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Some Remarks on Infrared Spectroscopy of Astronomically Interesting Silicates

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In this paper the influence of the embedding medium in KBr pellet technique on spectral appearance is investigated. Especially, the case of two amorphous silicates is discussed.

V této práci je studován vliv materiálu použitého při technice tablet lisovaných z KBr na vzhled spektra. Zvlášť je diskutován případ dvou amorfních silikátů.

В настоящей работе исследуется влияние материала примененного при технике прессования таблеток из KBr на вид спектра. В частности дискутируется случай двух аморфных силикатов.

1. Introduction

An important observational result of infrared astronomy was the detection of broad emission features at the wavelength of about 10 and 20 μm in the spectra of oxygen-rich giants and supergiants. Similar absorption features at these wavelength positions were found in the spectra of infrared objects in star-forming regions. There is now a general consensus that the two features are due to stretching and bending vibrations, respectively, of SiO_4 tetrahedra in the lattices of silicate grains.

Laboratory spectroscopy is an important tool for identifying the mineralogical and chemical structure of cosmic silicates. Recent work focused on both synthesis of astronomically interesting substances and spectroscopy of grains made from material of terrestrial, lunar, and meteoritic origin (see Gürtler et al., 1985 and Dorschner et al., 1985 for recent results). A common technique applied for infrared absorption spectroscopy of powders is the KBr pellet method. In this technique a small amount of silicate particles dispersed in KBr powder is pressed into a pellet, the transmission spectrum of which is easily recorded. Potassium bromide can be used because of its softness and its transparency between about 0.2 μm and 40 μm . For a comparison between the measured spectra with the observed ones it is necessary to estimate the influence of the embedding medium (KBr) on the appearance of the

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spectrum. First steps in this direction were done by Dorschner et al. (1978) and Schmidt (1981). The detailed paper by Schmidt (1981) does not take into account surface modes on small particles. Furthermore the optical constants of the astronomical silicates considered were not given. We wish to emphasize that reliable optical constants obtained from measurements on bulk samples must be available for an estimate of KBr effects. Additionally, in the equations derived in the paper by Schmidt (1981) we found several errors (e.g. in equations (3), (6), and (11)).

For these reasons we reinvestigate the influence of the embedding in KBr for two amorphous silicates – forsterite (Mg_2SiO_4) and enstatite (MgSiO_3), the optical constants of which are given by Day (1979).

It should be mentioned that another major problem in laboratory spectroscopy which is not usually dealt with, is the shape effect. Both nonsphericities of the individual particles and their almost unavoidable clustering in laboratory samples must be taken into account. These effects of nonsphericity are often more dominant than the KBr effects (Huffman, 1985).

2. Mie theory, surface modes and KBr effects

We will apply Mie's theory of the interaction of light with spherical particles to obtain quantitative results about the influence of KBr. Excellent presentations of this theory can be found in the books by van de Hulst (1957) and Bohren and Huffman (1983).

At infrared wavelengths extinction by submicron-sized particles is dominated by absorption. The absorption efficiency $Q_{\text{abs}}(a, \lambda)$ depends on the two dimensionless parameters

$$(1) \quad x = 2\pi a/\lambda \quad \text{and} \quad y = mx,$$

where a is the particle radius, λ the wavelength and m the complex refractive index of the material.

$$(2) \quad m = n + ik.$$

The relation between m and the complex dielectric function ε is given by

$$(3) \quad \varepsilon = \varepsilon' + i\varepsilon'' = m^2.$$

Mie's formulae can be generalized for the case of particles embedded in a medium. The complex index of refraction and the wavelength must be simply divided by the real index of (non-absorbing) KBr:

$$(4) \quad m_{\text{rel}} = n/n_{\text{KBr}} + ik/n_{\text{KBr}}, \quad \lambda_{\text{rel}} = \lambda/n_{\text{KBr}}.$$

