

Investigation of the Crystallinity of the Modifications of Silica by their IR-Reflectance Spectra

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Infrared reflectance spectroscopy has been used for the identification of the different modifications of silica and for the determination of their crystallinity.

Infrared reflectance spectroscopy is not as widely used as infrared transmission spectroscopy (KBr-Pellet-Method). The main advantage of the former method lies in the fact that it is non-destructive and does not require any special sample preparation. The only requirement is that the sample has a flat and polished surface. The IR-reflectance spectrum of a sample is homologous to its absorption spectrum, with the exception that certain peaks are shifted minutely to longer or shorter wavenumbers.

The IR-reflectance spectrum of a single crystal is dependent on its structural orientation. Therefore several spectra have to be measured for the different orientations of the single crystal. According to [1], amorphous materials and glasses, and also fine grained polycrystalline materials if their grain size is small relative to the area being measured, do of course not show these differences.

The present paper demonstrates the application of IR-reflectance spectroscopy for the identification of the different types of microcrystalline and amorphous modifications of silica. Moreover, it is observed that there is a correlation between the crystallinity and the shape and intensity of certain particular bands in the IR-spectra of the samples.

The spectra were measured using an FTIR-Spectralphotometer (Perkin-Elmer, Model 1760), equipped with an accessory for the measurement of reflectance. The sample area used was 3 mm in diameter. All samples were ground and highly polished before measurement.

The IR-reflectance spectrum of chalcedony, which is a cryptocrystalline modification of silica, is very similar to that of quartz. Both of them show five peaks at or near 1176, 1108, 800, 780 and 690 cm^{-1} with the difference that the peaks at 780 and 800 cm^{-1} for chalcedony are not as sharp as in the case of quartz. In addition to that, an additional peak near 537 cm^{-1} is found to occur in case of chalcedony. Similar differences were also found between the spectra of chalcedony and jasper, a microcrystalline modification of silica. Jasper can be distinguished from chalcedony with the help of a broad peak occurring between 497 and 452 cm^{-1} .

The IR-reflectance spectra of opals vary considerably from those of quartz, chalcedony and jasper. According to [2] the structure of opals varies from almost perfect crystalline opal-CT, to nearly amorphous opal-A. Accordingly, opal-CT can be distinguished from opal-A with the help of their characteristic spectra. The two main peaks for opal-CT are at or near 1107 and 480 cm^{-1} , while those for opal-A are shifted to 1116 and 470 cm^{-1} , according to the degree of crystallinity. Furthermore, the two peaks at 780 and 800 cm^{-1} , which are typical of quartz, chalcedony and jasper merge to a single broad peak in the case of opals.

IR-reflectance spectroscopy is also very suitable for the investigation of silica glasses. According to [3], glasses show infrared spectra whose pattern changes with composition and progressive ordering. The two prominent peaks of quartz occurring at or near 1176 and 1109 cm^{-1} merge to a single peak at about 1088 cm^{-1} in the case of silica glasses and obsidians. Simultaneously, the peak between 800 and 780 cm^{-1} becomes even broader than it is in the case of opals.

As far as the structural similarity is concerned, the different modifications of silica consist of SiO_4 -tetrahedra which are linked together at their corners. According to [4], the peaks between 800 cm^{-1} and 780 cm^{-1} represent the ordered or disordered arrangement of the SiO_4 -tetrahedra in the different modifications of silica. As it has been shown in [5], the crystallinity and also the ordered arrangement of the SiO_4 -tetrahedra decreases from quartz to obsidian (glass) as follows:

quartz → chalcedony → opal-CT → opal-A
→ obsidian (glass).

