Photospheric Dust Grains Formation in Brown Dwarfs

F. Allard, D. R. Alexander
Dept. of Physics, Wichita State University, Wichita, KS 67260

A. Tamanai, and P. H. Hauschildt
Dept. of Physics and Astronomy, University of Georgia, Athens, GA 30602

Abstract. We have constructed a grid of brown dwarf model atmospheres with $T_{\text{eff}} \leq 3000$ K that includes (i) the formation of over 600 gas phase species, and 1000 liquids and crystals, and (ii) the opacities of corundum ($\text{Al}_2\text{O}_3$), iron, enstatite ($\text{MgSiO}_3$) and forsterite ($\text{Mg}_2\text{SiO}_4$), as well as amorphous carbon and SiC. We confirm earlier findings of Tsuji, Ohnaka & Aoki (1996) that grains are abundant in the outer photospheric layers of red and brown dwarfs with spectral type later than M8. We identify hot temperature condensates including perovskite ($\text{CaTiO}_3$) that depletes the photospheres of important absorbers including TiO, and we confirm the disappearance of TiO bands in the observed spectra of cool dwarfs.

1. Introduction

While it has been long suspected that grains could form in the cool atmospheres of late-type dwarfs (Sharp & Huebner 1990, Burrows et al. 1993), the intensivity of such computation prevented until recently their inclusions to already extensive model atmospheres calculations. Using the free Gibbs energies of formation from the work of Sharp & Huebner, and a simple sphere approximation for the mie opacity of the grains, Tsuji et al. (1996a) explored recently the formation of the three dust grain species $\text{Al}_2\text{O}_3$, Fe, and $\text{MgSiO}_3$ in model atmospheres of late-type dwarfs. They found the hot condensate $\text{Al}_2\text{O}_3$ to be a very abundant and a powerful continuous absorber in red dwarf stars with spectral type later than M8.

In this paper we present new model calculations which present significant improvements upon the work of Tsuji et al.: (1) hundreds of grain species are included to allow identify the hot condensates that are most abundant in the atmospheres of late-type M dwarfs and brown dwarfs; (2) a detailed treatment of the grain opacities is included based on the principle of continuous distributions of ellipsoidal shapes and sizes (Borhen 1983, see also Alexander & Ferguson 1994); and (3) these grain formation and opacities are incorporated to the best opacity sampling model atmospheres currently available (see Allard, this volume).
2. Dust clouds: formation

We have included the equation of state of the code Phoenix version 8, the complete series of over 1000 liquids and crystals from the work of Sharp & Huebner (1990). To do this, we used the free Gibbs energy of formation ($F_{gibbs}$) generously provided by Walter Huebner (private communication), and computed the fictitious pressures $P = NkT$ of each grain species by filling the condition that the grains be in equilibrium with the surrounding gas phase. For corundum:

$$P(Al_2O_3) = \frac{P(Al)^2P(O)^3}{F_{gibbs}} P(Al_2O_3)^{max}; \quad \text{for } F_{gibbs} \leq P(Al)^2P(O)^3$$

where the $max$ refers to the maximum concentration of grain cores (one core of corundum = one Al$_2$O$_3$) given the conservations of the cores of each element. As can be seen from left to right in Figure 1, the first dust grain species to form are ZrO$_2$ for $T < 2000K$ and corundum i.e. Al$_2$O$_3$ for $T < 1800K$. Other stable species to appear at $T < 1600K$ are Ca$_2$Al$_2$SiO$_7$, Ca$_2$MgSi$_2$O$_7$, and CaMgSi$_2$O$_6$, as well as Ti$_4$O$_7$ and Ti$_2$O$_3$. These grains all compete with the formation of the perovskite CaTiO$_3$ and corundum, and form an intricated layer of clouds in the outer photospheres of late type dwarfs. Note that, contrary to Tsuji et al’s findings, corundum is not the most abundant grain species and even disappears in central regions of the clouds. For cooler models, the situation complicates very rapidly with dozens of new grain species including iron, enstatite and forsterite begin to form and the clouds move further inside to higher optical depths of the atmosphere. This shows the importance of accounting for a complete composition of grain species in the equation of state.

