FORMATION, GROWTH AND EVAPORATION OF HETEROGENEOUS DUST GRAINS IN OXYGEN-RICH ENVIRONMENTS UNDER OSCILLATING THERMODYNAMIC CONDITIONS

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I. INTRODUCTION

In order to understand the physical processes determining the dynamical structure and behaviour of circumstellar dust shells (CDS) around long-period variables (LPVs), it is inevitable to take consistently into account the complex interplay among dust formation, hydrodynamics, chemistry, and thermodynamics. Since the dust component, due to its huge absorption cross section with respect to the stellar radiation field, plays a decisive role for the structure and dynamics of the circumstellar shell, a proper description of formation and growth of the dust grains is a necessary prerequisite to model the CDS around LPVs.

In contrast to the carbon-rich situation, where mainly homogeneous amorphous carbon grains are formed (Gail & Sedlmayr 1988), in an oxygen-rich environment almost all carbon is locked up in the chemically inert CO molecule. Therefore, the grains only can be formed from molecules containing the remaining oxygen and the less abundant elements Mg, Si, S, Fe, Al. In this case a heterogeneous element composition of the emerging dust component has to be expected (Sedlmayr 1994, Dominik et al. 1993).

To focus the investigation on the heterogeneous condensation of these elements, in this poster we consider two gas elements which are subject to periodic variations of temperature and density in order to simulate the varying conditions encountered by gas elements moving through the circumstellar shell of an oxygenrich LPV.

II. MODELING METHOD

Assuming chemical equilibrium in the gas phase, we describe the nucleation process of the seed particles according to the equations given in Gail et al. (1984). The seed nuclei of these particles (homogeneous SiO and Fe clusters, Gail & Sedlmayr 1986) grow by addition of those molecular species which have a stable solid phase under the local thermodynamic conditions prevailing in the circumstellar environment. Heterogeneous growth of the particles is treated by means of a moment method (Dominik et al. 1993), while grain evaporation is described by the formalism developed in Gauger et al. (1990).

We consider an adiabatic gas element with a prescribed sinusoidal temporal variation of the temperature. Correspondingly, also the density varies sinusoidally in time. The numerical values of the parameters are: period P=300 days, mean temperature

 $\bar{T}=1100K$, temperature amplitude $\Delta T=700K$, mean density $\bar{\rho}=10^{-13}gcm^{-3}$ and adiabatic exponent $\gamma=5/3$. Two cases are calculated: case A with constant temperature amplitude and case B with damped temperature amplitude.

III. RESULTS

Case A: Nucleation of Fe starts around $T = 920 \,\mathrm{K}$, with a maximum nucleation rate around $T = 690 \,\mathrm{K}$; see Fig. 1. The different species successively contribute to grain growth, according to a stability hierarchy established by the thermodynamic conditions. The last element contributing to growth is sulphur. Growth of particles is up to an average size of $\langle r \rangle \approx 7 \, 10^{-3} \mu \text{m}$. All dust-forming elements, with the exception of oxygen, become completely depleted from the gas phase. Evaporation of S around $T = 680 \,\mathrm{K}$, of Fe around $T = 1200 \,\mathrm{K}$, and of Si around $T = 1360 \,\mathrm{K}$. Complete destruction of grains occurs at $T = 1600 \,\mathrm{K}$. After evaporation of Fe in the grain mantle at $T = 1200 \,\mathrm{K}$, the Fe core is still stable up to $T = 1600 \,\mathrm{K}$, since it is surrounded by the very stable aluminium bearing molecules. Finally, destruction of the cores occurs in a very narrow range of temperature.

Case B: Phase of nucleation and growth is similar to Case A (Fig. 3). Caused by the higher density, the mean particle radius becomes larger than in case A. Evaporation of S-bearing molecules, but no complete destruction of grains.

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Fig. 1.— Thermodynamic and dust quantities for Case A.

upper diagram: mass density ρ (blue line, l.h.s. ordinate) and Temperature T (red line, r.h.s. ordinate);

middle diagram: nucleation and evaporation rate J_* and $J_{\rm ev}$ ($J_{*,\rm Fe}$: black line, $J_{\rm ev}$ red line, l.h.s. ordinate) and number of dust particles per H-atom $n_{\rm D}/n_{<{\rm H}>}$ (blue line, r.h.s. ordinate); lower diagram: mean particle radius $\langle r \rangle$.

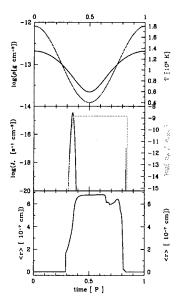
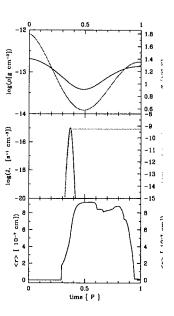


Fig. 3.— Thermodynamic and dust quantities for Case B.

upper diagram: mass density ρ (blue line, l.h.s. ordinate) and Temperature T (red line, r.h.s. ordinate);

middle diagram: nucleation and evaporation rate J_{\star} and $J_{\rm ev}$ ($J_{\star, \rm Fe}$: black line, $J_{\rm ev}$ red line, l.h.s. ordinate) and number of dust particles per H-atom $n_{\rm D}/n_{\rm < H>}$ (blue line, r.h.s. ordinate); lower diagram: mean particle radius $\langle r \rangle$.



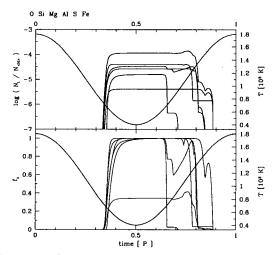


Fig. 2.— Chemical composition of the dust grains as a function of time for Case A. upper diagram: number of condensed atoms of element i per H-atom $n_i/n_{< H>}$, lower diagram: Degree of condensation f_c of the elements.

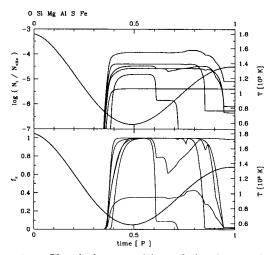


Fig. 4.— Chemical composition of the dust grains as a function of time for Case B. upper diagram: number of condensed atoms of element i per H-atom $n_i/n_{\text{CH}>}$, lower diagram: Degree of condensation f_c of the elements.