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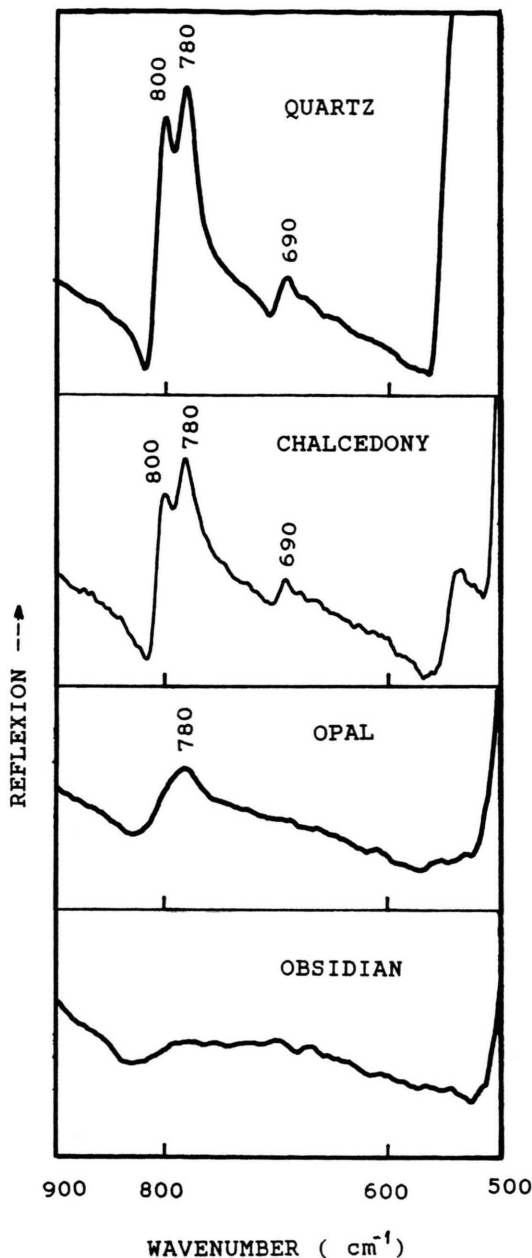


Fig. 1. Gradual changes of the shape and intensity of the peaks between 500 and 800 cm^{-1} in the sequence quartz–chalcedony–opal–obsidian (a natural glass). Note also that the peak at 690 cm^{-1} , which is quite prominent in the case of quartz, becomes gradually broader from opal to obsidian.

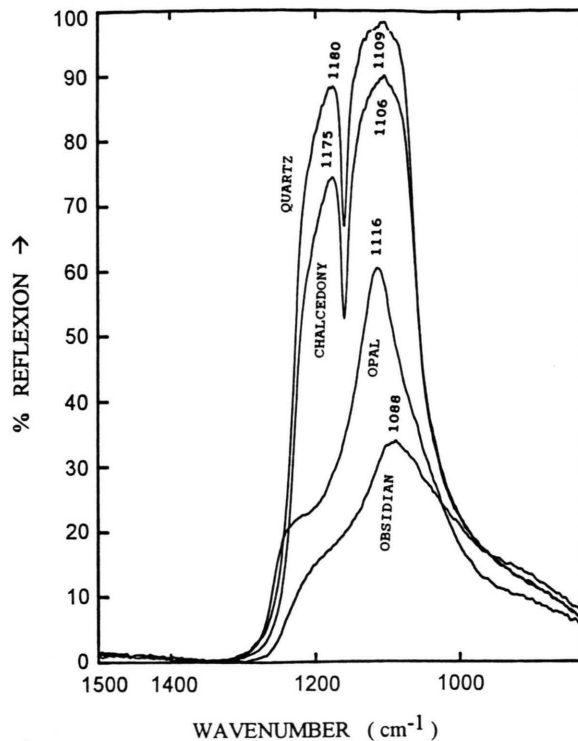


Fig. 2. Shift of the major peaks between 1180 and 1088 cm^{-1} from quartz to obsidian (glass) according to the change in the degree of crystallinity.

The shape and intensity of the two peaks at 800 and 780 cm^{-1} in the IR-reflectance spectra change gradually from quartz to obsidian (glass) as the crystallinity decreases according to the sequence mentioned above (Figure 1). In addition to that, a systematic shift of peaks is noted between 1176 cm^{-1} and 1088 cm^{-1} from quartz to obsidian (glass) as the crystallinity of the samples gradually decreases (Figure 2).

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