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Letter to the Editor

FeSi as a possible new circumstellar dust component

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Abstract. We performed chemical equilibrium calculations for a solid-gas mixture in order to determine the possible condensates for the peculiar element mixture of S-stars and Luminous Blue Variables (LBV's). Some compounds of abundant elements where included in the calculation which seem to have been not considered in previous condensation calculations. It turned out that solid FeSi is the first condensate of the abundant refractory elements in S-stars with abundance ratios of C/O≈ 1 and also for the element mixture in LBV winds when stellar layers having burnt H via the CNO-cycle are exposed after serious mass-loss. The unusual material FeSi has recently attracted much attention in solid state physics and its optical properties have been carefully determined in that context. For temperatures below approx. 300 K FeSi shows two strong and comparatively narrow absorption bands located at $\lambda\lambda = 32, 50\,\mu$m for the pure substance and several weak bands. We propose that a strong narrow and presently not identified emission band around $\lambda = 47.5\,\mu$m seen in AFGL 4106 (Molster et al. 1999) and possibly in some other highly evolved objects may be due to FeSi dust grains.

Key words: stars: circumstellar matter – stars: mass-loss – stars: AGB and post-AGB – stars: winds, outflows – ISM: dust, extinction

1. Introduction

Advanced stages of stellar evolution are generally accompanied by heavy mass-loss either by explosive events or during phases of a massive stellar wind. Tiny solid particles condense from the gas phase which are easely detected by their infrared emission. The chemical composition and the mineralogical properties of the condensed material are not easely determined since such dust cannot simply be analysed in the laboratory, except for the rare presolar grains detected in certain meteorites (see Zinner 1998 for a review). From the limited spectroscopic information it was, nontheless, possible to show that essentially two different compositions of solid material in circumstellar dust shells exist for stars loosing mass by a stellar wind: (i) stars with the standard cosmic element abundance form Mg-Fe-silicate dust and (ii) stars with a carbon rich element mixture form soot and SiC. In both cases the precise composition of the material remains an open question since the observable absorption or emission bands are rather unspecific. This situation changed since the ISO satellite came into operation, and now a lot of well resolved solid state bands are detected (e.g. Waters et al. 1996; Barlow 1998; Molster et al. 1999), especially in the formerly non-accessible IR region longwards of $23\,\mu$m.

Table 1. Abundances of some elements used in the condensation calculations for S-stars and stars with CNO-cycle equilibrium abundances exposed by mass-loss. Last column shows solar system abundances for comparison.

El.	$\epsilon_{\text{S-star}}$	$\epsilon_{\text{CNO-cycle}}$	ϵ_{solar}
He	1.04×10^{-1}	1.48×10^{-1}	9.75×10^{-2}
C	2.33×10^{-4}	1.54×10^{-5}	3.55×10^{-4}
N	2.52×10^{-4}	1.15×10^{-3}	9.33×10^{-5}
O	6.87×10^{-4}	2.55×10^{-5}	7.41×10^{-4}

Calculations of condensation sequences for the relevant element mixtures have been used from the beginning to constrain the possible materials which are formed in the outflow. Gilman (1969) showed that olivine and pyroxene in M–stars and carbon dust and SiC in C–stars are expected to be the main dust components. More recent calculations for the oxygen rich mixture of M–stars (e.g. Grossman 1972; Sharp & Huebner 1990) and the carbon rich mixture of C–stars (e.g. Lodders & Fegley 1993; Bernatowicz et al. 1996) predict several additional dust materials to condense from the gas phase, some of which have now been detected spectroscopically or as presolar grains in meteorites.

In an attempt to determine the possible condensates of (i) S-stars during the transition from M- to C-stars and (ii) of LBV outflows, we calculated the chemical equilibrium compositions of gas-solid mixtures for the element compositions of such stars. We used the set of solids listed in the JANAF tables (Chase et al. 1985) and added additional compounds with high melting or boiling points from Barin (1992), Kubaschewski and Alcock (1983), especially FeSi, $FeSi_2$, and Fe_3Si_7. We found that FeSi

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in chemical equilibrium is the first abundant condensate for the two peculiar element mixtures, which both are characterised by a lack of oxygen and of carbon available for mineral formation. FeSi, thus, is an unexpected new candidate for forming an abundant dust component in stars with the peculiar surface element compositions in highly evolved stars of medium and high mass stars.

