

A new method for measuring the crystallinity index of quartz by infrared spectroscopy

S. SHOVAL

Open University of Israel, 16 Klausner St., Tel-Aviv 61392, Israel

Y. GINOTT AND Y. NATHAN*

Geological Survey of Israel, 30 Malkhei Israel St., Jerusalem 95501, Israel

Abstract

A new method for measuring the crystallinity index of quartz is presented. It is based on the measurement of the intensity of the first derivative of the infrared absorption spectrum at the shoulder at $c. 1145 \text{ cm}^{-1}$. The results correlate well with X-ray and D.T.A. crystallinity measurements.

KEYWORDS: quartz, chert, infrared spectroscopy, crystallinity index, IR first derivative.

Introduction

QUARTZ, in sedimentary rocks, has a very wide range of crystallinity which is characteristic of its origin and diagenesis. Murata and Norman (1976) have described a semi-quantitative X-ray method for measuring quartz crystallinity. They suggested a crystallinity index of quartz on a scale of 10 based on the intensity of the (212) peak. Plyusnina (1978) has also described a method for measuring quartz crystallinity using infrared spectroscopy. Her method is based on the intensity of the absorption band at 780 cm^{-1} . Czaja and Paluszkiwicz (1987), quoting earlier unpublished work of Czaja, found no simple correlation between results obtained by the two methods. They recorded the far-infrared spectra of quartz samples of different crystallinities and showed that quartz with a low degree of crystallinity has less intense bands in this range; they did not however propose any quantitative scale. This paper proposes a semi-quantitative infrared method for measuring quartz crystallinity based on the intensity of the absorption shoulder at $c. 1145 \text{ cm}^{-1}$. The intensity is measured by using the first derivative of the absorbance curve. These infrared results correlate well with crystallinities determined by X-ray and DTA methods.

Experimental

Two quartz and 26 chert samples, 20 of which were previously used in a DTA study (Deutsch

* To whom correspondence should be addressed.

et al., 1989) were analysed. All the chert samples were collected either from the Campanian Mishash Formation or the Neogene Hazeva conglomerate. Alkali halide disks were prepared by mixing 1 mg of the ground sample with 150 mg KBr. The mixtures were ground manually in an agate mortar and mixed manually before the disk was pressed. To obtain better-resolved spectra, the disks were re-ground and re-pressed. The infrared absorption spectra were recorded on a Nicolet ZDX FT-IR spectrometer immediately after the preparation of the disks. The derivatives of the curve were obtained using the 'DERIVE.FTN' program (Compton *et al.*, 1984). The first derivative curve was used since it enhances the shoulder height and makes it possible to obtain a quantitative measurement (Fig. 1), while the second derivative enables one to obtain the shoulder exact position. It should be noted that the software inverts the first derivative curve, allowing peaks in the absorption curve to appear as peaks in the derivative curve. Therefore the derivative curves shown in Figs. 1 and 2 are inverted. They have been multiplied by -1 (or they are the reflection of the true derivative curves).

Results and discussion

The quartz band at $c. 1145 \text{ cm}^{-1}$ (Rey, 1966, p. 272 places it at 1141 cm^{-1} , and Moenke, 1974, p. 369, at 1150 cm^{-1}) occurs as a shoulder because it partly overlaps the strongest absorp-

