust. Experience with former model calculations of dust formation has shown that the degree of condensation of the dust forming elements in a stellar outflow is far from being complete. Hence, the fraction of Ca being consumed by pyroxene-type dust formation before the onset of calcite growth is unlikely to exceed 50% and the over-estimation of the rate of calcite growth is not severe.

Equation (6) for calcite growth is solved from that point on in the outflow, where n_{Ca} first exceeds p_{eq}/kT.

3. Results

We have calculated some simple models for the stellar wind of oxygen rich luminous giant stars, assuming a spherically symmetric and stationary outflow. The method for calculating the stellar wind and the dust formation of the more common dust species is described in Gail & Sedlmayr (1999) and Ferrarotti & Gail (2001, 2002, 2003). The model considers condensation of olivine-type and pyroxene-type silicate dust, solid iron dust, and magnesium-iron-oxide dust. Calcite is added to this dust mixture and its condensation is calculated as described in the preceding section.

Figure 3 shows the resulting fraction f of the Ca condensed into calcite. For comparison the degrees of condensation of the abundant silicates and of solid iron also are shown. In the left part of the figure the variation of f with distance r from the star and in the right part of the figure the variation of f

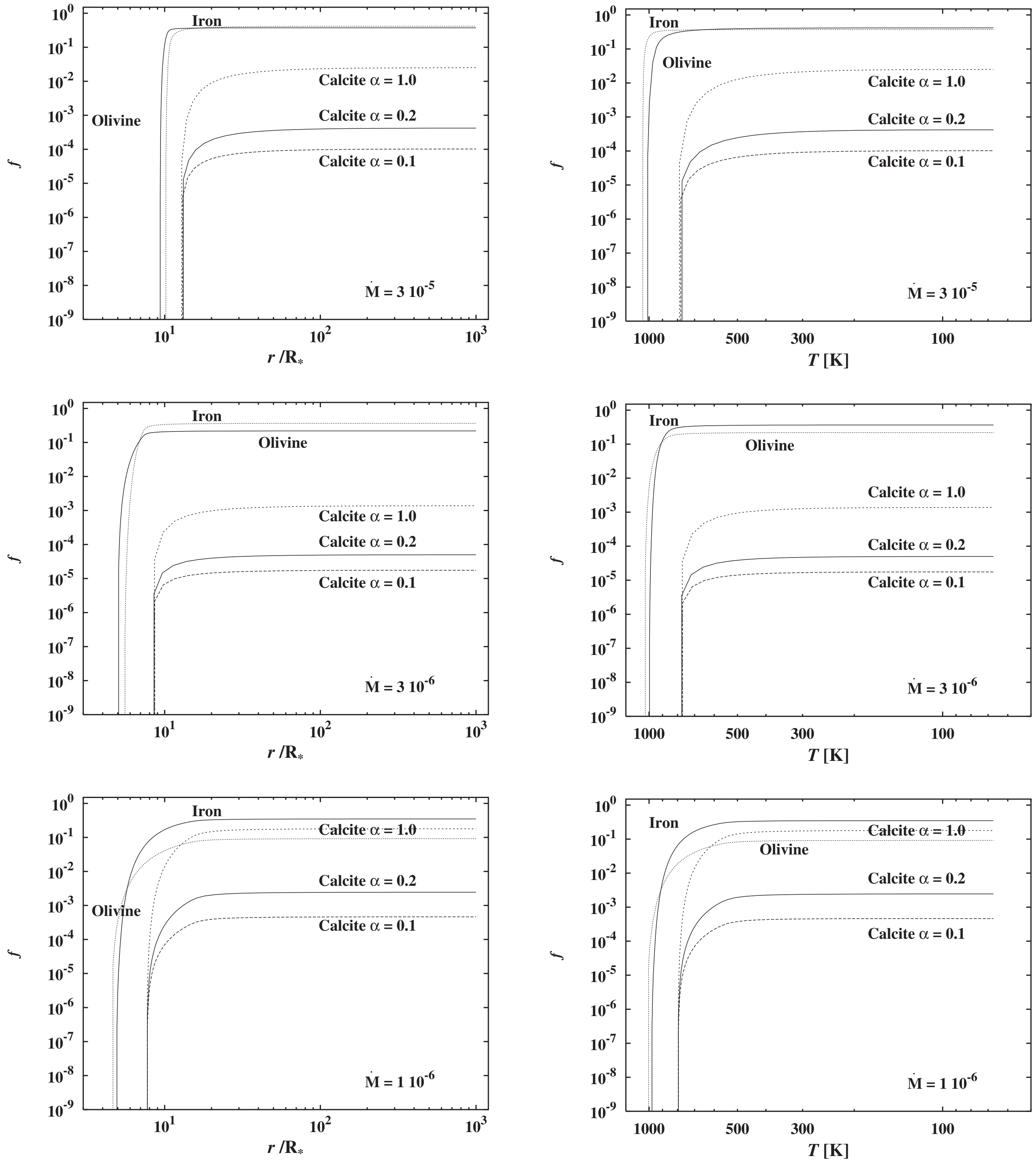

Fig. 3. Degree of condensation of carbonates and of the main dust components olivine and iron in a stellar outflow for three different mass-loss rates. *Left*: variation of the degree of condensation with radial distance from the star. *Right*: variation of the degree of condensation with the local temperature in the outflow.

with local temperature T is shown. The models are calculated for mass-loss rates of $\dot{M} = 1 \times 10^{-6}$, $\dot{M} = 3 \times 10^{-6}$, and $\dot{M} = 3 \times 10^{-5}\,M_\odot\,\mathrm{yr}^{-1}$, which correspond to a slow wind and a thin dust shell, a normal dusty object with a thick dust shell, and an object in the final super-wind phase of AGB stars with a very thick dust shell, respectively. The quite different radii for the inner boundary of the dust shell for different mass-loss rates result from the strongly different optical depths of the dust shells (note that radiative transfer is accounted for in the models, though in a simple analytical approximation). In fact, the onset of dust condensation occurs at nearly the same temperature in all cases, as can be seen from the right part of the figure.

