Molecular dynamics simulations of structurally incorporated hydroxyls in quartz, coupled with IR spectroscopy

Satoru Suzuki [1], Katsuyuki Kawamura [2]

[1] Earth and Planetary Sci., Hokkaido Univ., [2] Earth and Planetary Sci., Tokyo Inst. Technology

Molecular dynamic simulations of incorporated OH species in quartz are conducted with the NTP ensemble. OH near Al impurity in quartz (OH(Al)) was simulated at 100K to 1000K and 0.1MPa. Stretching direction of OH(Al) by the MD was perpendicular to c-axis of quartz. This was consistent with the result by the polarized-IR measurements. S<=>4H defect in quartz was also simulated. Stretching vibrational spectrum showed an asymmetric band with its peak at around 3100cm-1.