SiO COOLING INSTABILITY IN THE ENVELOPES OF COOL GIANT STARS

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ABSTRACT

In the outer atmospheres of oxygen-rich giant and supergiant stars, the formation of the silicon monoxide molecule not only represents a first step toward the production of dust but may also produce an efficient radiative cooling agent. Molecular cooling occurs as a thermal instability in many cases with an onset at 2000 to 3500 K, rapidly reducing the temperature by as much as 1000 K. This process may occur in the upper photosphere-lower chromosphere of such stars and can have profound dynamical consequences. The process occurs far from LTE, on a time scale controlled by the reaction rates for SiO formation. SiO masers may be indicative of this process. The molecule CS which may play a similar role in carbon stars and serve as the basis for carbonaceous dust production.

Subject headings: masers — molecular processes — radiation mechanisms — stars: circumstellar shells — stars: late-type — stars: supergiants

I. INTRODUCTION

Tsuji (1968) originally described a process by which radiation in infrared molecular bands can lead to strong surface cooling in stellar atmospheres. The extreme temperature sensitivity of molecular opacities can lead to thermal instabilities with large temperature excursions and resultant dynamic effects (Kneer 1983; Muchmore and Ulmschneider 1985). Within restricted ranges of effective temperature this can cause a bifurcation in the solutions for an atmosphere (Muchmore 1986), as has probably been observed in the Sun (Ayres and Testerman 1981; Deming et al. 1984; Ayres, Testerman, and Brault 1986) and in Arcturus (Heasley et al. 1978; Ayres 1986).

Dust in red giants can be expelled by radiation pressure (Jura 1984; Gail and Sedlmayr 1986). However, one classic problem has been how to form dust near a warm photosphere and chromosphere (cf. Stencel, Carpenter, and Hagen 1986). We describe here an autocatalytic molecule formation process in conjunction with molecular cooling of the gas as a significant step in reducing the temperature of the atmospheric material to the point at which molecules and dust can begin forming. We present estimates for the rates of the relevant gas and radiation processes.

In § II we discuss the SiO cooling and the associated thermal instability in LTE. Then in § III we discuss briefly the rates of chemical reactions and collisional excitations which guarantee that cooling rates at low densities will be slower than the LTE rates, and compare these with the dynamical time scale.

II. SiO RADIATIVE COOLING AND INSTABILITY IN LTE

The SiO molecule has a strong fundamental rotation-vibration band extending from 7.5 to about 10 μm. Here we discuss the radiative equilibrium of gas with SiO, analogous to the treatment of CO (Muchmore and Ulmschneider 1985). In general, strong sources of IR opacity are effective in removing energy from a warm plasma. We first derive an approximation for a radiative cooling function and then perform a stability analysis on it.

For the SiO opacity, we used the Einstein A-coefficient

$$A_{v_j, v_{j'}/j} = (5.25 - 0.15v) v (J + J' + 1)/(4J + 1),$$

for the transition from the state with quantum numbers $v, J$ to $v' = v - 1, J' = J ± 1$. The formula $(5.25 - 0.15v)v$ s$^{-1}$ provides an excellent fit to the values of Hedelund and Lambert (1972) for $v = 1$ to 5, lying between their two cases. We assume that it also yields a valid extrapolation for somewhat larger $v (= 10)$, although it is clearly not valid for still larger $v$ since it becomes negative for $v > 35$. Hönl-London factors for $^1Σ - ^1Σ$ bands are from Kovacs (1969) and Herzberg (1950, p. 126). A
Fig. 1.—Radiative cooling function with SiO at various densities for $T_{\text{eff}} = 3000$ K; each curve is labeled with the logarithm of the density

restricted Planck mean opacity over this band is defined by

$$\langle \kappa \rangle_p = \int_{\nu_1}^{\nu_2} \kappa_\nu B_\nu \, d\nu \left/ \int_{\nu_1}^{\nu_2} B_\nu \, d\nu \right.,$$

(2)

using the molecular constants of Huber and Herzberg (1979) and the SiO partition function of Rossi, Maciel, and Benevides-Soares (1985). We assume the gas has cosmic abundances in which half of the oxygen is already bound in CO.