The impact of condensation on the atmospheres and spectra of cool dwarf is therefore to gradually deplete them from their refractory elements, especially zirconium, titanium, silicium, calcium, magnesium, aluminium and iron. Ignoring for the moment the opacity of the grains, the result is a more transparent optical spectral distribution since the abundances of TiO, VO, FeH and metal-lines opacities decline with decreasing effective temperature of the star. This is reflected by a saturation of these features in the latest-type M dwarfs and brown dwarfs, a behavior which is presently observed in brown dwarf candidates as late as BRI0021 and GD165B.

3. Dust clouds: opacities

Early attempts to compute the opacity of grains were made by Cameron & Pine (1973) and Alexander (1975). More detailed calculations, including the effects of chemical equilibrium calculations and grain size distributions were reported by Alexander et al. (1983) and Pollack et al. (1985). Alexander et al. (1994) have described the computation of the opacity of grains with the inclusion of equilibrium condensation abundances, the effects of the distribution of grain sizes, and the effect of grain shape through the continuous distribution of ellipsoid model of Bohren & Huffman (1983). These calculations include the absorption and scattering due to magnesium silicates, iron, carbon, and silicon carbide grains for a wide range of chemical compositions down to temperatures of 700 K. We have
Figure 1. Run of the relative abundances of gas phase (full lines) and crystallized species across a $T_{\text{eff}} = 2600$ K NextGen-dusty model atmosphere. The condensation of perovskite (CaTiO$_3$, dashed line) is the principal cause of TiO depletion in the atmospheres of dwarfs later than about M6.

Figure 2. Opacity profiles of dust grains are compared to the total opacity (including atomic and molecular transitions) for the outermost layers ($T \approx 800$K) of a 2000K NG-dusty model atmospheres. Forsterite and enstatite dominate completely the total continuous opacity among the six species considered in the present calculations.
included these grain opacities, as well as those of corundum to the Phoenix opacity database. Using the number densities of grain cores provided by Phoenix's equation of state as described above, we compute the opacities of the six grain species Al2O3, MgSiO3, Mg2SiO4, Fe, SiC, an amorphous C in the model atmosphere calculations. The opacity profile of these grains are shown in Figure 2 for a typical outermost layer of a cool dwarf atmosphere. Magnesium silicates such as forsterite and enstatite dominate the opacity at these low temperatures. Figure 1 also suggests that calcium silicates dominate at the higher photospheric temperatures. In fact, the competition among calcium silicates causes an interruption of the opacity of corundum and an artificial drop in the total opacity in the layers where these grains dominate. This shows the importance of including opacities for all grain species, especially silicates, in the model atmosphere calculations. The inclusion of high temperature condensates such as ZrO2 and CaTiO3 may also have significant effects on the opacity in stellar atmospheres, even though their abundance is quite small, because of the high absorption and scattering efficiency of grains. For lower temperatures, the optical effects of species such as FeS, Fe3O4, and H2O need also to be included.

The extinction caused by grains in a stellar atmosphere may also depend critically on the rate of grain formation and the resulting size distribution. The effect of grain formation and of its opacity on the atmospheric structure of red and brown dwarf atmospheres will, therefore, not be fully understood until grain formation and time-dependent grain growth calculations incorporating the effects of sedimentation, diffusion, coagulation and coalescence are included.

Acknowledgments. This research is supported by a NASA LTSA NAG5-3435 and a NASA EPSCoR grant to Wichita State University. It was also supported in part by NASA ATP grant NAG 5-3018 and LTSA grant NAG 5-3619 to the University of Georgia. Some of the calculations presented in this paper were performed on the IBM SP2 of the UGA UCNS, at the San Diego Supercomputer Center (SDSC) and the Cornell Theory Center (CTC), with support from the National Science Foundation. We thank all these institutions for a generous allocation of computer time.

References