The strength of the KBr effect depends on the strength of the infrared absorption band in the solid. Very strong bands result in strong surface modes in small particles, and there are considerable shifts of the peak wavelength and changes in maximum absorption. The reason for surface modes in small particles can be seen in the equation

of the absorption efficiency for a small sphere ($x \ll 1$; $|m| x \ll 1$):

$$(5) \quad Q_{\text{abs}} = 4x \operatorname{Im} \left\{ \frac{\varepsilon - \varepsilon_m}{\varepsilon + 2\varepsilon_m} \right\};$$

ε_m denotes the dielectric function of the embedding medium. The resonance condition for the surface modes (denominator approaches zero) is given by

$$(6) \quad \varepsilon' = -2\varepsilon_m; \quad \varepsilon'' = 0.$$

From these equations it can be seen that surface modes occur if ε' becomes strongly negative. This is the case for SiC and MgO which Bohren and Huffman (1983) discussed as examples. They showed that the absorption maxima for these particles in KBr are higher and shifted toward shorter wavelengths. The absorption bands due to surface modes are rather narrow. Therefore the surface modes may be overlooked in Mie calculations.

Henning et al. (1983) gave strong arguments in favour of the interstellar/circumstellar grains being amorphous. Experimental investigations of synthetic Mg and Fe silicates matching the composition of pyroxene and olivine (Day 1979, Day 1981, Nuth and Donn 1982) as well as of melted or irradiated pyroxene and olivine (Rose 1979, Krätschmer and Huffman 1979, Dorschner et al. 1986) confirm these conclusions. Additional support comes from stability calculations of amorphous circumstellar silicate grains (Henning and Svatoš 1986). Absorption bands in disordered silicates are sufficiently weak compared with those in SiC so that shape effects and KBr effects should be not very important. For weak bands in which ε' never goes close to zero, the KBr matrix effects are smaller. Experimental support for this view is given by Day (1976). He showed that the spectra of amorphous silicates looked similar whether the particles were encased in KBr or in air on top of a substrate.

In the next section we describe the results of our Mie calculations for amorphous silicates.

3. Results of Mie calculations for amorphous silicates

For estimating the KBr effects in the case of amorphous silicates we will use the optical constants for amorphous MgSiO_3 and Mg_2SiO_4 given by Day (1979). At first we proved that the ε' of these silicates never becomes negative. Thus, we do not expect strong surface modes.

The index of refraction of KBr is taken as 1.5264. We assumed $\delta = 3.3 \text{ g cm}^{-3}$ for the internal density of the material, the particles are made of. The mass absorption coefficient is given by

$$(7) \quad \kappa_{m,a}(\lambda_c) = 3Q_{\text{abs}}(a, \lambda_c)/4a\delta.$$

Here λ_c denotes the wavelength of the band's centres. Following Schmidt (1981) we describe the influence of the KBr on the band with the help of three parameters:

1. The wavelength shift of the band's centre $D = \lambda_c(\text{vac.}) - \lambda_c(\text{KBr})$;
2. the ratio of the mass absorption coefficients at the corresponding band's centre $h = \kappa_{m,a}(\lambda_c(\text{vac.}))/\kappa_{m,a}(\lambda_c(\text{KBr}))$;
3. the difference of the band's width $g = \text{FWHM}(\text{vac.}) - \text{FWHM}(\text{KBr})$.

To derive these parameters we represented analytically the absorption coefficient by two dispersion profiles. The results of Mie calculations for the two bands are given in Table 1.

Table 1. Influence of KBr on the spectral appearance

| band | material | a [μm] | $Q_{\text{abs}}(\lambda_c(\text{vac.}))$ | $\kappa_{m,a}(\lambda_c(\text{vac.}))$ [cm^2/g] | D [μm] | h | g [μm] |
|-------------------|----------------------------------|-----------------------|--|--|-----------------------|------|-----------------------|
| 10- μm | MgSiO ₃ | 0.1 | 0.1316 | 2991 | -0.21 | 0.68 | -0.07 |
| | Mg ₂ SiO ₄ | 0.1 | 0.1014 | 2305 | -0.16 | 0.71 | -0.04 |
| | Mg ₂ SiO ₄ | 1.0 | 1.1050 | 2511 | -0.22 | 1.01 | -0.14 |
| 20- μm | MgSiO ₃ | 0.1 | 0.0373 | 848 | -0.63 | 0.61 | -0.20 |
| | Mg ₂ SiO ₄ | 0.1 | 0.0351 | 798 | -0.90 | 0.60 | -0.82 |
| | Mg ₂ SiO ₄ | 1.0 | 0.3788 | 861 | -1.09 | 0.64 | -1.13 |

