Dust Formation in the Inner Wind of the Oxygen-rich AGB Star IK Tau

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Abstract. The purpose of this study is to understand the processes underpinning the formation of dust in oxygen-rich AGB stars, reproduce molecular abundances in the dust-formation zone, and derive dust-to-gas mass ratios for specific condensates. We model the inner wind of the O-rich Mira IK Tau by considering layers of gas above the stellar photosphere that are periodically crossed by pulsation-induced shocks. The formation of molecules and dust clusters follows a chemical kinetic approach, which includes the formation pathways to small clusters of silicates, alumina, and metal oxides. In order to derive grain size distributions, the dust nucleation phase is coupled to the condensation phase, which is described by a Brownian formalism.

Our results on molecules agree well with the most recent observations and confirm the crucial role of shocks in the making of carbon-rich molecules, such as HCN, CO₂ and CS, in O-rich AGB inner winds. Alumina grains readily form in the shocked photosphere and the gas layers just above it. The nucleation of small silicate grains with forsterite stoichiometry proceeds through a new chemical route involving the dimerisation of HSiO. These clusters grow and condense around 4 R_{*} and keep growing over several pulsation periods. The dust-to-gas mass ratio for silicates is ~ 2 × 10⁻³, in good agreement with values characteristic of O-rich AGB stars.

1. Introduction

The circumstellar envelopes of AGB stars are sites of active dust formation, wind acceleration, and mass loss close to the star. These stars thus play a major role in galactic chemical evolution. We study the inner winds of oxygen-rich AGB stars (M type, C/O < 1), which are characterised by cool and dense gas layers where dust forms and the stellar wind is accelerated. Dust grains of forsterite (Mg₂SiO₄), enstatite (MgSiO₃), alumina (Al₂O₃) and spinel (Mg₂AlO₄) have been observed in O-rich Mira stars (Hackwell et al. 1970; Onaka et al. 1989; Posch et al. 1999), but the synthesis of such dust grains remains poorly understood. Furthermore, large abundances of carbon-bearing species such as HCN, CS, and CO₂, which cannot be explained by thermodynamic equilibrium (TE) conditions, are detected and relate to shock activity close to the photosphere (Duari et al. 1999; Cherchneff 2006). In this study, we build up a nonequilibrium physico-chemical model that also reproduces molecules in the gas-phase. In order to understand how dust grains form close to the star, we focus on the nearby galactic M-type star IK Tau, which is known for its chemical diversity.

2. Model

The wind of IK Tau is modelled between $1 R_*$ and $10 R_*$ with the parameters listed in Table 1. The inner gas layers experience the passage of periodic shocks with an initial

velocity of 32 kms⁻¹, where the post-shock gas is composed of a chemical cooling layer and an adiabatic excursion (Willacy & Cherchneff 1998; Duari et al. 1999; Cherchneff 2006; Cherchneff 2012). We use a chemical-kinetic approach to describe the formation of 105 molecules pertaining to O-rich environments and the synthesis of dust clusters of silicates (forsterite, enstatite), metal oxides (alumina, MgO, AlO, TiO, SiO) and pure metal clusters (Fe₂, Si₂, Al₂). We grow small silicate clusters according to Goumans & Bromley (2012) and implement a new silicate formation pathway, which proceeds via HSiO and its dimerisation to $H_2Si_2O_2$. Reactions involved in this new route were studied by Zachariah & Tsang (1995). Moreover, a condensation formalism is coupled to the gas phase in order to grow clusters to dust grains (Sarangi & Cherchneff 2015).

Table 1. Parameters used for modelling IK Tau.

T_*	2200 K	M_*	$1 \ \mathrm{M}_{\odot}$	α	0.6
R_*	2.5×10^{13} cm	v _s	20-32 km/s	v _{term}	18 km/s
Р	470 days	$n(r_{\rm s})$	$3.62 \times 10^{14} \text{ cm}^{-3}$	М	$1 \times 10^{-5} - 8 \times 10^{-6}$
r _s	1 R _*	C/O	0.75	$\Psi = m_{\rm dust}/m_{\rm gas}$	$4 \times 10^{-3} - 9 \times 10^{-2}$

3. Results

Our modelled abundances for the prevalent species such as CO, H₂O, SiO, HCN, CS, SiS, PN, and SO well agree with observations, as illustrated in Figure 1. On the other hand, our modelled abundances for SO₂ and PO are lower by a factor of ~ 100-1000. However, the observational abundance of SO₂ is derived for lines probing the $50 - 400 R_*$ wind region, which do not constrain the SO₂ abundance in the inner wind. Regarding PO, the chemistry of P-bearing species is very poorly characterised. Thus, our results indicate that the shocked, inner regions above the photosphere have non-equilibrium conditions that are conducive to molecular formation.

