Infrared absorption spectroscopy of SiO$_2$-moganite

MING ZHANG$^{1,2,*}$ AND TERRY MOXON$^3$

$^1$Frontier Institute of Science and Technology, Xi’an Jiaotong University, 710054, Xi’an, China  
$^2$Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge CB2 3EQ, U.K.  
$^3$55 Common Lane, Auckley, Doncaster DN9 3HX, U.K.

ABSTRACT

Moganite, a newly approved mineral, is microcrystalline silica. Samples of microcrystalline silica varieties containing variable amounts of moganite have been analyzed using absorption infrared spectroscopy (IR). The main spectral differences between moganite and α-quartz occur in the wavenumber region below 650 cm$^{-1}$. Above this wavenumber, the frequencies of Si-O stretching vibrations of moganite are almost identical to those of quartz. Additional moganite bands were recorded near 165, 207, 296, 343, 419, 576, and 612 cm$^{-1}$, and several of these extra IR bands have been identified for the first time in moganite. The results indicate that moganite and quartz have different crystal structures and symmetries in terms of different tetrahedral linkages. Infrared spectra obtained from samples with different moganite contents cannot be simply explained by mechanical mixing of the two moganite and quartz end phases. The change in moganite content leads to not only a variation of spectral intensity, but also a systematic modification in band position and full-width at half maximum. This unusual behavior is attributed to grain size, strains, and stacking faults in moganite and the intergrowth of moganite with fine-grained quartz. The close correlation between band width and moganite content is indicative of an improved crystallinity with decreasing in moganite concentration that has been identified in natural quartz variations. The results imply that moganite may play a role in the formation or crystallization of microcrystalline quartz. The present IR application offers a new method to estimate the moganite content in microcrystalline silica varieties.  

Keywords: Moganite, SiO$_2$, infrared spectroscopy, phonon modes, quartz

INTRODUCTION

Moganite is a microcrystalline silica polymorph (Flörke et al. 1984). It has recently been approved as a valid mineral species (CNMMN no. 99-035) by the Commission on New Minerals and Mineral Names of the International Mineralogical Association. The crystal structure of moganite has been described as monoclinic (Miehe et al. 1988) with alternate stacking of layers of [101] slices of left- and right-handed α-quartz corresponding to a periodic Brazil-law twinning on the unit-cell scale (Miehe and Graetsch 1992). Moganite is reported to have cell parameters of $a = 8.758$, $b = 4.876$, $c = 10.715$ Å, and $\beta = 90.08^\circ$ and space group $I2_1/a$ ($Z = 12$) (Miehe and Graetsch 1992), compared with $a = 4.913$, $b = 4.913$, $c = 5.404$ Å, and space group $P3_{1}2_{1}$ ($Z = 3$) for α-quartz (Deer et al. 1992). Physical properties and crystal structure of moganite have been explored by some investigators (Graetsch et al. 1987, 1994; Miehe and Graetsch 1992; Petrovic et al. 1996; Götze et al. 1998; Heaney and Post 2001; Hantsch et al. 2005; Heaney et al. 2007). Moganite is found to coexist and form intergrowths with fine-grained quartz varieties, e.g., chert, agate, and chalcedony from around the world (Heaney and Post 1992; Parthasarathy et al. 2001; Rodgers and Cressy 2001; Moxon and Rios 2004). Moganite-type phases have been identified in the silica analog phosphorus oxynitride (PON) (Chateau et al. 1999), zinc borophosphate (Huang et al. 2008), and AlPO$_4$ (Kanzaki and Xue 2012).

Quartz shows a varied distribution and high abundance in the Earth’s rocks. Hence, a better understanding of the structural relationship with other minerals is of scientific interest. The relatively recent discovery of moganite means that knowledge of its optical properties [such as infrared (IR) spectra] and comparison with other well-known crystalline polymorphs of silica may offer important information on the degree of diagenesis in microcrystalline silica. Moganite is suggested as an indicator for crystallization in evaporitic environments (Heaney 1995). Although IR spectra of moganite have been reported by several groups, the spectra acquired in these investigations offered limited lattice phonon modes and some were mainly focused on the near infrared (NIR) region (Graetsch et al. 1987, 1994; Miehe and Graetsch 1992; Parthasarathy et al. 2001; Zhang and Moxon 2012; Hardgrove and Rogers 2013).

Additionally, some of the previously reported infrared spectra of moganite showed inconsistent features. For example, the work of Parthasarathy et al. (2001) gave a relatively strong IR band near 600 cm$^{-1}$; however, this absorption was not clearly revealed in the study of Miehe and Graetsch (1992). There was also a lack of comprehension or detailed analysis on how IR spectra may change with varying moganite content. Therefore, the present study also aimed to gain a good understanding of the vibrational phonons of moganite and to compare the spec-

* E-mail: mzhanguk@gmail.com