2. Condensation calculations

2.1. Element abundances

Condensation calculations are done for two non-standard element mixtures: For S-stars and for stars where heavy mass-loss has exposed layers which formerly have burnt hydrogen by the CNO cycle. The element abundances used in our model calculations are shown in Table 1 for some important elements. For all elements not shown in this table the standard cosmic abundances of Anders & Grevesse (1989) and Grevesse & Noels (1993) are used.

For S-stars all photospheric element abundances up to the iron peak are not changed during stellar evolution up to the TP-AGB except for He, C, N, and O. For these we scaled the standard abundances according to the change in stellar surface abundances found in the evolutionary calculations of Schaller et al. (1992) for stars of small and intermediate masses. The result agrees with observationally determined mean abundances in AGB stars (Smith & Lambert 1990).

The second element mixture in Table 1 is relevant for very massive and luminous stars, like η Car, which loose considerable amounts of mass during their life time by a hot stellar wind and start to expose layers of CNO-cycle processed material after a few million years. The model calculations of Maeder & Meynet (1987, 1988) show that after several million years of stellar evolution the abundances of C and O start to drop considerably below their initial abundances while the abundance of N increases. If we take their final abundance ratios after the sudden C, O depletion and N enrichment of the surface and scale the standard abundances of C, N, and O, we obtain the abundances given in Table 1.

2.2. Condensation sequences

We have calculated chemical equilibrium compositions of a solid-gas mixture which considers the 25 most abundant elements, their first two ionisation stages, their approx. 100 most stable molecules, and approx. 90 solid compounds. Data for equilibrium constants are taken from Sharp & Huebner (1990), Chase et al. (1985), Binnewies (1996), and Tsuji (1973).

Fig. 1 shows the stability limits for the stable condensates of the abundant refractory elements C, Si, Fe, Mg, and Al for a fixed pressure $P = 10^{-4}\,\mathrm{dyn\,cm^{-2}}$ which is representative for the condensation zone in circumstellar dust shells. For M-stars ($\epsilon_{\rm C} < \epsilon_{\rm O}$) and C-stars ($\epsilon_{\rm C} > \epsilon_{\rm O}$) the results agree with the results of previous calculations (e.g. Grossman 1972; Sharp & Huebner 1990; Lodders & Fegley 1993). For S-stars ($\epsilon_{\rm C} \approx \epsilon_{\rm O}$) we find that FeSi is the most stable condensate formed from

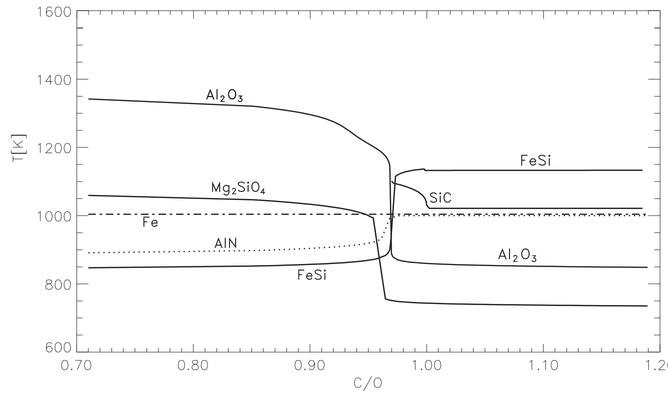

Fig. 1. Stability limits of condensates of some of the most abundant elements for varying C/O abundance ratio. The pressure is fixed at $P = 10^{-4}\,\mathrm{dyn\,cm^{-2}}$.

abundant elements (for C-stars carbon dust, not shown in Fig. 1, is the most stable condensate). The compounds FeSi, $FeSi_2$, and Fe_3Si_7, considered in our calculation, have not been included in earlier chemical equilibrium calculations.

