Nucleation studies under the conditions of carbon-rich AGB star envelopes: TiC

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Abstract. Many studies of especially dust nucleation in winds of carbon-rich AGB stars consider primarily carbon as dust forming material. But dust grains formed in such circumstellar envelopes are rather a mixture of several chemical elements such as titanium or silicon in addition to the main component carbon as verified by many investigations of pre-solar grains enclosed in meteorites, for example. In this contribution we focus on the study of the nucleation of titanium carbide particles from the gas phase. Therefore, the necessary properties of molecular titanium carbide clusters have been estimated within density functional approaches and first implications on the homogeneous nucleation of TiC are studied for conditions being representative for circumstellar dust shells around carbon-rich AGB stars.

1. Constrains from pre–solar TiC grain analysis

Analyses of meteorites revealed the existence of pre–solar TiC grains with characteristic isotopic signatures originating from AGB stars as dust sources (e.g. Bernatowicz et al. 2005, Croat et al. 2005). The detection of central inclusions of such TiC particles in carbon material implicate titanium carbide condensation before carbon dust formation, thus constraining the dust condensation sequence. Phase stability lines (S=1) of different carbon materials have been analysed by Bernatowicz et al. (2005) especially in view of this sequence. They conclude that TiC before C dust formation is in principle possible at high temperatures (ca. 1570 K – 1780 K) but low C/O ratios (C/O < 1.2) depending only weakly on the pressure. However, these considerations are not taking any details of the nucleation process of titanium carbide itself into account.

2. Molecular properties of small titanium carbide clusters and implications for nucleation studies under the conditions of carbon–rich AGB stars

The investigation of the properties of molecular clusters is essential for the understanding of dust nucleation in circumstellar environments of AGB stars. They can be obtained theoretically by electronic structure techniques to determine the required data of the microphysical processes involved, which are often not at hand (see also Patzer 2007). Here, we focus on the properties of small titanium carbide clusters of mainly stoichiometric composition, which were studied within the density functional approach (DFT) (cf. e.g. Paar & Yang 1989) at the bpl level of theory in conjunction with the standard medium sized all–electron split valence 6–31G(d) basis set (Frisch et al.
1984). This theoretical level of approximation is a reasonable compromise between computational effort and desired numerical accuracy (cf. Wendt 2008).

The small titanium carbide cluster systems investigated so far show structural motives of the bulk TiC lattice (fcc). The calculated positions of the main active IR modes around 15.7 µm and ~ 21 µm of these titanium carbide clusters, which are caused by vibrating carbon atoms in a titanium atom ‘grid’, are in very good agreement with the results of the TiC cluster measurements of von Helden et al. (2000). This does not necessarily imply, that the ‘21’ µm feature is caused by TiC dust particles. Strong objections are given by e.g. Henning & Mutschke 2001, Chigai et al. 2003, Li 2003.

The nucleation of titanium carbide in AGB winds has been previously investigated by e.g. Chigai et al. (1999) using a special key species concept. Studying first implications we apply here our findings to the most simple nucleation process, to determine an upper limit on the stationary homogeneous TiC nucleation rate (see e.g. Patzer 2004 for more details on nucleation theory). Therefore, only the addition of monomers is taken into account and depletion effects are not yet considered. It turns out, that effective TiC nucleation is possible at high temperatures (see above), but high supersaturation ratios are absolutely necessary!

3. Concluding remarks

Properties of small titanium carbide clusters have been determined from elaborate DFT studies. A simple application to the homogeneous process reveals, that in cool and expanding outflows of carbon–rich AGB stars effective TiC nucleation is in principle possible at high temperatures, but highly supersaturated conditions are required.

First implications according to the condensation sequence are therefore: Is TiC condensation before C dust formation really possible only at low C/O ratios, especially if high S values are necessary prerequisites? Can such highly supersaturated conditions only occur in inhomogeneous AGB winds? Are other different TiC nucleation mechanisms more important, that operate at (maybe) lower supersaturation? To address these questions TiC clusters in further, chemically more complex TiC nucleation studies have to be considered.

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