Next we analyze the radiative energy balance. We assume the gas to be optically thin, in LTE, and that it is irradiated by a star with effective temperature $T_{\text{eff}}$, so that the mean intensity, $J_\nu$, is $\frac{1}{2} B_\nu (T_{\text{eff}})$. We split the radiation field into two frequency bands, one of which (IR) corresponds to the $\Delta \nu = 1$ band of SiO (7.5–10 μm) while the other (opt) represents all other frequencies, and define the cooling function $\phi = \langle \kappa \rangle_{\text{IR}} (S_{\text{IR}} - J_{\text{IR}}) + \kappa_{\text{opt}} (S_{\text{opt}} - J_{\text{opt}})$, where $S$ is the source function. The opacity in the optical band, $\kappa_{\text{opt}}$, is taken from the Rosseland mean opacity table of Kurucz (1979) and extrapolated where necessary to lower temperatures and densities. $\kappa_{\text{IR}}$ is the sum of this continuum opacity with the molecular opacity defined in equation (2). Because we are discussing an emission process in the IR, the Planck mean is the appropriate choice; the Rosseland mean is suitable to the extent that the optical continuum is gray.

Assuming $S_\nu = B_\nu$ and introducing the function $w(T)$ which is the fraction of the Planck function in the IR band, the cooling function becomes

$$\phi = \kappa_{\text{IR}} \left[ B(T) w(T) - \frac{1}{2} B(T_{\text{eff}}) w(T_{\text{eff}}) \right] + \kappa_{\text{opt}} \left[ B(T) \left( 1 - w(T) \right) \right] - \frac{1}{2} \left[ B(T_{\text{eff}})(1 - w(T_{\text{eff}})) \right],$$

(3)

which is illustrated in Figure 1 for various densities when $T_{\text{eff}} = 3000$ K.

When $\kappa_{\text{IR}}$ greatly exceeds $\kappa_{\text{opt}}$, substantial cooling will occur so long as $T_{\text{gas}}$ is above the radiative equilibrium value, $T_{\text{RE}}$, at which $\phi = 0$. At log $\rho = -10$ and $T = 2500$ K, for example, SiO produces a large peak of $5 \times 10^7$ ergs g$^{-1}$ s$^{-1}$ in the cooling function—emphasizing the efficacy of this process in cooling a stellar envelope. At yet lower densities (e.g., log $\rho = -20$) SiO forms in appreciable quantity in LTE only at very low $T$—below $T_{\text{RE}}$. When $T_{\text{eff}} = 3000$ K, $T_{\text{RE}}$ is 1890, 1850, 1850, and 2360 K, for log $\rho = -5$, -10, -15, and -20, respectively, illustrating the dichotomy in temperatures of the outer atmospheres of stars with and without molecular cooling.

When the slope of the cooling function, $d\phi/dT$, is negative, the gas is thermally unstable—cooling enhances molecule formation, which accelerates the cooling. While equilibrium might occur under such conditions, the gas would be unstable against temperature perturbations. In Figure 2 we show the domain of the instability in the $(T, \rho)$ plane along with models for the solar temperature minimum and for Betelgeuse. The semiempirical Betelgeuse model of Hartmann and Avrett (1984) has a temperature minimum region which is clearly subject to this instability. The result is analogous to the destabilizing role of CO in the solar atmosphere (Muchmore and Ulmschneider 1985).
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III. RADIATIVE AND CHEMICAL TIME SCALES

At some point in the outer atmosphere of red supergiant stars SiO forms, as evidenced by the presence of SiO masers within a few stellar radii of objects like VX Sgr (Chapman and Cohen 1986). If we imagine a steady, spherical outflow in LTE, the arguments of the last section suggest that SiO formation and its associated cooling would occur rapidly, yielding a steep radial gradient in the temperature—nearly a discontinuity on the scale of a circumstellar shell. But the assumption of LTE is not warranted for such low densities; the slow rate of the chemical reactions which form SiO will spread the temperature gradient significantly. This can be estimated by comparing time scales for chemical reactions, cooling, collisional excitation and outflow.

