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Circumstellar Grain Formation

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1. Principal Classes of Grain-Forming Stars

It is now evident that grains are present in the outflows from many cool giant and supergiant stars. In addition to these cool evolved stars, nova explosions are also known to sometimes show evidence for dust condensation (Gehrz *et al.* 1984 and references therein). Less is known about dust formation in the neighborhood of protostars, but this may play a significant role in grain reprocessing (Burke and Silk 1976). The present paper will concentrate on dust formation around cool giants and supergiants.

Cool stellar atmospheres and envelopes are quite cleanly separated into two very different classes: those in which oxygen is more abundant than carbon ($C/O < 1$), and those in which carbon is more abundant than oxygen ($C/O > 1$). In both cases, the cool atmosphere forms CO to the point of almost fully locking whichever of the two elements is least abundant; the remaining atoms of the more abundant of C or O then dominates the chemistry of the cool atmosphere.

(a) Oxygen-Rich Outflows

The first abundant condensate expected in a cooling atmosphere with cosmic abundances ($C/O \approx 0.5$) and densities $n_H \approx 10^8 \mathrm{cm}^{-3}$ would be silicate minerals such as olivine $(Mg,Fe)_2SiO_4$ and enstatite $MgSiO_3$ (see the review article by Salpeter 1977). These silicates appear at $T \approx 1000$K. Dusty outflows from oxygen-rich stars commonly show the 10μm "silicate feature" -- due to the Si-O stretching mode -- in either emission or absorption, thus confirming the condensation of silicates in these outflows. Betelgeuse (α Ori) is an example of a red supergiant star with a silicate emission feature; OH 0739-14 is an example of an oxygen-rich outflow with

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so much dust that the silicate feature appears in absorption (Soifer *et al.* 1981).

(b) Carbon-Rich Outflows

In a carbon-rich atmosphere, some form of solid carbon will be the dominant condensate. Ideal monocrystalline graphite is the thermodynamically favored condensate, but kinetic factors will probably result in the formation of some polycrystalline carbon solid -- such as "turbostratic" graphite -- or "amorphous" or glassy carbon. Graphite and amorphous carbon have no strong infrared spectral features permitting unambigous identification, although crystalline graphite does have weak infrared resonances (Draine 1984). In addition to graphite, SiC (silicon carbide) can also condense (although somewhat later than graphite if in LTE). Silicon carbide has a spectral band in the 10.5$-$12μm region which was first identified in the spectrum of IRC+10216 (Treffers and Cohen 1974). IRC+10216 is perhaps the best example of a carbon-rich outflow, showing a nearly featureless infrared spectrum.

2. Grain Nucleation in Steady, Spherically-Symmetric Outflows

(a) Temperatures of Circumstellar Grains

The temperature of a circumstellar dust grain is essentially determined by a balance between the rate of absorption of radiation from the stellar surface and the rate of thermal infrared emission by the grain. The temperature therefore is quite strongly dependent upon the absorptive properties of the particle at the wavelengths where most of the stellar radiation is -- typically $\sim$1μm for the cool stars which concern us here. Clean terrestrial silicates have relatively small absorption coefficients in this wavelength region. For a star with a temperature T_*=3000K, a clean olivine grain at a radius $r \approx 1.6 R_*$ will be at the condensation temperature $T \approx$1000K. For a star emitting as a T=2500K blackbody, a clean olivine grain at $r = 1.3 R_*$ will have T=1000K. Thus clean olivine particles can exist relatively close to the surfaces of cool stars.

However, there is strong evidence that the silicate dust surrounding at least some stars must be much "dirtier" than the clean olivine discussed above. This is because the grains must be sufficiently absorptive to absorb enough of the stellar radiation to reprocess it into the observed infrared emission (Jones and Merrill 1976). For a star with T_*=3000K, these dirty silicate particles would have T=1000K at $r \approx 4.5 R_*$. Thus we see that the "condensation radius" depends quite sensitively on the assumed grain optical properties.

(b) Kinetic Considerations

Consider a spherically-symmetric steady outflow with mass loss rate $\dot{M}$. Suppose that a grain is injected into the outflow at radius r_1. If the sticking probability is s, and depletion of the vapor is neglected, the amount Δa by which the grain radius will increase is

$$\Delta a = 200\text{Å}\, f_{-4} s \left(\frac{R_*}{r_1}\right) \left(\frac{\dot{M}}{10^{-6} M_\odot\, \text{yr}^{-1}}\right) \left(\frac{L}{10^4 L_\odot}\right)^{-1} \left(\frac{T_{eff}}{2500\text{K}}\right)^{2} \left(\frac{v}{10 \text{km}\,\text{s}^{-1}}\right)^{-2} \qquad (1)$$

I have assumed a grain density $3\,\text{g}\,\text{cm}^{-3}$, an average atomic mass 25 amu, and a mean speed of $1 \text{km}\,\text{s}^{-1}$ for the condensible gas atoms. The condensible gas atoms are assumed to have a density $n = 10^{-4} f_{-4} n_{\text{H}}$ ($f_{-4} \approx 1$ being appropriate for condensation of silicate grains from gas of cosmic abundances: Si/H= 3.3×10^{-5} Mg/H = 2.6×10^{-5}, Fe/H =4.0×10^{-5}). It is clear that grain growth in such an outflow is severely limited by kinetic considerations, completely aside from the question of grain nucleation.