The condensation of dust clusters is described by a formalism that involves Brownian motion, attractive van-der-Waals forces, and spherical dust particles with the corresponding dust dimer stoichiometry (Sarangi & Cherchneff 2015). The number density of available dimers and the timescales are most crucial for cluster condensation and grain growth. Assuming radial drift velocities of 0.5 km s⁻¹ and 1.5 km s⁻¹ at 1 R_{*} and 4 R_{*}, respectively, the grains keep growing over 12 pulsations each 1 R_{*} close to the star, and over 4 pulsations each 1 R_{*} at radius > 4 R_{*}.

As seen from Figures 2 and 3, alumina grains readily start forming in the first excursion and at late pulsation phases in the post-shock gas and grow up to an average size of ~ 1000 Å, whereas forsterite grains form around 4 R_{*} with sizes of ~ 400 Å. In Table 2, we list the dust-to-gas mass ratio derived at various radii in the inner wind. Silicates form with larger dust masses than alumina. Our results for alumina and silicates are consistent with the most recent interferometric observations of oxygen-rich AGBs (Karovicova et al. 2013). These observations indicate the presence of the alumina dust shell around 2 R_{*}, and that of silicates around 4 R_{*}. Silicates form in an amount characteristic of O-rich AGB stars (~ 10⁻³). When a higher gas density is considered, larger grains and masses of silicate and alumina are formed (see Figure 3 and Table 2).

We conclude that the non-equilibrium chemistry induced by the passage of periodic shocks in the inner wind of IK Tau reproduces well the gas phase and provides clues to the formation of dust grains in oxygen-rich AGB stars.



Figure 1. Modelled abundances at $6R_*$ (with respect to H_2) compared with the most recent observational abundances. Vertical bars indicate a range of observational values.



Figure 2. Alumina dust grain size distribution between $1 R_*$ and $2 R_*$.



Figure 3. Forsterite dust grain size distribution for the photospheric density listed in Table 1 (*upper*) and for the case of $10 \times$ greater photospheric number density (*lower*).

$R(\mathbf{R}_*)$	Alumina		Silicate	
	Standard	High	Standard	High
1.0	2.1×10^{-5}	4.3×10^{-4}	_	_
1.5	2.7×10^{-5}	5.3×10^{-4}	_	_
2.0	3.3×10^{-5}	6.5×10^{-4}	_	_
3.5	_	_	1.3×10^{-4}	4.7×10^{-4}
4.0	_	_	4.6×10^{-4}	1.1×10^{-3}
5.0	_	_	7.3×10^{-4}	2.9×10^{-3}
6.0	_	_	1.0×10^{-3}	5.3×10^{-3}

Table 2. Derived dust-to-gas mass ratio for alumina and silicate dust grains as a function of radius for IK Tau and for a 10× greater photospheric gas number density.

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Discussion

Olofsson: What are the implications of your results for the possibility of having a dustdriven wind for IK Tau?

Gobrecht: That the dust forms within the inner wind with the help of stellar pulsations which are responsible for warm and dense gas layers.

Posch: Is it possible to constrain from your models whether Al_2O_3 grains will form in crystalline or in amorphous structure?

Gobrecht: From the clusters (dimers) it is possible, as they are crystalline. For the larger condensed grains I cannot constrain whether they are crystalline or not.

Uttenthaler: You mentioned that you *assumed* a C/O ratio of 0.75 for IK Tau. Has this been constrained by observations? Have you tried to vary it, and what was the result?

Gobrecht: The exact C/O ratio of IK Tau is unknown. However, we know that IK Tau is an oxygen-rich AGB star. A greater C/O ratio results in a higher CO abundance.

Höfner: How do you determine (or set) the temperature of the clusters and dust grains? This will have strong implications for the condensation distances.

Gobrecht: We assume that the grains and the clusters have the same temperature as the gas (for instance). This is a simplification and it is certainly possible that the gas and the dust decouple thermally.



David Gobrecht on the mic.