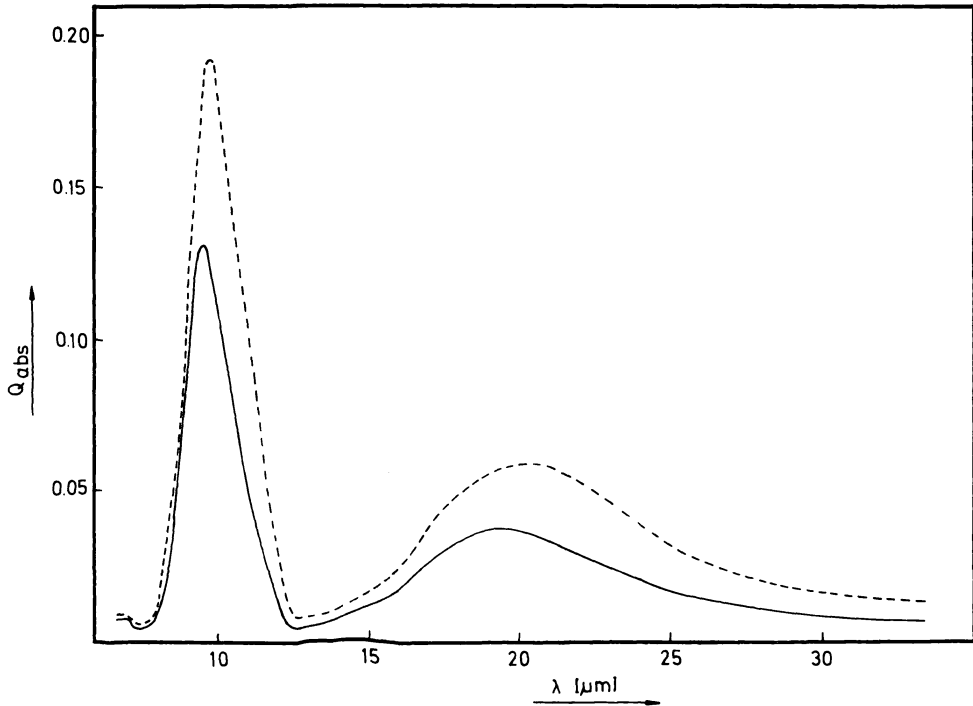


Fig. 1. Absorption efficiency $Q_{\text{abs}}(0.1 \mu\text{m}, \lambda)$ for MgSiO₃ (solid line: in vacuum; dashed line: in KBr).