(c) Nucleation Theory and Its Limitations

As seen above, grain *growth* is subject to severe kinetic limitations. Perhaps an even more severe limitation is that posed by the need to nucleate solid particles out of the vapor. The problem here is that small particles or clusters are not as stable as bulk material, because surface free energy makes a substantial contribution to the overall free energy of the cluster. Thus, at a given degree of supersaturation, there is a minimum particle size (the "critical cluster size") below which clusters are more likely to evaporate than to grow. Statistical fluctuations are responsible for a finite rate of formation of clusters exceeding the critical cluster size; once having attained this size, the cluster becomes stable and will continue growing until the vapor ceases to be supersaturated.

The idealized problem of nucleation out of a *slowly* cooling vapor, always close to LTE, has been the subject of so-called "classical" nucleation theory (Draine and Salpeter 1977; Yamamoto and Hasegawa 1977). When account is taken of depletion of the vapor by cluster nucleation and growth, it turns out that specific predictions can be made of, for example, the supercooling which the vapor will undergo before the nucleation rate peaks, and the final sizes of the clusters which will form.

The theory makes a number of simplifying assumptions. One is that the "vibrational" temperature of the clusters and the kinetic temperature of the gas are the same. This condition is certainly *not* satisfied in a circumstellar flow. It is relatively easy, however, to make allowance for nonequality of the vibrational temperature and the gas kinetic temperature (Draine 1981). A second assumption is that grain growth consists of addition of monomers from the vapor, and that chemical distinctions among these monomers may be overlooked. This is certainly not correct in detail for growth of silicates, for example, as has been emphasized by Donn (1976). A third questionable assumption is that the "critical" cluster size is large enough that the free energies of these clusters may be sensibly estimated. This is a controversial issue; Draine (1979) has argued that existing information concerning the thermodynamics of small clusters suggests that their free energies *can* be meaningfully estimated, but others have disagreed (Donn and Nuth 1985). A fourth assumption is that the critical-sized clusters are large enough so that the internal degrees of freedom of the cluster are able to absorb the latent heat released when a new chemical bond is formed at the grain surface; this latent heat can in fact lead to very small effective "sticking" coefficients for growth of small clusters (Salpeter 1973).

The applicability of "classical" nucleation theory to the nucleation of refractory materials is not clear. Donn and Nuth (1985) have argued that existing experimental studies of the nucleation of refractory materials are inconsistent with the predictions of classical nucleation theory. My own view is that "classical" nucleation theory must of course be employed with extreme caution when the critical cluster size is small, but that the theory -- for all its limitations -- is better than nothing. Obviously it would be most desirable to have a full kinetic model with state-to-state transition rates, but this is far beyond our grasp at the present time. I am also not persuaded that the experimental data really rule out the applicability of "classical" nucleation theory to refractory systems -- the experiments are extremely difficult and demanding, and I hope that more work will be done in this area. In any case, as indicated below, the chemical physics of grain nucleation -- as incompletely understood as it is -- may perhaps not be the greatest source of uncertainty in our present understanding of circumstellar grain formation.

3. Real Circumstellar Mass Flows

(a) What drives mass loss?

We observe mass loss from many cool stars, but it must be said that the mass loss mechanism remains a mystery. In extremely cool stars, grain formation itself could in principle drive the mass loss: grains could nucleate within the stellar atmosphere, and radiation pressure acting on the grains could then "lift off" the upper layers of the atmosphere. The physics of this has been discussed by Salpeter (1974a,b). Model calculations of steady mass loss from very cool

(T_{eff} =2000K) stars have been done by Deguchi (1980); Woodrow and Auman (1982) have modelled the time-dependent mass loss from cool pulsating Mira variable stars.

Convection in the envelopes of giant stars is expected to lead to substantial variations in temperature over the stellar surface. As a result, Salpeter proposed that grain formation might take place within cool patches on the stellar surface. This idea continues to have appeal, particularly for understanding mass loss from the coolest stars. However, many mass-losing stars -- such as α Ori -- are now believed to have such high effective temperatures that it is hard to believe that there could be patches cool enough for grains to form right in the stellar atmosphere, or, indeed, that grains so formed could survive as they moved away from the local cool patch and were exposed to radiation from hotter regions of the stellar surface. Remember that silicate grains cannot survive heating to temperatures significantly in excess of 1000 K.