Clegg, van Ijzendoorn, and Allamandola (1983) discuss a network of chemical reactions relevant to the formation of SiO in circumstellar material. For the direct reaction Si + O → SiO, they give a rate constant of \( k_1 = 10^{-17} \text{ cm}^3 \text{ s}^{-1} \). We adopt this value, although such rate constants are uncertain by 1 to 2 orders of magnitude. Furthermore, this reaction is not necessarily the dominant producer of SiO. Among pure gas phase reactions, the pathway Si + H → SiH followed by SiH + O → SiO + H may produce SiO faster, depending on the relative reaction rates and the steady state abundance of SiH. However, since the reaction rates are so uncertain, we simply adopt the direct reaction for our discussion. In the presence of a UV radiation field, the photoinduced reactions which Clegg et al. discuss can accelerate molecule formation by several orders of magnitude. The actual rates of these reactions depend on the details of the stellar envelope model and upon moderately large networks of reactions and are thus beyond the scope of our discussion.

We define a time scale for the binding of one-half of the Si to SiO by

\[
\tau_{\text{chem}} \approx \ln 2/(k_1 n_0) = 4 \times 10^{-4} \rho^{-1} \text{ g cm}^{-3} \text{ s},
\]

where \( n_0 \) is the number density of oxygen atoms. We have again assumed cosmic abundances, with one-half of the oxygen bound in CO.

Next, we evaluated the radiative cooling time scale, \( \tau_{\text{cool}} = -\frac{1}{2} \int Nk/\phi(T, \rho) dT \), evaluated from a temperature just above the onset of molecular cooling (LTE) to the equilibrium temperature, using equation (3) and assuming \( T_{\text{eff}} = 3000 \text{ K} \). Table 1 presents SiO formation time scales, \( \tau_{\text{chem}} \), and SiO radiative cooling time scales. Only for the intermediate densities does rapid molecular cooling set in, so only in these cases is \( \tau_{\text{cool}} \) either well-defined or significant. These results show that the reaction rates for the formation of SiO are much slower than the LTE cooling; they will control the actual cooling rate in circumstellar shells. For a stellar envelope with the structure of the Hartmann and Avrett model illustrated in Figure 2, SiO would form in the temperature minimum region, then be destroyed in the chromosphere. When the temperature above the chromosphere in this model falls enough so that SiO would be stable, the density is so low that molecules could only form on time scales of millions of years—inconsistent with any reasonable wind flow. There may well be alternatives to the destruction of molecules in such a chromosphere. They may nucleate into grains rather than being destroyed. Or if the chromosphere begins at sufficiently low density, gas phase reactions may be frozen out by decreasing density and reduced dissociative reaction rates due to molecular
vibrational disequilibrium (Nuth, Wiant, and Allen 1985) before molecules can be destroyed. Molecules may survive in self-cooling, self-shielding clumps of material wherein chromospheric heating processes are thwarted, where polymerization of SiO can commence, and where radiation force can accelerate the SiO-rich protodust away from the star.

Table 1 also presents estimated time scales for the excitation of vibrational levels, \( t_{\text{exc}} \), and for the dynamics of the wind, \( t_{\text{dyn}} \). The actual molecular cooling rate is influenced at low densities by the rate of collisional excitation of the vibrational levels. These rates are poorly known, but for an order of magnitude estimate, we take the rate given by Nuth and Donn (1981). A minimum value for the collision coefficient is

\[
C_{1,0} = \frac{P}{\exp \left[ 1.16 \times 10^{-3} \mu^{1/2} \theta^{2/3} (T^{-1/3} - 0.015 \mu^{1/4}) - 18.42 \right] \left[ 1 - \exp \left( -\theta/T \right) \right]},
\]

with excitation energy \( \theta = 1782 \) K for excitation of the first vibrational level by collisions with H, where \( \mu \) is the reduced mass.