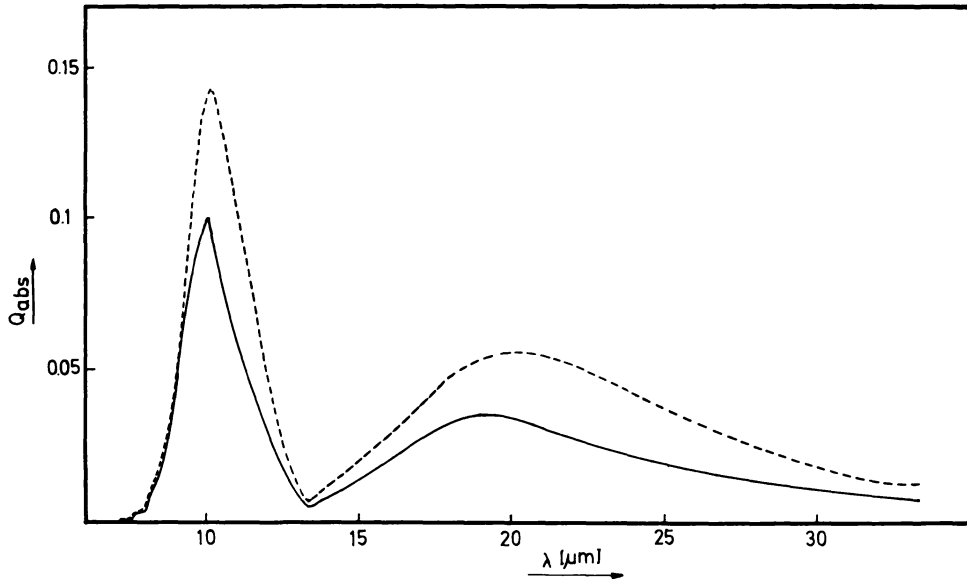


Fig. 2. Absorption efficiency $Q_{abs}(0.1 \mu\text{m}, \lambda)$ for Mg_2SiO_4 (solid line: in vacuum; dashed line: in KBr).

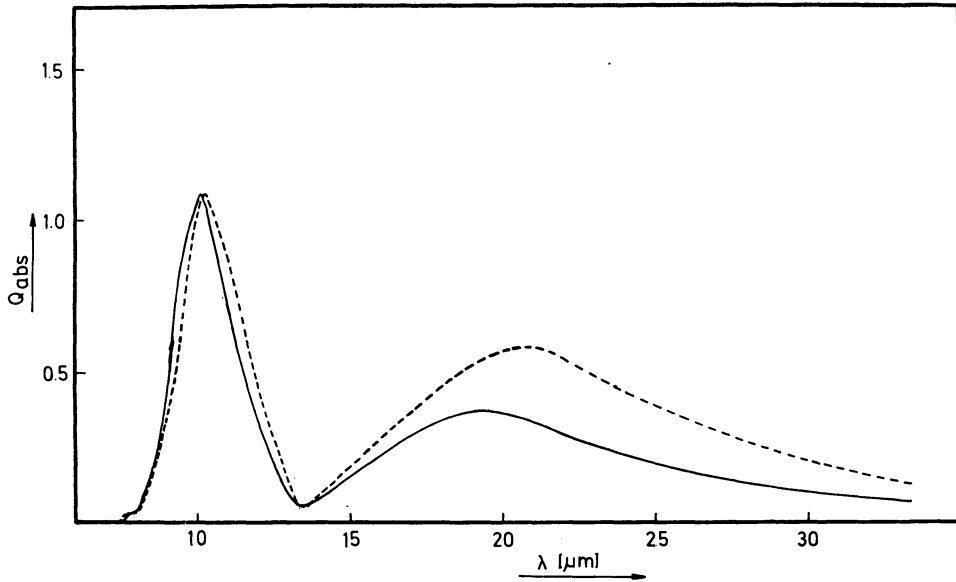


Fig. 3. Absorption efficiency $Q_{abs}(1 \mu\text{m}, \lambda)$ for Mg_2SiO_4 (solid line: in vacuum; dashed line: in KBr).

It can be seen that the 10- μm maximum absorption of the silicate particles with a radius of $a = 0.1 \mu\text{m}$ in vacuum is 70% of the value for grains in KBr. In the case of the 20- μm band we found a value of about 60%. The wavelength centre of the 10- μm band is shifted in KBr to longer wavelengths by about 0.2 μm . A remarkable change of the FWHM could not be observed. In general it can be seen that in the 20- μm band the KBr effects are more pronounced. For comparison we should mention that the peak extinction for SiC ($a = 0.1 \mu\text{m}$) in KBr is three times higher as in air (Bohren and Huffman 1983). The results for MgSiO_3 and Mg_2SiO_4 are displayed in Fig. 1, Fig. 2, and Fig. 3.

4. Conclusions

The paper showed that KBr effects must be taken into account if laboratory spectra of astronomically interesting amorphous silicates with weak absorption bands are considered. This is true especially for the peak absorption. Thus the influence of KBr must be accounted for if the ratio of maximum absorption in the 10- μm and 20- μm band is used as a criterion for the selection of a silicate that matches the observations most favorably.

Before estimating KBr effects in infrared spectroscopy it is necessary to check the appearance of surface modes. For quantitative calculations the optical constants of the bulk matter must be available.

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