(b) Observational Evidence for Complex Gas Flows Around Mass-Losing Stars

Accumulating observational evidence is leading to a picture where the gas flows around mass-losing stars are extremely complex. In the case of α Ori, Boesgaard (1979) has observed FeII emission lines which she interprets as originating from material at $\sim 1.8 R_*$ *falling inward* onto the star. This is hardly comforting to proponents of steady, spherically-symmetric outflow models!

Red giants with SiO masers provide another independent piece of evidence for complex outflows. Attempts to model the observed SiO maser emission from VX Sag and R Cas lead to the conclusion that the maser emission originates in clumps of gas with densities a factor of $\sim 10^2$ times greater than the density which would be appropriate to a spherically-symmetric, steady outflow (Alcock and Ross 1985).

It is evident that we are a long way from understanding the nature of the near-star gas flows in these mass losing stars.

(c) Application to α Ori

Now let us consider α Ori as a particular, well-observed, example. For reasonable parameters ($\dot{M} \approx 2\times10^{-6} M_{\odot}$ yr^{-1}, $L \approx 2\times10^{5} L_{\odot}$, $T_{eff}=3600$K, $v=8$km s^{-1}) we find $\Delta a = 65$Å $f_{-4} s(R_{*}/r_1)$. It is clear that *if* grain formation does not take place until, say, $r_1 = 6.5R_{*}$ (the minimum distance at which *dirty* silicate grains can survive), then (from eq. (1)) the resulting grains must be *very* small: $a < 10$Å . In fact, infrared interferometric observations (McCarthy, Low, and Howell 1977; Sutton 1977; Howell, McCarthy, and Low 1981; Bloemhof, Townes, and Vanderwyck 1984) have been interpreted as showing that grain formation around α Ori does not occur within $\sim 10R_{*}$. The observations of Bloemhof *et al.* appear to indicate that the peak 10μm emission occurs approximately 0.9 arcsec from the star -- 40 stellar radii (for an assumed stellar angular diameter of 0.046 arcsec). On the other hand, scattering of starlight by circumstellar dust has been observed (McMillan and Tapia 1978), which requires the grains to be at least $\sim$100Å or so in size. Thus we conclude that one or more of the assumptions made above must not be correct. It appears most likely that the assumption of a spherically-symmetric, steady outflow is unrealistic, and that the actual gas flow in the grain-forming region is time-dependent and possibly not spherically-symmetric. This of course is a serious complication, and one which poses a serious obstacle to progress in understanding the grain formation in this outflow.

Even so, it is difficult to see how grain nucleation and growth can be deferred until the gas reaches such large distances from the star. One possibility, of course, is that the outflow is strongly time-dependent, with little grain formation at the present time. At a velocity of 8km s^{-1}, the time scale for flowing one stellar radius is ~3 year, so that this interpretation would suppose that the star last produced dust a few decades ago. In this connection, it may be noted that the dust emission around α Ori appears to be asymmetric: Bloemhof *et al.* report greater emission on the west side of the star. Furthermore, two distinct velocity components are observed in the outflow, with a $14 \mathrm{km s}^{-1}$ component present exterior to the $8 \mathrm{km s}^{-1}$ component (the 8 and $14 \mathrm{km s}^{-1}$ components have CO rotational temperatures of 200 and 70K, repectively; Bernat *et al.* 1979), suggesting that the outflow properties have changed within the past 1000 years (Ridgway 1981).

Another possibility for trying to understand the peaking of the $10 \mu m$ emission at such large distances from the star is the following idea: the grains may nucleate relatively close to the star, as "clean" silicate grains. After the nuclei are present, grain growth may proceed in a self-limiting fashion: when the growing grain incorporates an "impurity" from the gas which enhances the grain absorptivity in the $\sim 1 \mu m$ region, the grain may heat up and begin evaporating atoms from the surface until it succeeds in removing the "impurity". The grain can obviously tolerate greater degrees of absorptivity as it is carried farther and farther from the star, until at $\sim 10 R_*$ it can exist in the fully dirty form. By this means grain nucleation can be carried out relatively close to the star, but grain growth will not be complete -- and the grains will not have attained their maximum absorptivity -- until the material has reached about 10 stellar radii from the star. This effect evidently helps in reconciling our theoretical expectations with infrared observations, though it seems incapable of accounting for the peaking of infrared emission at $30 R_*$ as reported by Bloemhof *et al.*.

4. Summary

Based on the above, we see that our understanding of the grain formation phenomenon is extremely limited: the optical properties of small clusters are uncertain; the molecular physics of cluster nucleation and growth is poorly understood; and the properties of the gas flows within which the nucleation occurs remain mysterious. Much remains to be done on both the observational and theoretical fronts.

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