Crystal structure of moganite: 
a new structure type for silica

GERHARD MIEHE1)* and HERIBERT GRAETSCH2)

1) Institut für Kristallographie, Goethe-Universität Frankfurt
Senckenberganlage 30, D 6000 Frankfurt/Main, F.R.G.
2) Institut für Mineralogie, Ruhr-Universität Bochum
Universitätsstraße 150, D 4630 Bochum, F.R.G.

Abstract: Structural characterization of the microcrystalline silica mineral moganite, using a combination of transmission and scanning electron microscopy, X-ray powder diffraction, infrared spectroscopy and chemical analyses, reveals that it represents a new AB2 structure type which is closely related to quartz. Moganite typically contains up to 3 wt% of water which is not a constituent of the structure. Rietveld refinement of the X-ray diffraction data leads to profile R-values R = 3.5 %, Rw = 4.5 %, GOF = 8.0. Moganite is essentially monoclinic with a = 8.758(2), b = 4.876(1), c = 10.715(2) Å, β = 90.88(3)°, space group I 1 2/a I, Z(SiO2) = 12, D = 2.55 g cm⁻³. The crystallites frequently display a triclinic superstructure which doubles the volume of the unit cell. The crystal structure can be thought of as consisting of alternating layers - resembling (101I)-slices through right- and left-handed quartz - which form a three dimensional framework of corner-sharing SiO4-tetrahedra. The structural principle is thus a periodic twinning according to the Brazil-law on a cell dimension scale. The topology of the quartz structure is transformed to the moganite topology if 1/6 of the Si-atoms occupies 14-positions of quartz. Besides the 6- and 8-rings, the structure contains 4-rings of SiO4-tetrahedra.

Key-words: moganite, silica structure, Brazil twin boundary.

Introduction

Moganite occurs in some of the ignimbrite flows of the Mogan formation on Gran Canaria as microcrystalline silica fillings of cavities, fissures and cooling cracks. The mineral was initially described by Flörke et al. (1976) under the working name "silica - G". Subsequently, additional chemical analyses, electron and X-ray powder diffraction data and a characterization of the thermal and optical properties were reported by Flörke et al. (1984). These authors introduced the mineral name moganite for this new silica polymorph.

Small amounts of structural elements with the same cell dimensions as moganite have been detected by transmission electron microscopy in the microcrystalline quartz varieties chalcedony, quartzine and flint. They are intergrowth structures located at the boundaries of polysynthetic lamellar Brazil twin domains (Miehe et al., 1984). Therefore the crystal structure is not only of interest as a new polymorph of silica, but also because of the light it sheds on our understanding of the structural state of the twin domain boundaries of chalcedony.

Experimental techniques

The morphology of moganite was studied by polarized light microscopy (PLM), scanning elec-