We note that the value of \( C_{1,0} \) could be as much as 1000 times higher due to interactions with molecular systems (von Rosenberg, Taylor, and Teare 1971; West, Weston, and Flynn 1977; MacDonald and Moore 1978). Thus the excitation time scale is

\[
t_{\text{exc}} = 1/C_{1,0} = 10^{-10} \rho^{-1} \text{ g cm}^{-3} \text{ s},
\]

for \( T = 2500 \) K. This excitation time is to be compared with the time scale for a radiative transition \( t_{\text{rad}} = 1/A \approx 0.2 \) s. Even after SiO forms, the cooling rate at densities lower than about \( 10^{-9} \) is reduced from the LTE cooling rate by the ratio \( t_{\text{rad}}/t_{\text{exc}} \).

We define the dynamical time scale, \( t_{\text{dyn}} \), for gas at any given density \( \rho \), as the time it spends moving from 10 \( \rho \) to \( \rho' \). These times, unlike the microphysical time scales, depend unavoidsly on the stellar model adopted. To indicate roughly the times involved, we assume \( M = 10^{-6} \) \( M_\odot \) yr \(^{-1} \) and \( v_p = 10 \) km s \(^{-1} \). These assumptions are enough to yield \( t_{\text{dyn}} \), wherever \( v = v_p \), such as at log \( \rho = -15 \) and -20. At higher densities, i.e., photospheric ones (where log \( \rho \geq -8 \)), \( t_{\text{dyn}} \) can be estimated since the density distribution is essentially hydrostatic and with a given \( \rho(r) \), the constancy of mass flux implies a mean outflow velocity. In this way we estimated \( t_{\text{dyn}} \) for log \( \rho = -5 \), assuming 1 \( M_\odot \) \( 100 \) \( R_\odot \) and \( T = 5000 \) K. Of course, in such a photosphere, convective velocities can be much faster than the 0.01 cm s \(^{-1} \) mean outflow speed. At any rate, the residence time at such densities is much longer than microphysical time scales. Between the photosphere and the outer envelope, we adopt an interpolating power law, \( \rho = \rho_0 (r/R_*)^{-\alpha} \), to fit between \( \rho_0 = 10^{-6} \) at \( R_\star \) and the density of the constant-velocity wind at some exterior point. This fitting point might plausibly lie between 2 and 100 \( R_\star \), so that the exponent \( \alpha \) might range from 20 to 4. By selecting an \( \alpha \) of 7, we obtain the \( t_{\text{dyn}} \) given in Table 1 for log \( \rho = -10 \) and also obtain values for log \( \rho = -5 \) and -15 corresponding fairly well with those derived above.

With our adopted parameters, \( t_{\text{dyn}} \) is longer than \( t_{\text{chem}} \), for densities greater than log \( \rho = -13 \). Beyond that point \( t_{\text{dyn}} \) becomes shorter so that the reaction Si + O is frozen out. Similarly, at very large distances from the star, when log \( \rho \) drops below -20, \( t_{\text{exc}} \) becomes longer than \( t_{\text{dyn}} \).

### IV. Conclusions and Discussion

In this Letter, we have demonstrated that when SiO molecules form in LTE they are very effective as radiative cooling agents, causing thermal instability. This phenomenon occurs at temperatures and densities similar to upper photospheric regions of red giant and supergiant atmospheres. We have estimated time scales for relevant chemical, collisional, and dynamical processes and find that the cooling is less than the LTE limit but that the chemistry can proceed faster than the outflow in the deeper parts of the circumstellar envelope. We suggest that this phenomenon may lead to important dynamical effects related to the origin of stellar winds driven by radiation pressure on newly formed protodust.

Radiation losses from the infrared fundamental vibration-rotation band of SiO molecules can strongly influence the thermal structure of the outer atmospheres of late-type stars. SiO formation in the temperature minimum region is attended by cooling of the gas. The existence of SiO masers and silicate dust in the envelopes of oxygen-rich red supergiants may be a natural consequence of this phenomenon (cf. Stencel 1986).