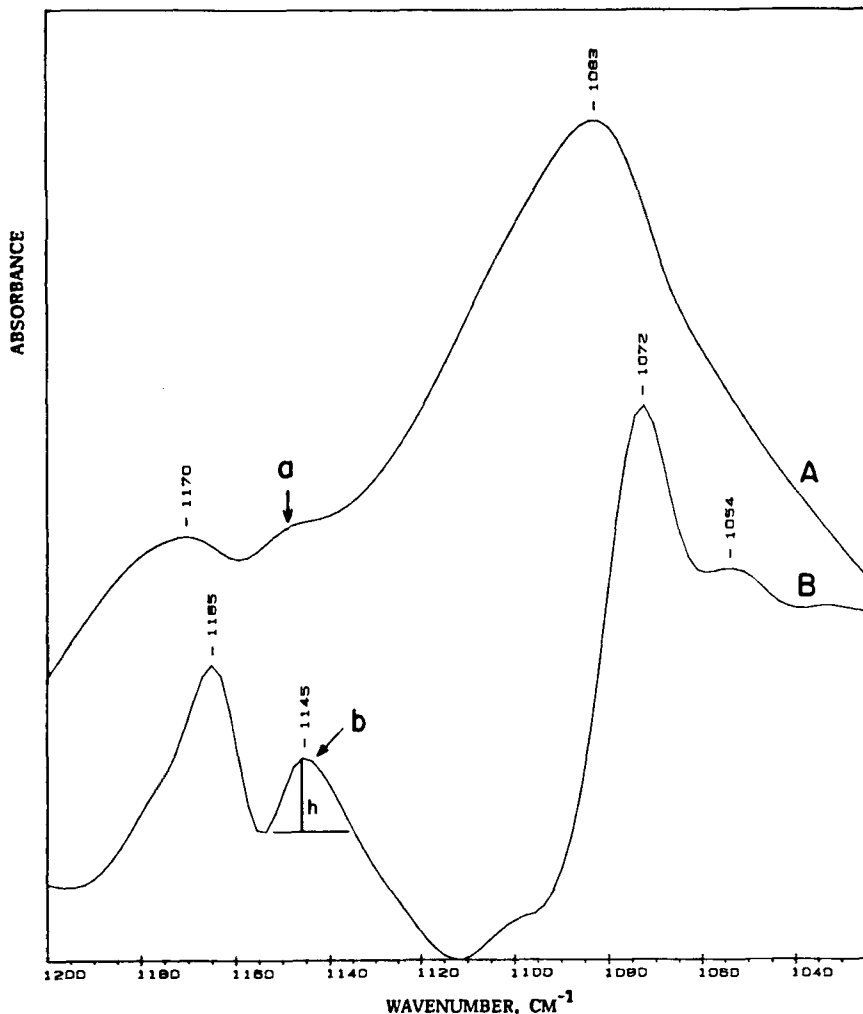


FIG. 1. IR spectrum of quartz and its first derivative: A, IR absorbance spectrum of quartz; B, first derivative of A; *a*, absorption shoulder at 1145 cm^{-1} ; *b*, first derivative of *a*; *h*, height of the first derivative peak *b* above background.

tion band of quartz at $c. 1085\text{ cm}^{-1}$. Examination of a number of quartz infrared spectra showed that the resolution of this shoulder appears to be very sensitive to the crystallinity of the quartz sample. Well-crystallised quartz shows a well-defined shoulder while the latter can hardly be recognised in poorly-crystallised samples. In order to quantify this often ill-defined shoulder (*a* in curve A, Fig. 1), the first derivative of the absorption spectrum was obtained. The height (*h* in curve B, Fig. 1) above the background was measured. The ratio of the height of this peak to the height of the peak obtained from the strongest quartz absorption band (at $c. 1085\text{ cm}^{-1}$), both measured on

the first derivative curve (the peak on the first derivative curve is at $c. 1075\text{ cm}^{-1}$) gives a good measure of the crystallinity of the sample. To simplify measurements, the strongest peak was kept at full scale and the absolute height of the derivative peak above background was taken as index. Fig. 2 shows the increase in height of this peak with crystallinity. A transparent rock-crystal pegmatite sample from Elat's Precambrian Massif was used as a standard. This sample was considered to be perfectly crystallised. In order to express the crystallinity index on the same scale as that proposed by Murata and Norman in 1976 (scale of 10), the crystallinity index determined for this sample, 2.55, was raised to 10 (using a