Fig. 2 shows the stability limits of the stable condensates for the abundant refractory elements Si, Fe, Mg, and Al for the peculiar element mixture (cf. Table 1) when the elements C, N, and O have obtained their equilibrium abundances if a star burns H to He via the CNO-cycle. The abundance of O and C is reduced, then, below the abundances of the refractory elements Mg, Si, and Fe. In our chemical equilibrium calculations we again find FeSi to be the first condensate of the abundant refractory elements in this case. These results indicate that solid FeSi may be formed as an abundant dust component in the outflows of highly evolved stars.

3. Properties of FeSi

The crystalline structure of FeSi is of cubic symmetry but with a rather unusual arrangement of the atoms in the unit cell, providing an example of coordination number 7. Each iron (silicon) atom is surrounded by 7 silicon (iron) atoms at distances between 2.28 and 2.50 Å. This arrangement seems to result from a particular distribution of the valence electrons in the bonding between the atoms (Pauling & Soldate 1948). This binary compound is not a line compound, implying that its chemical composition allows for some spread in the occupation of the atomic sites.

FeSi is also known for its unusual electronic and magnetic properties. Although it has been studied in some detail some 30 years ago (Jaccarino et al. 1967), it has recently enjoyed a renewed interest in relation with the general and topical issues of correlation effects among itinerant electrons in metals. The more recent investigations involved measurements of thermal, transport and optical properties of single crystalline FeSi. The results indicate that FeSi is a semiconductor with rather unusual features in the structure of the electronic excitation spectrum (Paschen et al. 1997 and references therein). Below room temperature, the electronic conductivity decreases by more than

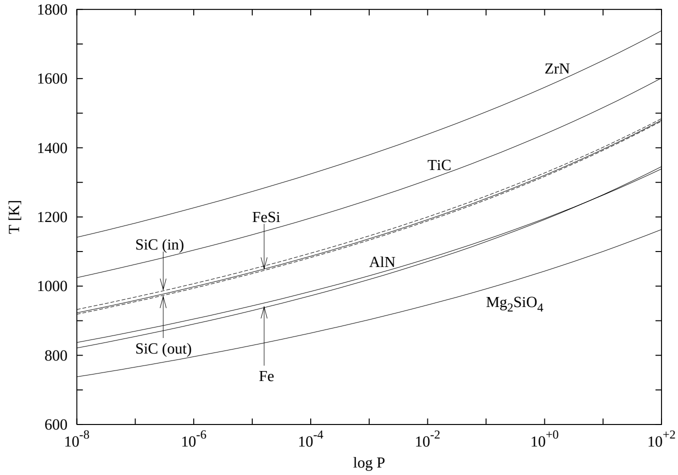

Fig. 2. Stability limits for condensates of the most abundant elements and for some less abundant refractory elements for the peculiar element mixture of CNO-cycle processes material. SiC(in) and SiC(out) denote the limits of appearance or disappearance of this material, respectively. ZrN and TiC may form the seed nuclei for the abundant dust components.

five orders of magnitude but a non zero conductivity persists at temperatures below 0.1 K. As may be seen in Fig. 3, the conductivity at 300 K is still high enough to effectively screen the lattice excitations in the far-IR region at approximately 30 and 50 μm, respectively. If the absorption at 47.5 μm shown in Fig. 4 is indeed due to solid FeSi, its observation implies that the temperature adopted by these dust particles must be below 200 K.

4. A possible detection of FeSi

4.1. Extinction properties of FeSi

Above $\approx$ 200 K the extinction by FeSi is rather smooth with wavelength (cf. Fig. 3) which makes it unlikely to detect FeSi in warm circumstellar dust shells, especially if at the same time there is emission from silicate dust from preceding mass-loss phases with normal element composition. For $T_{\rm dust} \lesssim 200$ K some sharp phonon modes become visible. Especially two modes at $\lambda \approx 50$ and 32μm become very strong. These two features may be identified in emission spectra if most of the dust is rather cold, i.e., for objects where most of the emission in the far IR comes from a detached shell.