The models are calculated for three different assumptions with respect to the growth coefficient α, since experimentally determined values for carbonates could not be found. A value of $\alpha = 0.2$ corresponds to our best estimate of α. The value $\alpha = 1$ corresponds to the highest possible value for α, which is only observed for metals, but not for other materials. The value $\alpha = 0.1$ for instance is the typical value for silicates (cf. Gail & Sedlmayr 1999; Ferrarotti & Gail 2001, 2002).

The figure shows that the fraction of carbonates formed is always very small, except for very small mass-loss rates. For mass-loss rates of $\dot{M} = 3 \times 10^{-6}$ and $\dot{M} = 3 \times 10^{-5}\,M_\odot\,\mathrm{yr}^{-1}$ and the unrealistically high growth coefficient $\alpha = 1$ the degree of condensation of Ca into carbonate is about a factor of 10^{-2} less than the degree of condensation of Si into silicate dust. In view of the fact that Ca is less abundant than Si by more than a factor of ten, the model calculation shows that carbonate forms, if ever, in completely negligible amounts. This holds the more for our best estimate $\alpha = 0.2$ and also for lower values of α. Our conclusion then is that carbonates cannot be formed in outflows from AGB stars with moderate to high mass-loss rates.

This results from the fact that the stability limit of $CaCO_3$ is more than 200 K below the stability limit of olivine. Once olivine starts to condense in the outflow the degree of condensation rapidly grows to such a value (typically $f = 0.1$) that radiation pressure on grains exceeds gravitational attraction by the star and rapid acceleration to highly supersonic outflow velocities begins. The outflowing gas is then rapidly diluted. If it enters the zone where carbonate formation becomes possible, the particle densities in this part are already so small that only insufficient numbers of collisions with Ca bearing particles occur during the further outflow. The early formation of olivine suppresses the formation of all significantly less stable dust species and in particular that of carbonates.

For very low mass-loss rates the timescale for olivine growth becomes rather long. Solid iron then may become a more abundant dust component because of the high condensation coefficient of metals ($\alpha \approx 0.9$ for iron) as compared to that of silicates ($\alpha \approx 0.1$). In this case the wind acceleration by radiation pressure on the abundant silicate and iron dust components is not sufficient to suppress the formation of less stable dust species. Our results in Ferrarotti & Gail (2003) have shown, for instance, that in this case compounds like magnesiowüstite may be formed, which cannot be formed in stellar winds with moderate to high mass-loss rates. In our present model calculation the degree of condensation f of Ca into carbonate is much higher than for the higher mass-loss rates, because it is not completely suppressed by an early acceleration of the wind. It is about 0.1 for the unrealistically high value of $\alpha = 1$, which would mean that some carbonate dust could be formed with at most 10% fractional abundance of the total dust. But for our best estimate $\alpha = 0.2$ it is lower by a factor of about 30, i.e. one expects that at most less than about 1% of the dust present could be carbonate dust. Such low amounts of dust in an optically thin dust shell are probably hardly detectable.

Our model calculation shows that carbonates in all likelihood are not formed in circumstellar dust shells, at least not in detectable amounts. With respect to the objects NGC 6302 and NGC 6537 for which an observed emission band at 92 μm has been proposed to be due to carbonates, this means that this identification is doubtful.

These two objects are planetary nebulae with fossil dust in their environment. The highly asymmetric nature of their circumstellar matter seems to result from their binarity and the existence of an accretion disk (Soker & Rappaport 2000), where much of the dust seems to reside (Kemper et al. 2002c). This dust is the remnant of the former superwind phase during the final stage of the AGB evolution of the stars. The carbonate dust cannot have been formed in the outflows from the AGB stars, as our calculations show. The claimed existence of carbonate dust in the cold dust component of NGC 6302 (Kemper et al. 2002c) however seems to require that the carbonate dust has formed in the superwind phase, which is impossible.

What then is the true nature of the 92 μm emission band? We presently cannot answer this question. One conspicuous feature of both objects by which they differ from other dusty objects is their unusual element mixture. The abundances determined from the planetary nebulae material clearly indicate that the progenitor stars were intermediate mass stars with initial masses $\gtrsim 4\,M_\odot$ and somewhat less than solar metallicity which experienced hot bottom burning (Marigo et al. 2003). The dredge-up of nuclear processed material may change not only the abundances of CNO elements but also may affect heavier abundant elements (e.g. Karakas & Lattanzio 2003). To find out the possible condensates in that element mixture would require a detailed study of the chemistry for the peculiar element mixture in both objects, which is out of the scope of the present paper.

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