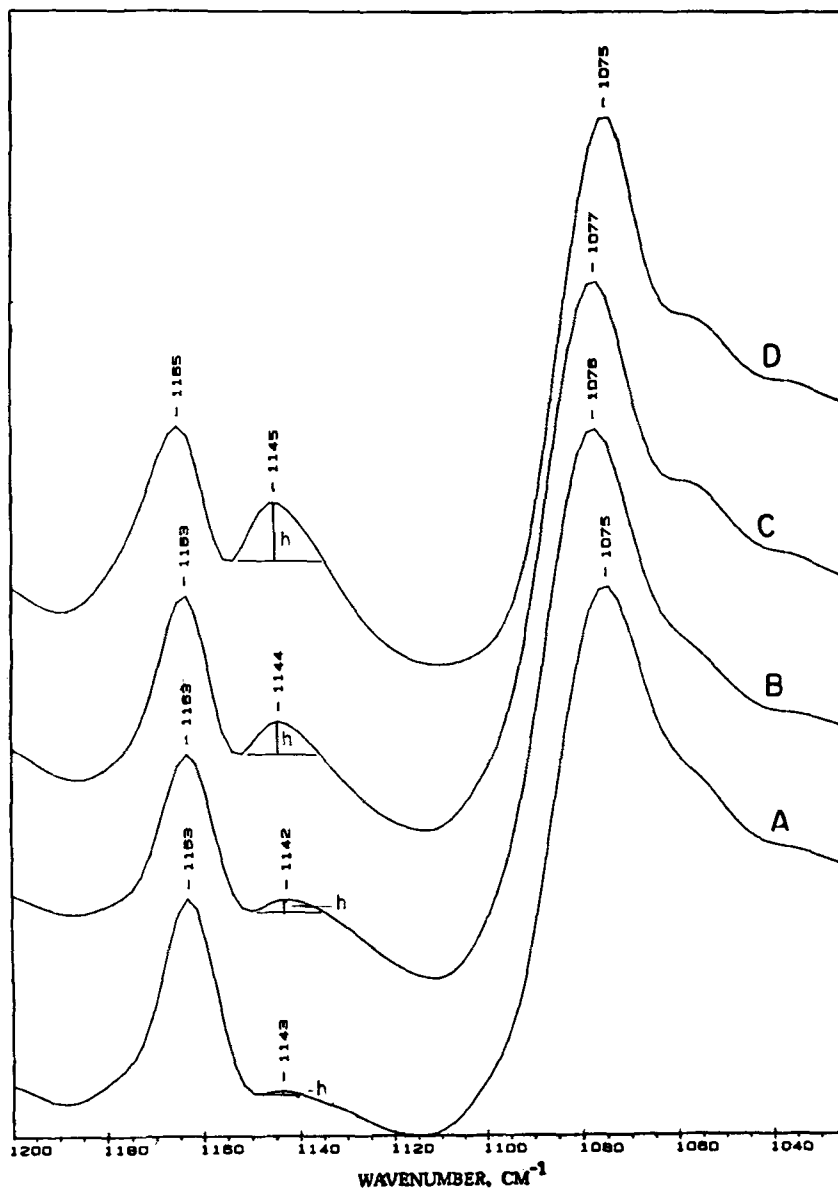


FIG. 2. First derivative curves of quartz with increasing crystallinity (A-D).

factor of 3.92). The same sample served as standard also for the X-ray and D.T.A. measurements (Deutsch *et al.*, 1989). Table 1 gives the results obtained for the crystallinity index of quartz by three different methods (X-ray, infrared and D.T.A.). Fig. 3 shows a plot of the infrared versus the X-ray results.

The results show a good correlation between the IR and X-ray results ($\rho = 0.9$). The advantage of the IR method is that it needs very small

samples; 1 mg is enough for a determination. This is important when only very small amounts of quartz are found in a sample or if more than one type of quartz occurs in a sample. It is then relatively simple to handpick, under a binocular microscope, enough enriched and homogeneous matter for an IR run. The IR method also appears to give better resolution for badly crystallised samples, in which the crystallinity index is less than 2 (Fig. 3).

QUARTZ CRYSTALLINITY X-ray vs Infra-red

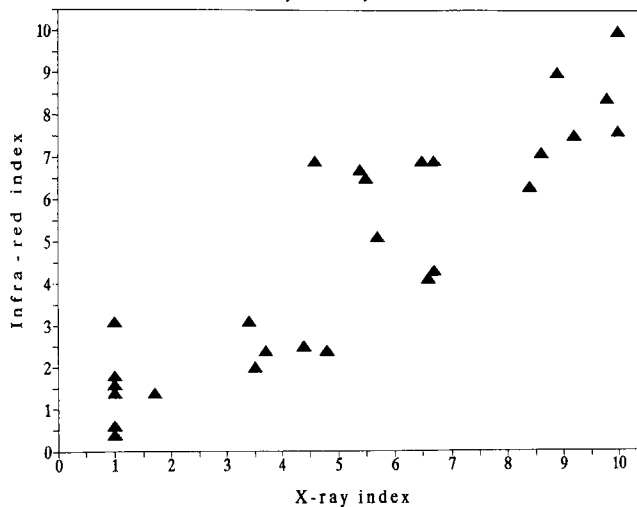


FIG. 3. Quartz crystallinity indices. Infra red vs. X-ray results.

Table 1

Comparison of crystallinity indices obtained by X-ray, infrared and D.T.A.

Sample No.	Locality	X-ray	Infrared	D.T.A.
YG-143.0	Nahal Mador	1.0	0.4	*
YG-156.1	Nahal Zin	1.0	0.6	0.3
YG-174.0	Arad	3.5	2.0	0.8
YG-172.0	Arad	4.8	2.4	0.6
YG- 59.2	E'n Fuar	1.0	1.4	0.3
YG-124.2	Nahal Mador	1.0	1.4	*
AB-611.0		1.7	1.4	0.5
YG- 48.0	E'n Fuar	1.0	1.6	0.3
YG-166.0	Han el Hatrur	1.0	1.8	0.3
YG-180.0	Arad	3.7	2.4	1.5
YG-152.0	Nahal Zin	4.4	2.5	*
YG-167.0	Han el Hatrur	3.4	3.1	*
YG-168.0	Han el Hatrur	1.0	3.1	0.6
YG-170.0	Arad	6.6	4.1	*
YG- 57.0	E'n Fuar	6.7	4.3	1.8
YG-187.0	Arad	5.7	5.1	1.9
YG-151.0	Nahal Zin	8.4	6.3	3.7
YG-173.0	Arad	5.5	6.5	*
YG-193.0	Arad	5.4	6.7	4.1
YG-182.0	Arad	6.7	6.9	4.3
YG-172.1	Arad	6.5	6.9	3.9
YG-188.0	Arad	4.6	6.9	2.7
AB-538.0	Arad	8.6	7.1	4.5
YG-176.0	Arad	9.2	7.5	*
MK-261	Arad	10.0	7.6	9.5
YN- 1.0	Jerusalem	9.8	8.4	8.6
YG-175.0	Arad	8.9	9.0	7.6
YN- 1.1	Quartz, Elat	10.0	10.0	10.0

* not determined

Frondel (1962, p. 195) applies the term 'chalcedonic silica' to fine-grained type of quartz with a fibrous microstructure. Following the work done on quartz crystallinity, a more precise definition for chalcedonic silica is suggested, namely, a fine-grained type of quartz with a crystallinity index less than 2.

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