In order to search for possible emission features from FeSi in IR spectra of evolved stars we have fitted the optical reflectivity data of FeSi measured at $T = 120$ K from Degiorgi et al. (1994) with a Drude-Lorentz model

$$\epsilon(\omega) = 1 - \frac{\omega_{pe}^2}{\omega^2 + i\gamma_e\omega} - \sum_j \frac{\omega_{pj}^2}{\omega^2 - \omega_j^2 + i\gamma_j\omega} \qquad (1)$$

(Bohren & Huffman 1983) and determined optical constants for FeSi in the far IR. From this we calculated the extinction efficiency Q_λ for 0.1 μm particles with $T = 120$ K in the small particle limit (see Fig. 4, bottom).

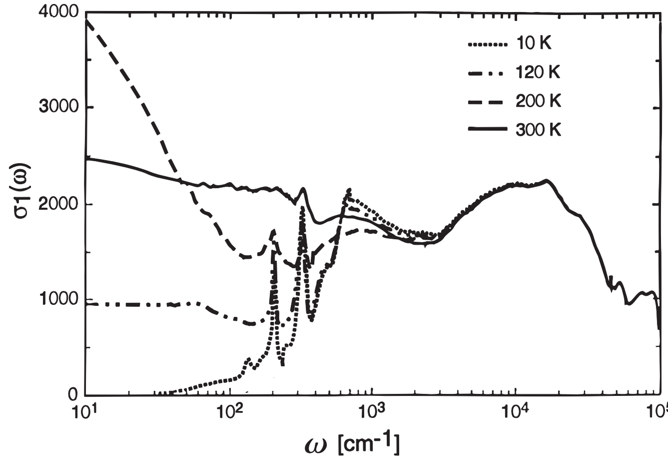

Fig. 3. Optical conductivity of FeSi at different temperatures (according to Degiorgi et al. 1994).

4.2. Comparison with AFGL 4106

The high abundances of Fe and Si suggests that FeSi, if it exists, should be identifiable by its two strong spectral features (see Fig. 3) at $\lambda\lambda = 32, 50\,\mu$m, which are accessible to the ISO satellite. The shorter wavelength band unfortunately is blended by a strong silicate feature, but the second one is located in a wavelength region free of strong silicate features and may be detectable.

We have searched for published ISO spectra of highly evolved objects since these seem to be the best candidates for looking for the spectral features of FeSi. In the far-IR spectrum of AFGL 4106 published by Molster et al. (1999) there is a strong band at $\approx 47.5\,\mu$m which is possibly also seen in some other highly evolved objects (Barlow 1998, Sylvester et al. 1999). This band is clearly seen in Fig. 4 which shows a sector from the spectrum of AFGL 4106 where the two strongest bands of FeSi should be visible. The band cannot be attributed to any other known dust species so far known to exist in circumstellar dust shells. A weak feature at $45\,\mu$m may also be due to FeSi.

AFGL 4106 is a double star with a late-A or early F-type member and an early M-type member. Both are massive stars $M \approx 15 \sin^{-3} i\, M_\odot$ (van Loon et al. 1999) and the earlier star is likely to be in the post red supergiant stage of evolution towards a WR star. The enhanced N abundance found in the spectrum (van Loon et al. 1999) indicates that CNO processed material is exposed by mass-loss. Temperatures of dust grains in the detached shell are estimated by Molster et al. (1999) from a radiative transfer model to be between 120 and 160 K, depending on the grain material. This makes AFGL 4106 a possible candidate (i) for the chemical peculiarity required for FeSi formation and (ii) for the low dust temperature required for visibility of the FeSi bands. We propose that the carrier of the 47.5 μm emission band in AFGL 4106 might be grains of FeSi.

The simultaneous presence of ice bands around 60 μm and of FeSi in AFGL 4106 shows that the detached shell also contains material from the preceding oxygen rich evolutionary phase.