Circumstellar densities are low enough that the rate of SiO molecule formation will generally be too slow to keep pace with the temperature decrease produced by radiative cooling while molecules are forming. However, for sufficiently long outflow time
scales, the reactions could approach the equilibrium SiO abundance thermodynamically expected at the lowest $T$ achieved in the outflow. The time scales for molecule formation and for collisional excitation in the outer parts of supergiant envelopes become very long. There, processes which we have not discussed will play important roles, i.e., the depopulation of excited vibrational levels will decrease the rate of chemical reactions compared to LTE, possibly by very large factors (Nuth, Wiant, and Allen 1985). Non–LTE occupation of vibrational levels may make it hard for molecules to be destroyed at low density—so that molecules formed near the temperature minimum could conceivably be transported through a warm chromosphere. Photodissociation and photoinionization of molecules can also change the scenario (Scalo and Slavsky 1980; Clegg et al.).

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SiO is only one example of a molecule which is important for the thermal structure of an atmosphere. At higher temperature CO can form with comparable cooling effects (cf. Muchmore and Ulmschneider 1985). We have also evaluated a cooling function similar to equation (3) but including a third band for CO opacity. In the regime where SiO forms, each of the two molecular bands provides comparable cooling. The instability locus in phase space shifts to somewhat higher $T$ but still encompasses the entire $T_{\text{min}}$ region of the $\alpha$ Ori model atmosphere. We find a tandem process in which CO can form and cool the gas to the point at which SiO begins to form. Similarly, the formation of SiO and its attendant cooling may reduce the temperature sufficiently that other molecules, such as OH or $H_2O$, form. The dissociation energies of these molecules, known to be important in red supergiant envelopes, are shown in Table 2. Each of the diatomic molecules has a strong fundamental vibration-rotation band (for which the wavelengths are tabulated), all with comparable oscillator strengths (Kirby-Docken and Liu 1978; Hedelund and Lambert 1972; Roux, d'Incan, and Cerny 1973). Because OH is so similar to SiO and CO, it should behave similarly in cooling the gas. $H_2O$ is known to form in abundance and because it has substantial IR opacity itself, we conjecture that it may also be an important coolant (cf. Goldreich and Scoville 1976 for a discussion of $H_2$ cooling in circumstellar shells).

Radiation force acting on dust appears to be important in accelerating the winds of cool supergiants to their terminal velocities. The formation of dust itself is quite sensitive to the gas temperature and density in the stellar atmosphere (see, e.g., Gail and Sedlmayr 1986). We speculate that the chain of molecular cooling episodes sketched above may contribute to the dynamics of the wind by reducing $T$ below the dust formation temperature in regions where the density is high. This can alleviate the problem described by Jura (1984) that the gas of the atmosphere must somehow be levitated to low temperature regions at high altitudes (in gray atmospheres) where dust can form.

In the envelopes of carbon-rich stars, the chemistry is different; there, a similar role may be played by the molecule CS which, with a dissociation energy of 7.35 eV, is almost as tightly bound as SiO and is the second most stable molecular species in C-rich stars (Tsuji 1973). The formation of CS might trigger the same sort of instability as SiO does in O-rich stars. The polymerization of CS could initiate the nucleation process in C-rich stars, although a more thorough theoretical investigation of the chemical reaction network in such atmospheres is needed before any definitive conclusion can be drawn. Such studies are planned in the near future.

Molecular cooling occurs primarily in line cores. Thus in an extended circumstellar envelope, where large optical depths arise in these lines, the cooling process will be shifted outward toward lower densities where departures from LTE are larger. In a realistic analysis, optical depth effects in the molecular lines and spherical dilution of the radiation field would be significant—but then a local stability analysis would no longer be possible.

A complete understanding of the physics in circumstellar shells around red supergiant stars involves the interactions of a wide range of processes. An intricate coupling occurs between hydrodynamical, chemical, and radiative processes with varying time scales and rates. A tremendous amount of additional work—both theoretical and in the lab—needs to be done to actually measure and understand the relevant reaction and collision cross sections. With the present discussion, we do not come closer to solving the whole system, but we do emphasize one element which must be added to the set of contributing processes.

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