

## Particle size effects on occurrence of Brazil twinning in microcrystalline quartz

# Koichi Momma[1]; Toshiro Nagase[2]; Yasuhiro Kudoh[1]; Takahiro Kuribayashi[3]; Masahiko Tanaka[4]

[1] Tohoku Univ; [2] Tohoku Univ. Muse.; [3] Tohoku Univ.; [4] Photon Factory, KEK

Brazil twinning in microcrystalline quartz was studied with Rietveld analysis, Raman spectroscopy, and molecular dynamics (MD) simulations. Although genesis of Brazil twinning and moganite in microcrystalline quartz varieties has long been argued, effects of surface energy on their occurrence have never been studied so far.

Rietveld analysis of synchrotron X-ray powder diffraction data for natural and synthetic microcrystalline quartz reveals that maximum lattice strain occurs along  $[101]^*$  regardless of the great differences in origin, crystallite size and texture. On the other hand, macroscopic quartz samples do not show anisotropic strain. The anisotropic lattice strain of microcrystal increases in proportion to decreasing of the crystallite size. Axial ratio ( $c/a$ ) also decreases in proportion to lattice strain and inverse of crystallite size. Quantitative analysis of moganite contents in microcrystalline silica samples was carried out by Raman spectroscopy. The result reveals that the sample having large lattice strain contains high amount of moganite, and that the lattice strain along  $[101]^*$  is resulted from Brazil twinning. A sample synthesized from aluminum-doped silica gel shows large lattice strain than that of samples synthesized from pure silica gel, whereas a sample synthesized from iron-doped silica gel does not. MD simulation of Brazil twinning reveals that twin boundary induces lattice strain along  $[101]^*$ . This result is consistent with the relation between lattice strain and moganite content. The relationship between the Brazil twinning and crystallite size shows that surface energy is the driving force for the formation of Brazil twinning in microcrystalline quartz. Although ferric iron is believed to cause Brazil twinning, its role in microcrystalline quartz is negligibly small compared to surface energy.