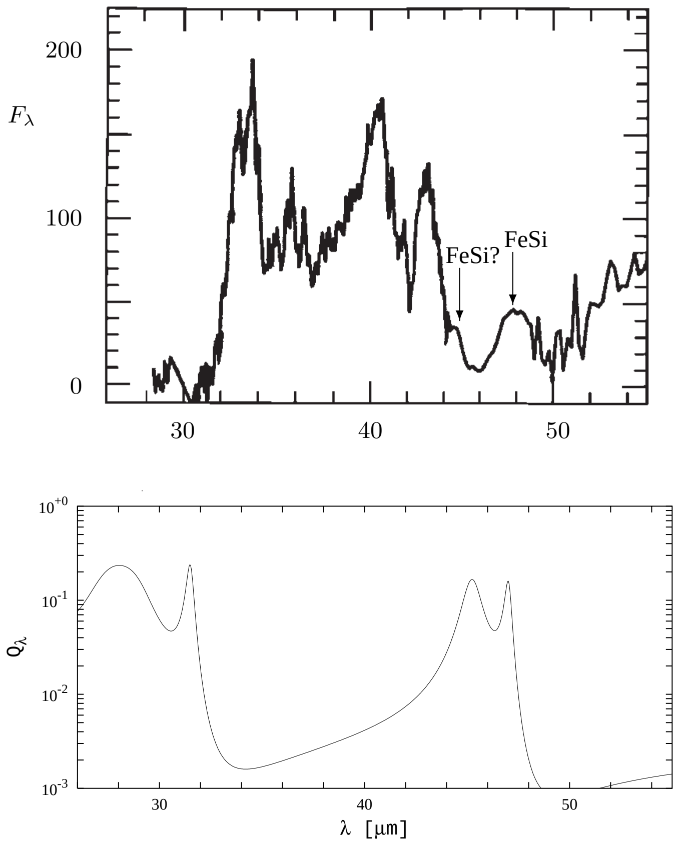

Fig. 4. *Upper Part:* Spectrum of AFGL 4106 (taken from Molster et al. 1999) in the far infrared wavelength region $28 \lesssim \lambda \lesssim 54\,\mu$m. The strong bands are due to forsterite and enstatite. *Lower part:* Absorption efficiency Q_λ of FeSi grains with 0.1μm radius at $T_{\rm dust} = 120\,$K. A broad distribution of grain radii would broaden the absorption bands.

This requires a change of the stellar surface abundances during shell ejection. Whether this is likely to happen depends on the details of the mass-loss process of red supergiants which are only badly known.

5. Concluding remarks

From thermodynamic equilibrium calculations of condensation sequences we have found that FeSi is the first condensate of the refractory abundant elements in element mixtures which can be characterised as being oxygen *and* carbon poor. Such environments occur during evolution of massive stars and at the transition to the PN-stage for medium-mass stars.

FeSi has two strong characteristic spectral features at ≈ 47 and 32μm which due to the temperature dependence of the optical conductivity of FeSi are visible only if the dust grains are cooler than $\approx 200\,$K. The 32μm feature is strongly blended by an enstatite feature and cannot be detected if silicate dust from earlier mass loss phases contributes significantly to the far IR emission. The $47.5\,\mu$m feature appears in a window free from strong features of other possible dust materials and should easely be detectable, if present. A resonance which occurs in small particles at $\epsilon_r(\omega) = -2$ at $\approx 45\,\mu$m falls on the shoulder of a strong enstatite band, but may also be detectable.

An inspection of a few recently published spectra of evolved stars taken with the LWS aboard the ISO satellite showed in one case (AFGL 4106) a rather strong feature at $47.5\,\mu$m and a second weaker feature at $45\,\mu$m on the shoulder of the strong $43\,\mu$m enstatite band. We propose that these two features in the spectrum of AFGL 4106 are due to FeSi grains. In some other cases there are also indications for the presence of the $47.5\,\mu$m feature of FeSi.

If this identification is true, it is for the first time that a material is found in a circumstellar dust shell with strongly temperature dependent spectral features, which can serve to some extent as thermometers for their environment.

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